

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
 Data File : BF092162.D
 Acq On : 10 Jan 2017 2:24
 Operator : UM/SJ
 Sample : I1055-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-31

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-BF122116.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	2.664	65	68	72	rBV	87835	155517	4.87%	0.467%
2	3.190	111	114	120	rVB	28840	60444	1.89%	0.182%
3	4.756	249	251	256	rBV	274226	367955	11.52%	1.105%
4	5.007	265	273	279	rBV4	10834	45950	1.44%	0.138%
5	5.247	292	294	302	rBV	1528422	1720684	53.87%	5.169%
6	5.784	336	341	347	rBV3	29922	63123	1.98%	0.190%
7	5.933	352	354	356	rBV	30229	35534	1.11%	0.107%
8	6.287	382	385	386	rBV	315014	378354	11.85%	1.137%
9	6.322	386	388	394	rVB	827899	1077790	33.74%	3.237%
10	6.413	394	396	399	rBV	1902401	2784390	87.18%	8.364%
11	6.596	409	412	414	rVB2	44146	65652	2.06%	0.197%
12	6.642	414	416	417	rBV	867546	809649	25.35%	2.432%
13	6.664	417	418	420	rVB	68819	61952	1.94%	0.186%
14	6.722	420	423	424	rBV2	51223	53936	1.69%	0.162%
15	6.802	427	430	432	rBV	1903526	2482444	77.72%	7.457%
16	6.893	437	438	441	rVB	58316	51688	1.62%	0.155%
17	6.984	443	446	449	rVB	68794	105581	3.31%	0.317%
18	7.053	449	452	456	rBV4	24085	57644	1.80%	0.173%
19	7.133	456	459	461	rBV	32576	50344	1.58%	0.151%
20	7.213	461	466	468	rBV	1916509	2187259	68.48%	6.570%
21	7.293	470	473	474	rBV2	51526	58800	1.84%	0.177%
22	7.327	474	476	478	rVB2	67087	99566	3.12%	0.299%
23	7.419	480	484	486	rVB2	211260	261543	8.19%	0.786%
24	7.510	486	492	493	rVB	48936	80412	2.52%	0.242%
25	7.590	496	499	501	rBV4	64778	112207	3.51%	0.337%
26	7.670	504	506	508	rBV	351048	363703	11.39%	1.092%
27	7.773	512	515	516	rVB2	81831	112858	3.53%	0.339%
28	7.807	516	518	520	rVB	30919	38542	1.21%	0.116%
29	7.865	520	523	526	rBV3	46723	107843	3.38%	0.324%
30	7.933	526	529	530	rVV	961575	1103273	34.54%	3.314%
31	7.979	530	533	536	rVB2	195547	305341	9.56%	0.917%
32	8.025	536	537	539	rVB2	34880	33918	1.06%	0.102%
33	8.093	541	543	545	rBV3	39553	65865	2.06%	0.198%
34	8.127	545	546	547	rVB	53466	36651	1.15%	0.110%

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35	8.162	547	549	550 rBV	340652	355174	11.12%	1.067%
36	8.207	550	553	557 rVB2	251833	557540	17.46%	1.675%
37	8.310	560	562	565 rBV4	47669	84406	2.64%	0.254%
38	8.367	565	567	569 rBV3	40090	68400	2.14%	0.205%
39	8.402	569	570	572 rVB	56158	40884	1.28%	0.123%
40	8.528	579	581	582 rBV	37656	36692	1.15%	0.110%
41	8.596	582	587	588 rVB3	84091	132621	4.15%	0.398%
42	8.630	588	590	593 rVB4	28229	52333	1.64%	0.157%
43	8.745	596	600	605 rBV3	104507	221323	6.93%	0.665%
44	8.848	605	609	610 rBV3	24201	50709	1.59%	0.152%
45	8.882	610	612	615 rVB3	46482	82400	2.58%	0.248%
46	8.939	615	617	621 rBV4	104217	194527	6.09%	0.584%
47	9.008	621	623	625 rVB	3458458	3193937	100.00%	9.594%
48	9.133	628	634	635 rBV5	57504	166365	5.21%	0.500%
49	9.373	650	655	656 rBV5	100215	196004	6.14%	0.589%
50	9.408	656	658	660 rVV	342665	309871	9.70%	0.931%
51	9.465	661	663	668 rVB5	55360	117744	3.69%	0.354%
52	9.590	673	674	676 rBV2	42922	44553	1.39%	0.134%
53	9.636	676	678	680 rVB3	22756	35603	1.11%	0.107%
54	9.682	680	682	684 rBV	1331496	1172378	36.71%	3.522%
55	9.762	688	689	691 rVB2	53269	46477	1.46%	0.140%
56	9.865	694	698	701 rBV4	67716	183505	5.75%	0.551%
57	9.911	701	702	704 rVB2	39971	41811	1.31%	0.126%
58	10.002	707	710	712 rBV2	47634	67793	2.12%	0.204%
59	10.059	712	715	717 rBV3	29322	60077	1.88%	0.180%
60	10.105	717	719	722 rVB	194365	214926	6.73%	0.646%
61	10.311	735	737	739 rBV2	50324	53213	1.67%	0.160%
62	10.368	741	742	744 rBV	30339	41163	1.29%	0.124%
63	10.471	749	751	754 rVV	1662750	1771674	55.47%	5.322%
64	10.539	755	757	760 rVV3	31225	61361	1.92%	0.184%
65	10.596	760	762	766 rVV4	173892	227639	7.13%	0.684%
66	10.665	766	768	769 rVV	67383	75280	2.36%	0.226%
67	10.699	769	771	772 rVV	64080	91896	2.88%	0.276%
68	10.733	772	774	777 rVV3	57926	133433	4.18%	0.401%
69	10.802	777	780	782 rVV3	43865	104977	3.29%	0.315%
70	10.848	782	784	785 rVV2	54709	89032	2.79%	0.267%
71	10.882	785	787	789 rVV	59557	105457	3.30%	0.317%

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72	10.916	789	790	794	rVB	51294	58718	1.84%	0.176%
73	11.065	799	803	807	rBV2	111983	226517	7.09%	0.680%
74	11.156	809	811	813	rVV2	836612	985589	30.86%	2.961%
75	11.191	813	814	819	rVB	66028	90992	2.85%	0.273%
76	11.351	826	828	829	rVB2	44393	44026	1.38%	0.132%
77	11.374	829	830	832	rBV	42929	61428	1.92%	0.185%
78	11.465	836	838	840	rBV	57619	69846	2.19%	0.210%
79	11.705	857	859	863	rBV4	101270	220447	6.90%	0.662%
80	11.762	863	864	865	rVV	60621	44273	1.39%	0.133%
81	11.785	865	866	869	rVV3	38447	73254	2.29%	0.220%
82	11.842	869	871	872	rBV2	39356	44735	1.40%	0.134%
83	11.876	872	874	875	rBV	68219	76767	2.40%	0.231%
84	11.968	880	882	884	rVV	39319	65768	2.06%	0.198%
85	12.265	907	908	909	rBV	45145	33744	1.06%	0.101%
86	12.299	909	911	913	rVV2	37945	51793	1.62%	0.156%
87	12.494	926	928	930	rBV3	52921	82379	2.58%	0.247%
88	12.528	930	931	934	rVB2	66551	63388	1.98%	0.190%
89	12.642	939	941	942	rBV2	56978	91580	2.87%	0.275%
90	12.745	948	950	952	rBV	2088579	2728806	85.44%	8.197%
91	12.791	952	954	957	rVB	61049	45997	1.44%	0.138%
92	12.859	957	960	962	rBV2	242417	444070	13.90%	1.334%
93	12.894	962	963	965	rVB2	73213	74899	2.35%	0.225%
94	13.031	973	975	977	rVB	178170	168426	5.27%	0.506%
95	13.077	977	979	981	rBV	82820	101745	3.19%	0.306%
96	13.328	998	1001	1003	rBV3	136592	242245	7.58%	0.728%
97	13.797	1039	1042	1044	rBV	711390	758629	23.75%	2.279%
98	15.168	1160	1162	1165	rBV	317837	461431	14.45%	1.386%

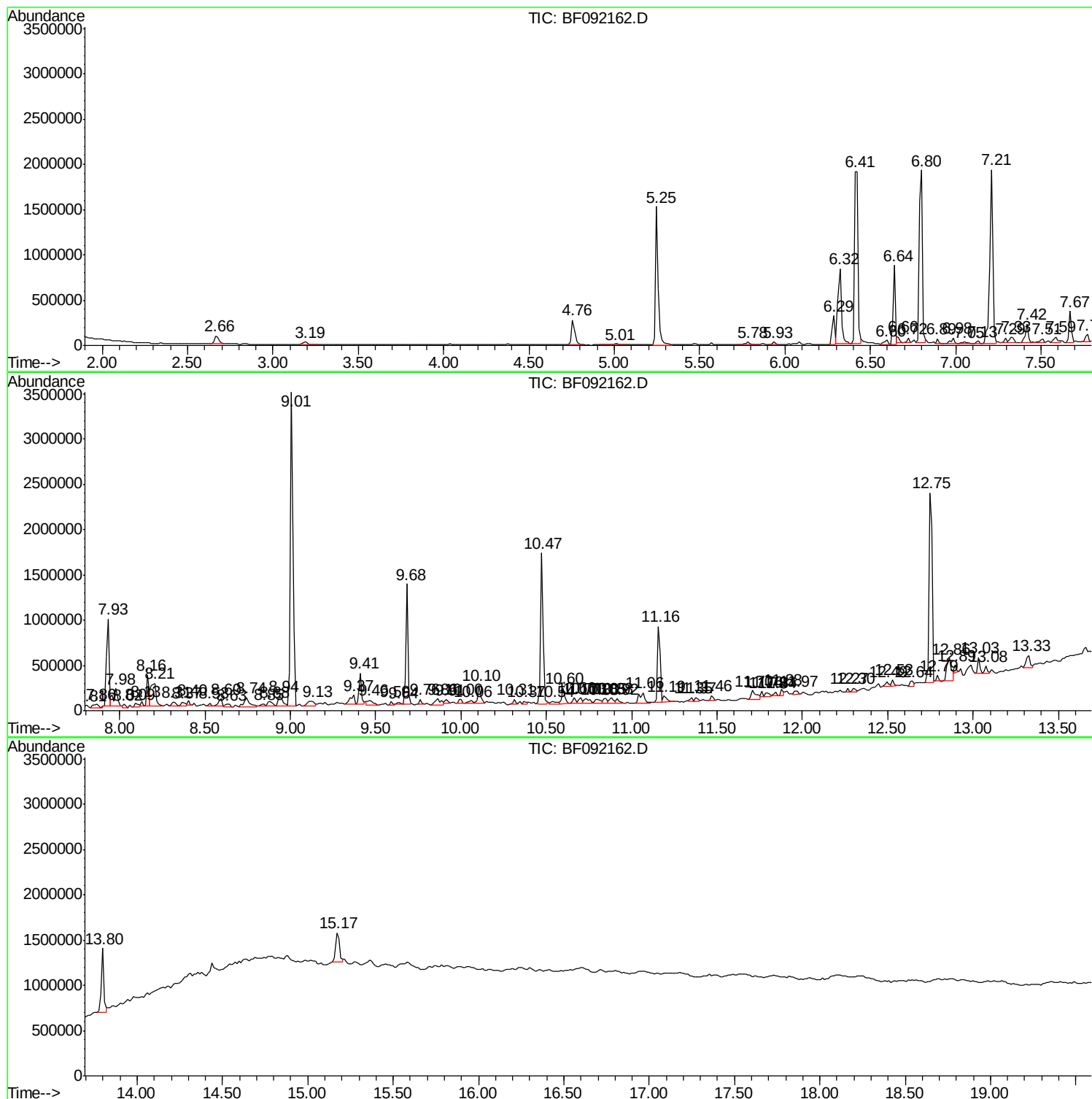
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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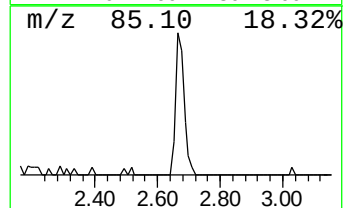
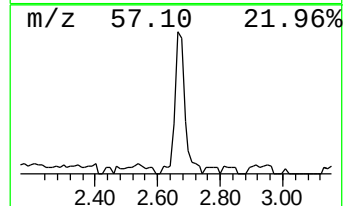
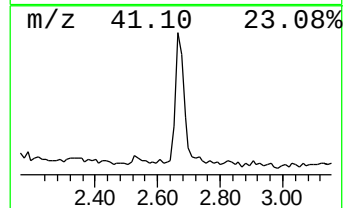
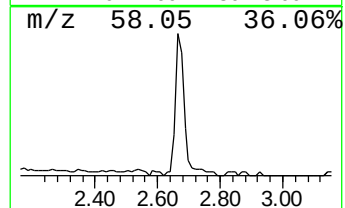
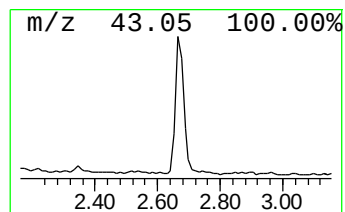
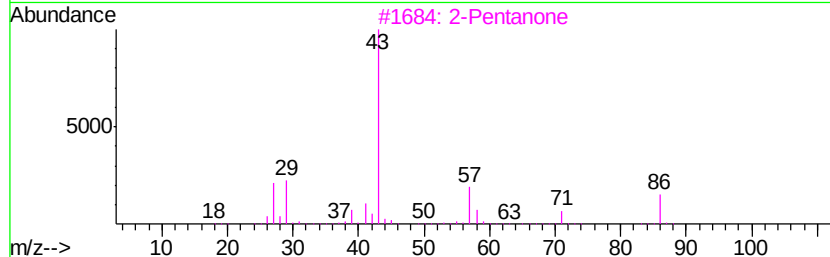
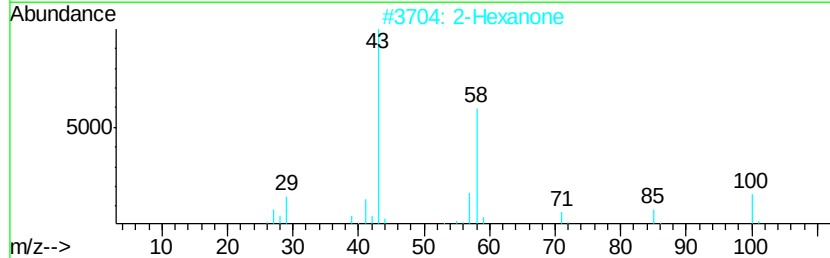
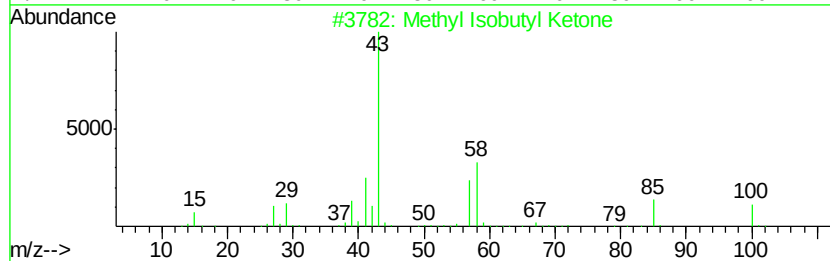
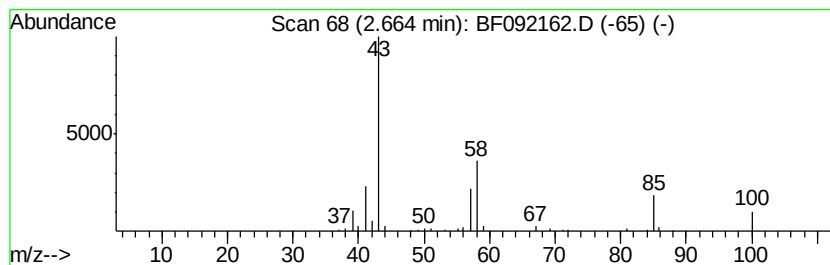
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.66	3.84 ng	155517	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	80
2			2-Hexanone	100	C6H12O	000591-78-6	78
3			2-Pentanone	86	C5H10O	000107-87-9	38
4			Tagetonol	170	C10H18O2	071547-63-2	33
5			2-Heptanone, 7,7,7-trichloro-	216	C7H11Cl3O	154264-40-1	28



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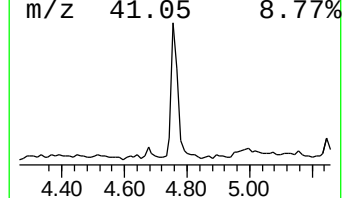
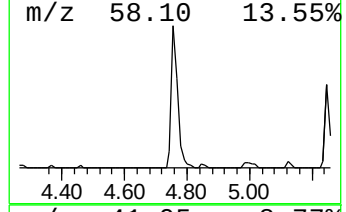
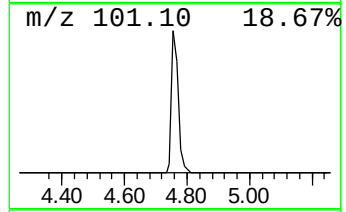
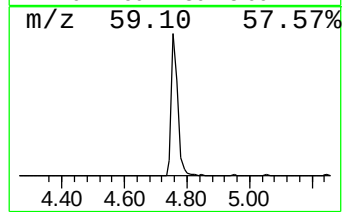
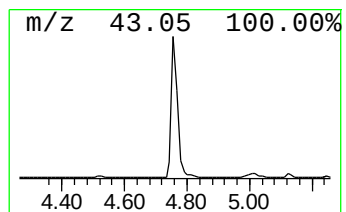
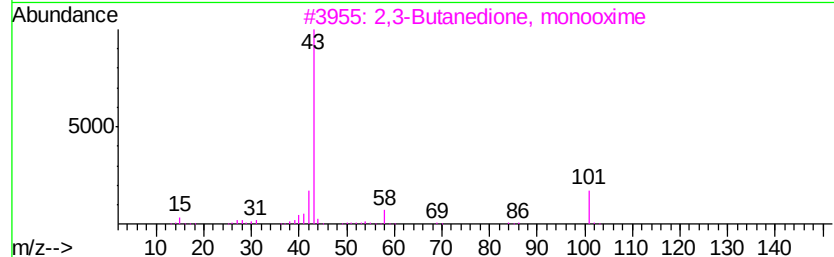
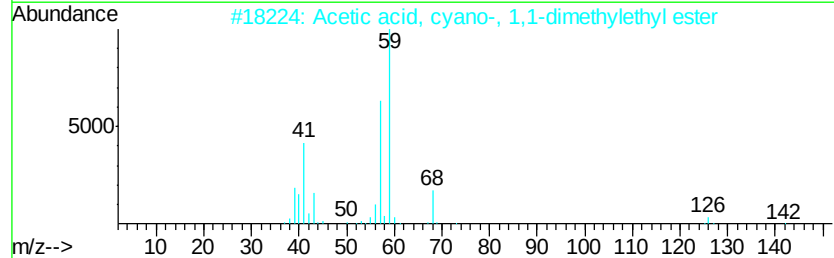
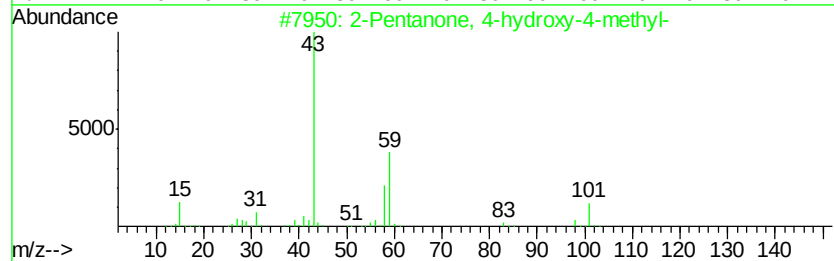
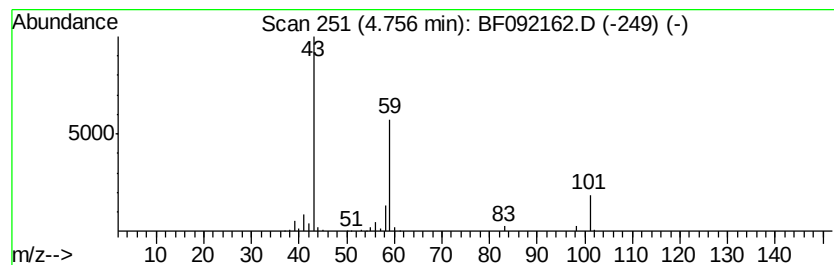
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	9.09 ng	367955	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9



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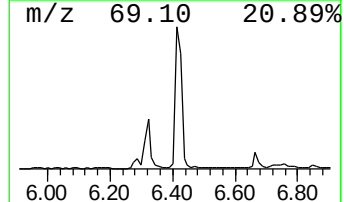
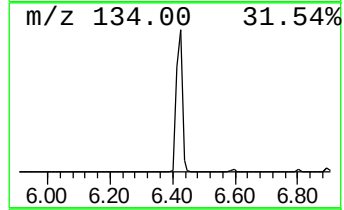
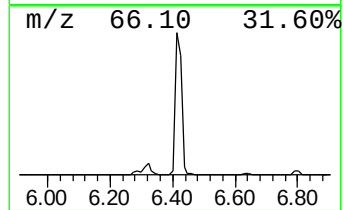
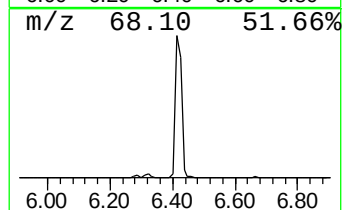
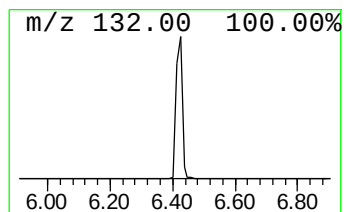
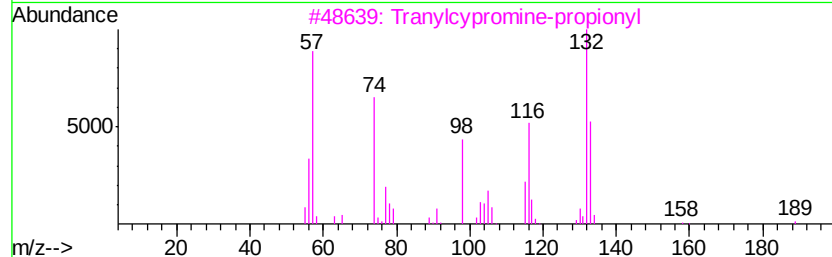
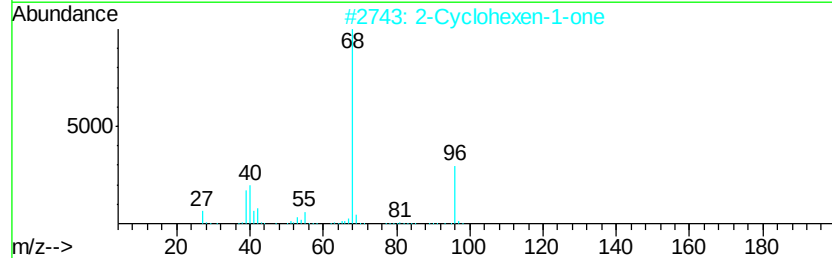
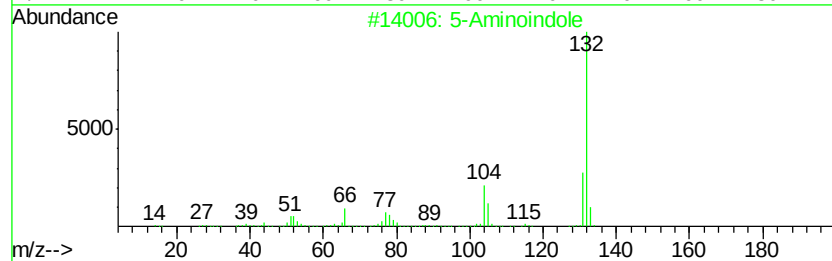
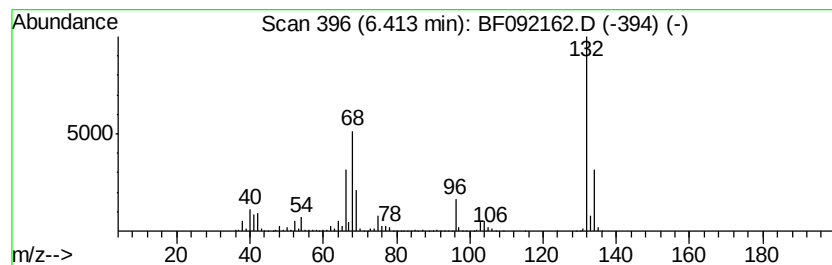
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	68.78 ng	2784390	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	10
2		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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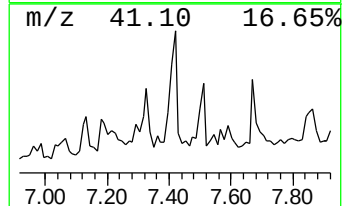
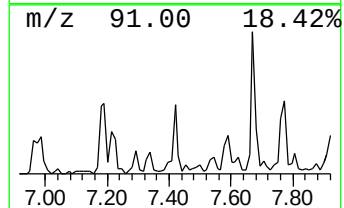
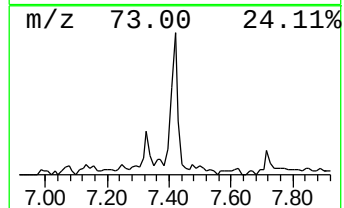
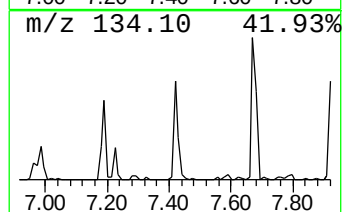
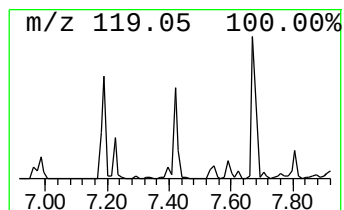
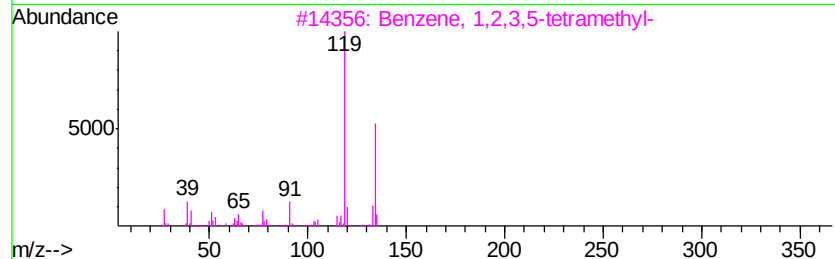
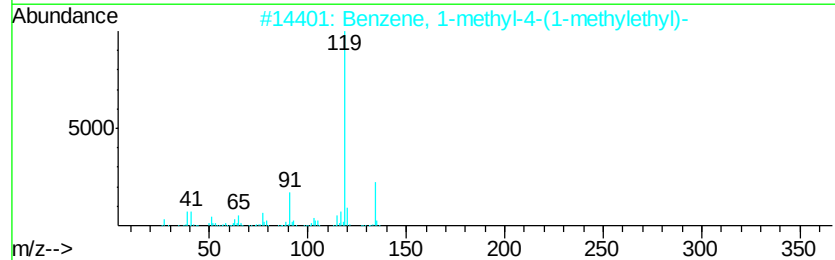
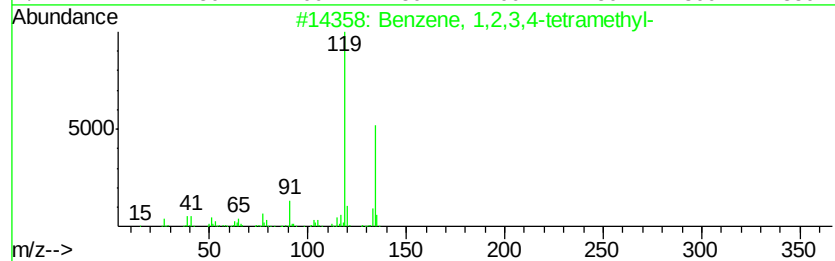
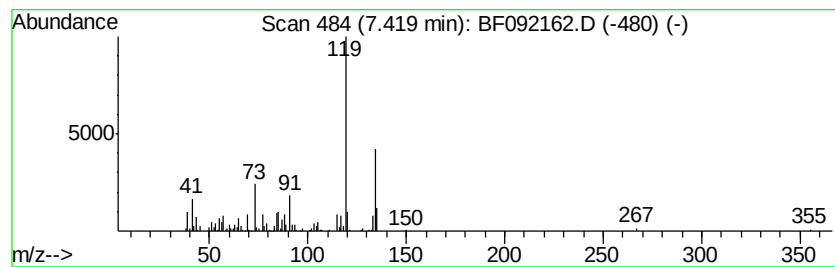
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	4.74 ng	261543	Naphthalene-d8	7.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
2		Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	89
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	76
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	76
5		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
Operator : UM/SJ
Sample : I1055-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

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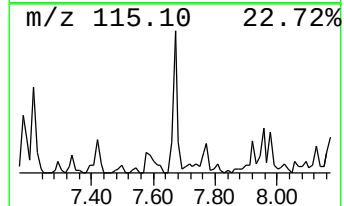
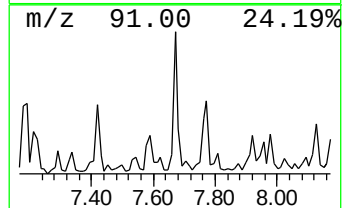
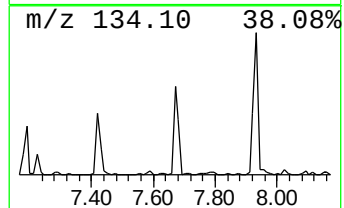
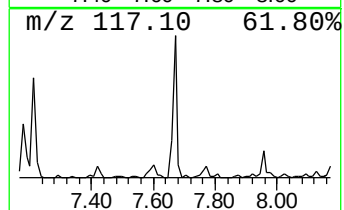
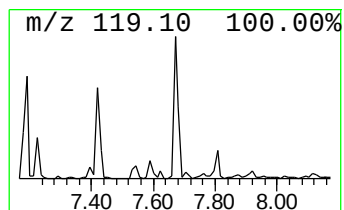
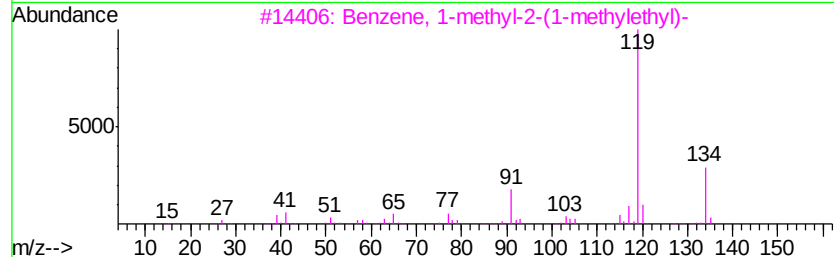
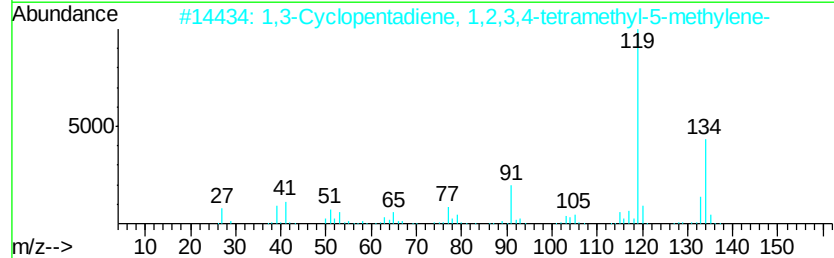
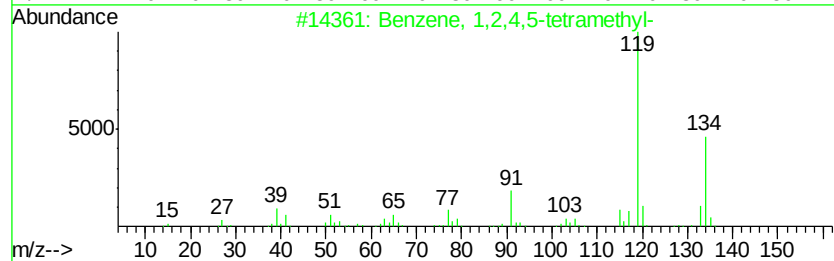
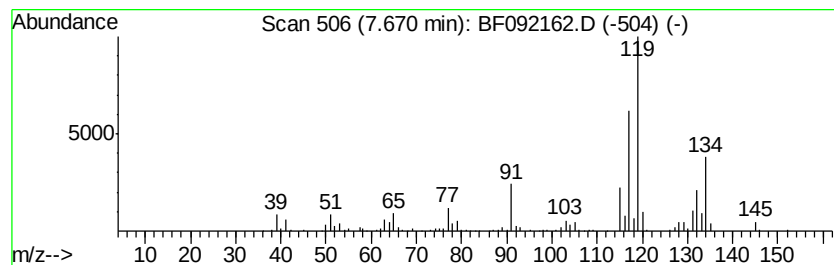
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	6.59 ng	363703	Napthalene-d8	7.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
2		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	64
3		Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	60
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	60



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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ALS Vial : 28 Sample Multiplier: 1

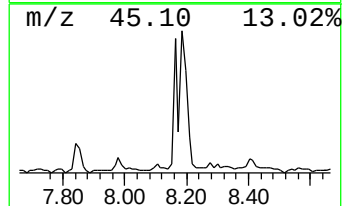
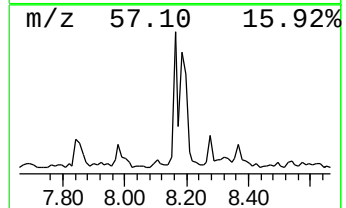
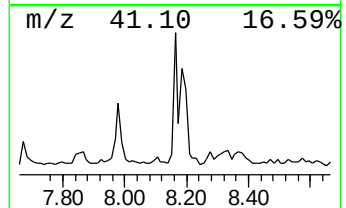
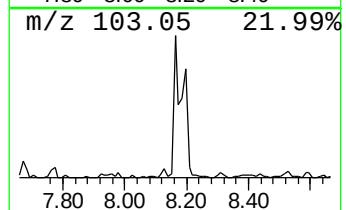
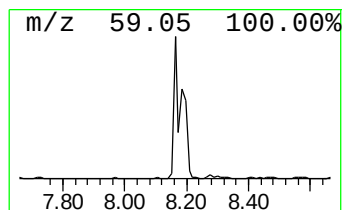
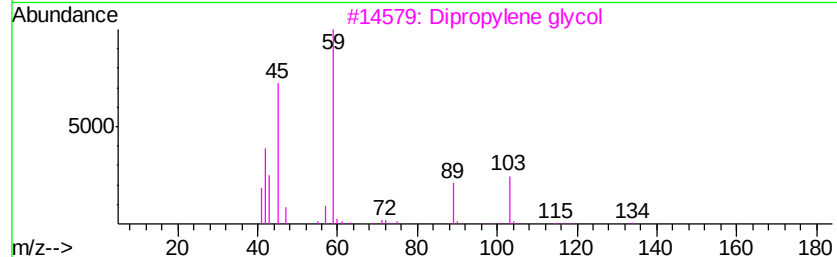
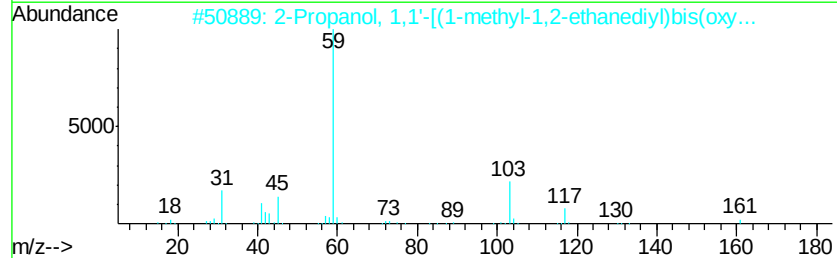
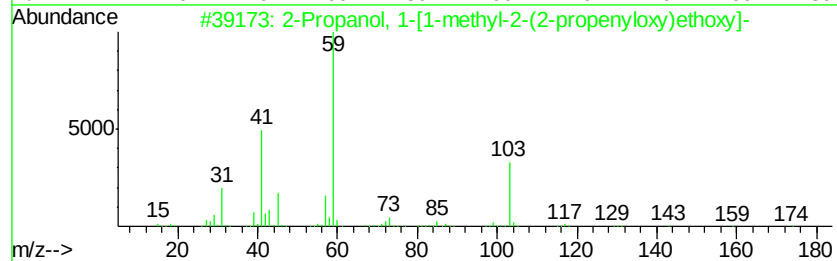
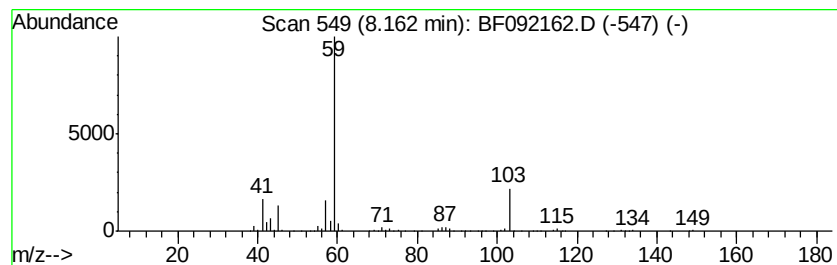
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.16	6.44 ng	355174	Napthalene-d8	7.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78	
2	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72	
3	Dipropylene glycol	134	C6H14O3	025265-71-8	64	
4	dl-Erythro-0-methylthreonine	133	C5H11NO3	1000214-70-7	59	
5	Butane, 2-methoxy-	88	C5H12O	006795-87-5	59	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
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Sample : I1055-06
Misc :
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Instrument :
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ClientSampleId :
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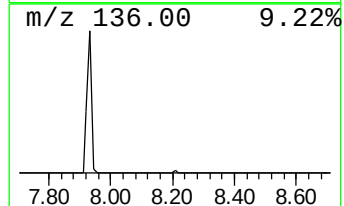
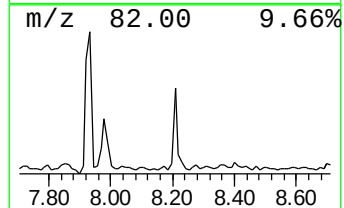
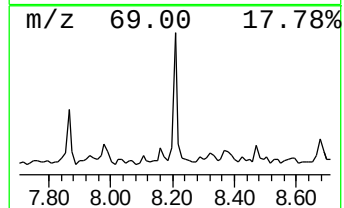
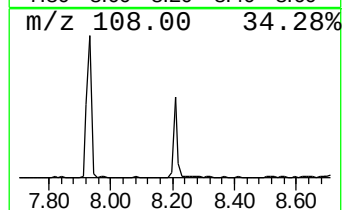
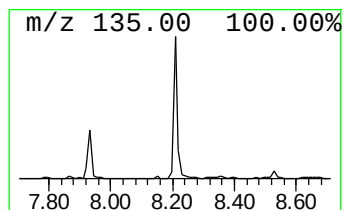
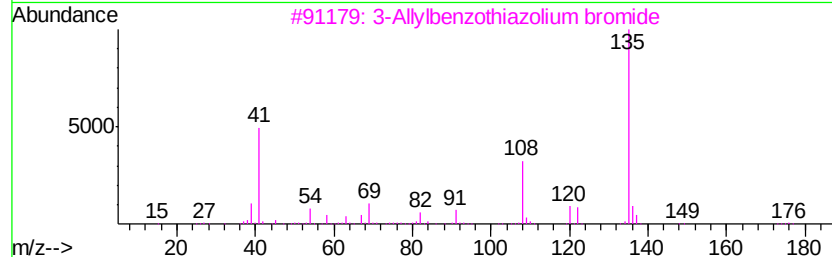
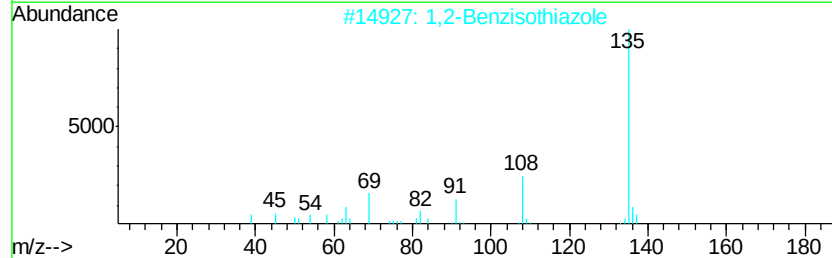
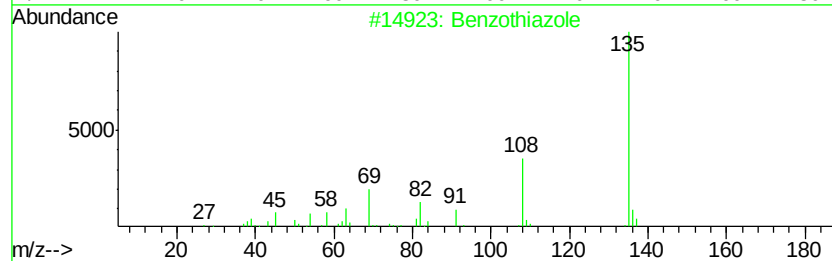
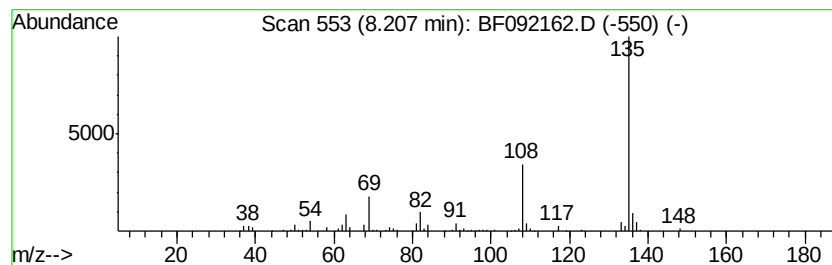
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.21	10.11 ng	557540	Naphthalene-d8	7.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	94
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
4		Adenine	135	C5H5N5	000073-24-5	64
5		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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Acq On : 10 Jan 2017 2:24
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Sample : I1055-06
Misc :
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Instrument :
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ClientSampleId :
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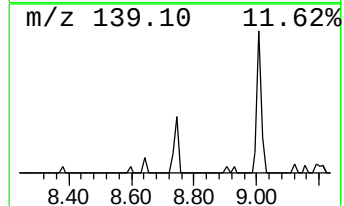
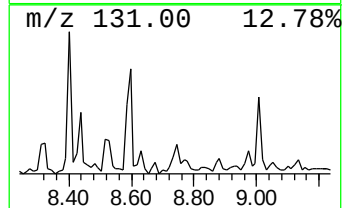
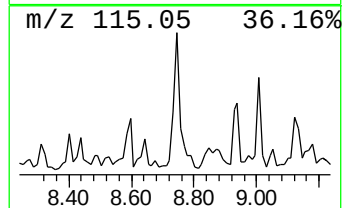
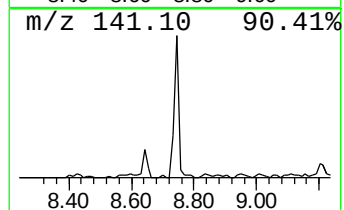
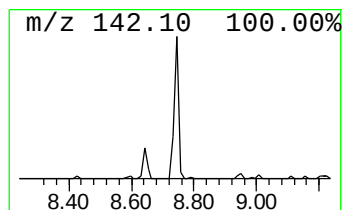
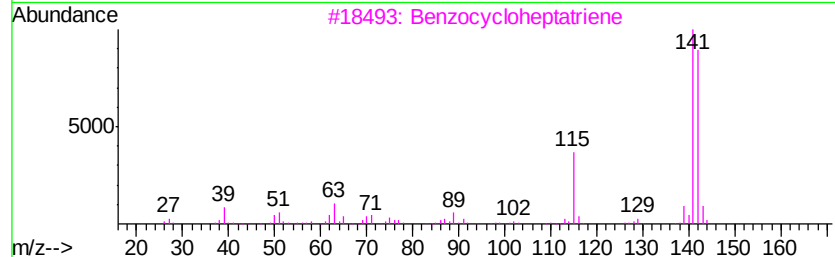
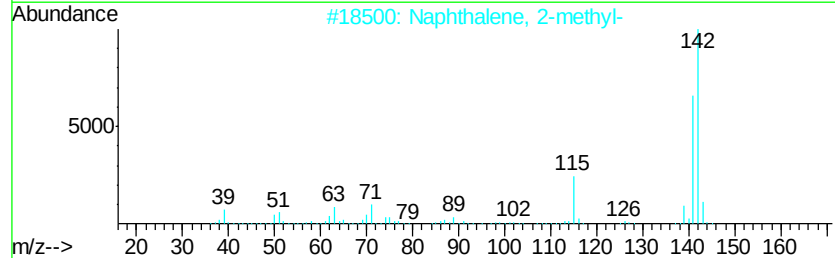
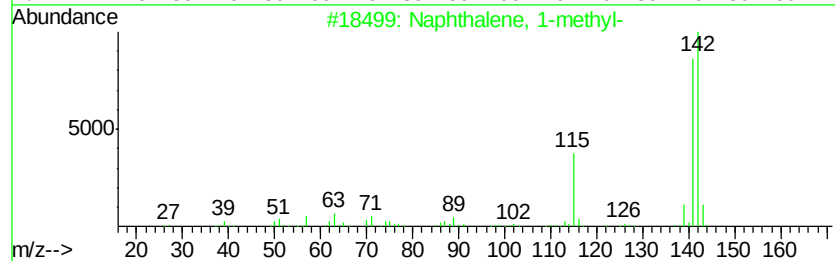
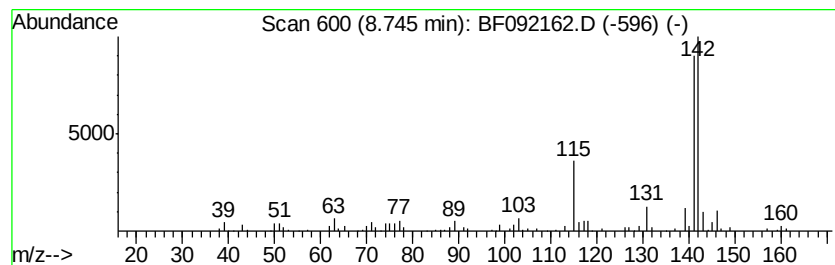
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.74	4.01 ng	221323	Naphthalene-d8	7.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	87
3		Benzocycloheptatriene	142	C11H10	000264-09-5	83
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	72
5		3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
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Sample : I1055-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

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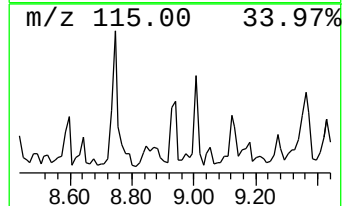
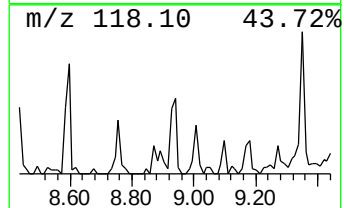
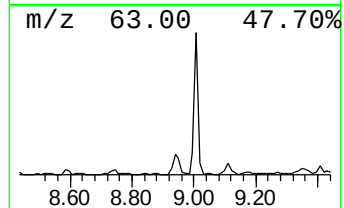
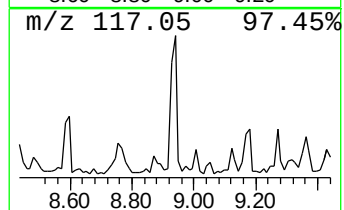
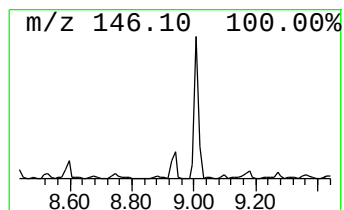
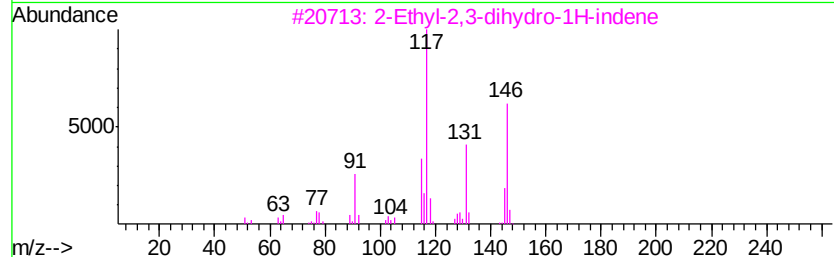
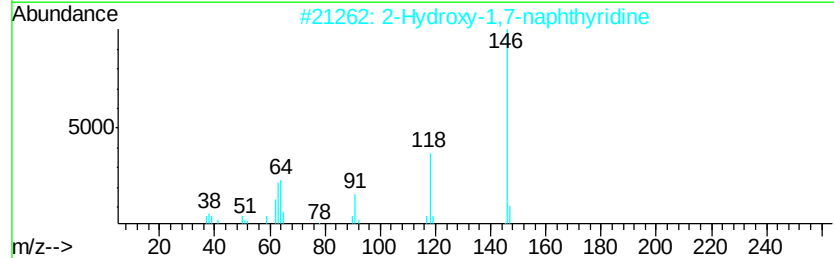
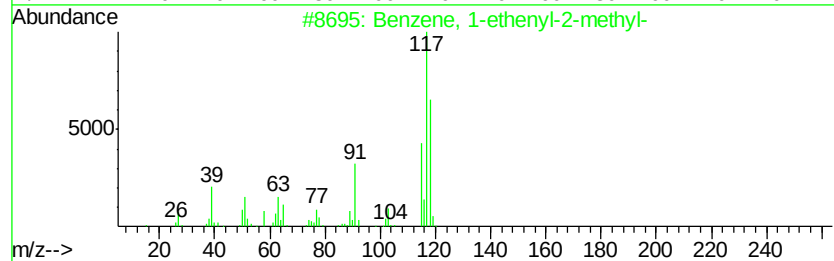
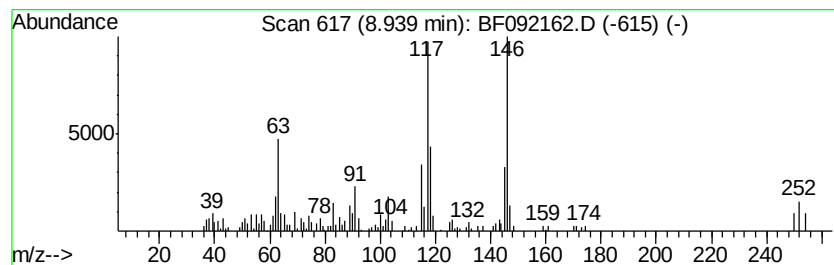
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.94 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	3.32 ng	194527	Acenaphthene-d10	9.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	42
2			2-Hydroxy-1,7-naphthyridine	146	C8H6N2O	054920-82-0	42
3			2-Ethyl-2,3-dihydro-1H-indene	146	C11H14	056147-63-8	38
4			7-Methylindan-1-one	146	C10H10O	039627-61-7	30
5			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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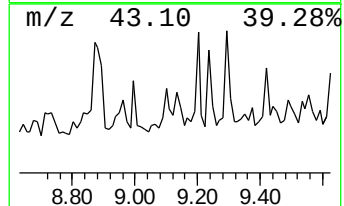
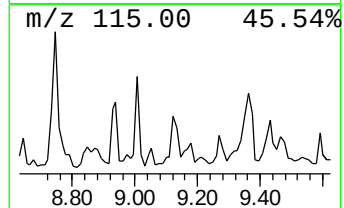
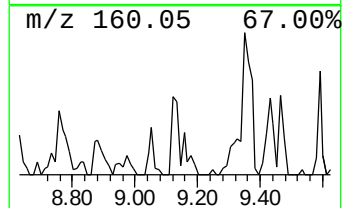
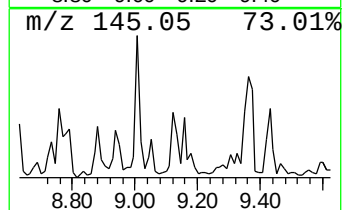
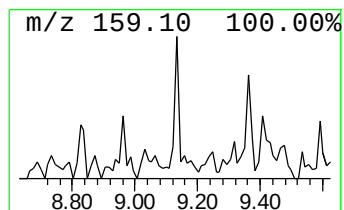
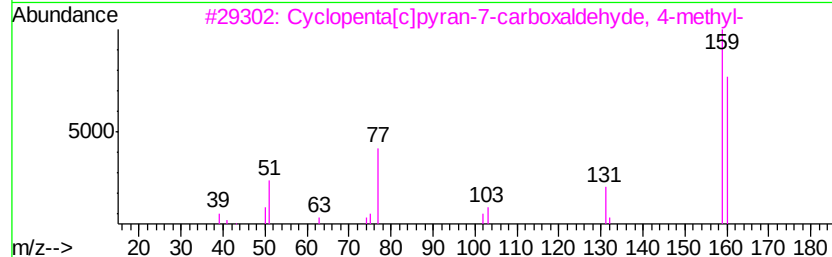
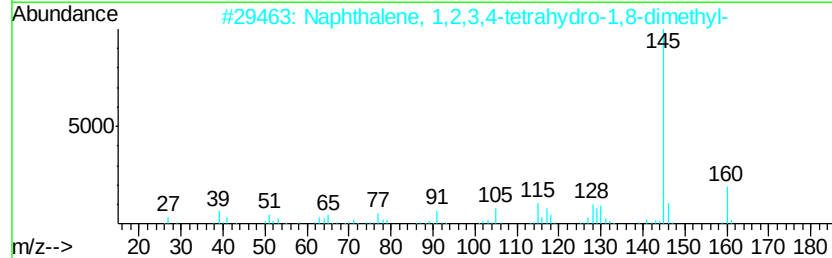
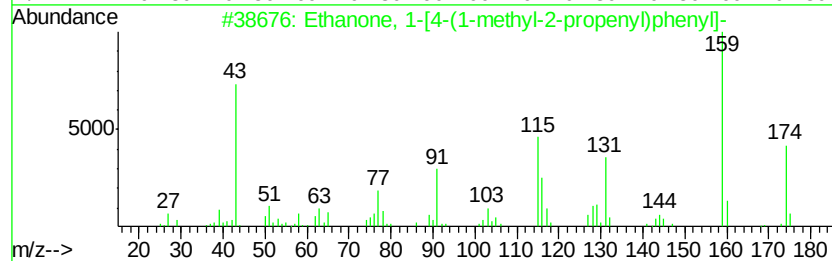
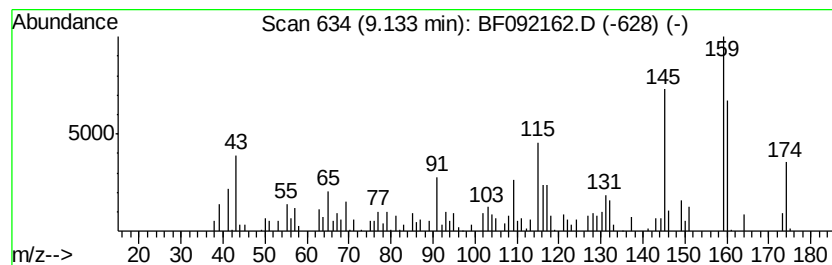
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanone, 1-[4-(1-methyl-2-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.13	2.84 ng	166365	Acenaphthene-d10	9.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ethanone, 1-[4-(1-methyl-2-prope...	174 C12H14O	109586-49-4	53
2	Naphthalene, 1,2,3,4-tetrahydro-...	160 C12H16	025419-33-4	38
3	Cyclopenta[c]pyran-7-carboxaldeh...	160 C10H8O2	063661-79-0	30
4	2,3,4-Trifluorobenzaldehyde	160 C7H3F3O	161793-17-5	30
5	Indan, 1,1,6,7-tetramethyl-	174 C13H18	016204-58-3	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
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Operator : UM/SJ
Sample : I1055-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

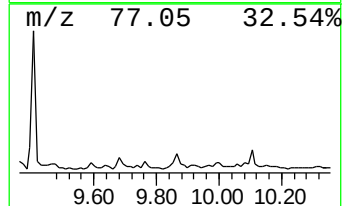
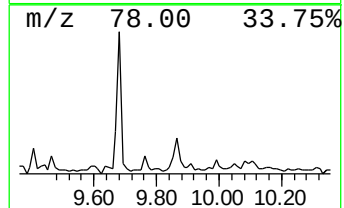
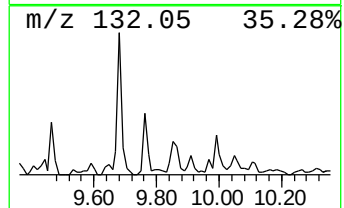
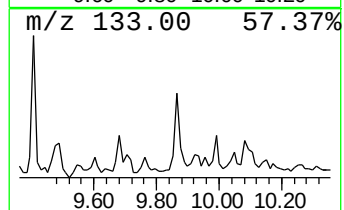
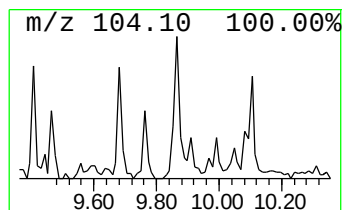
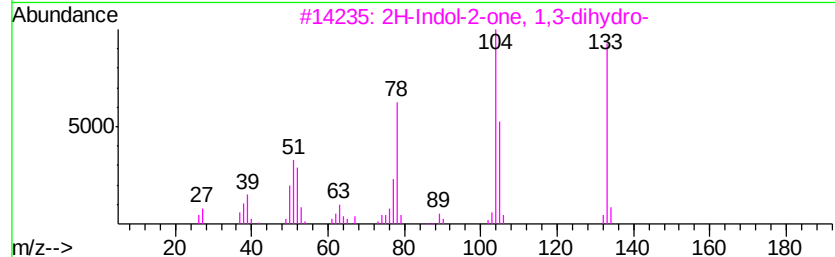
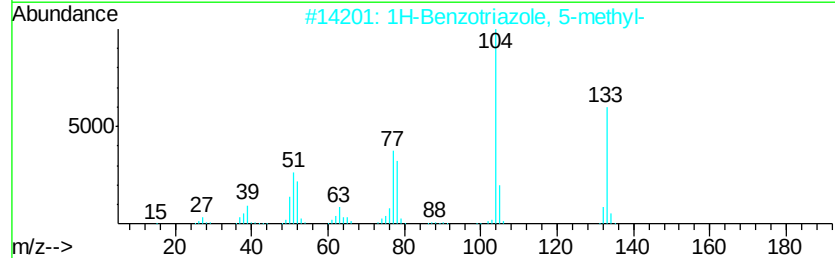
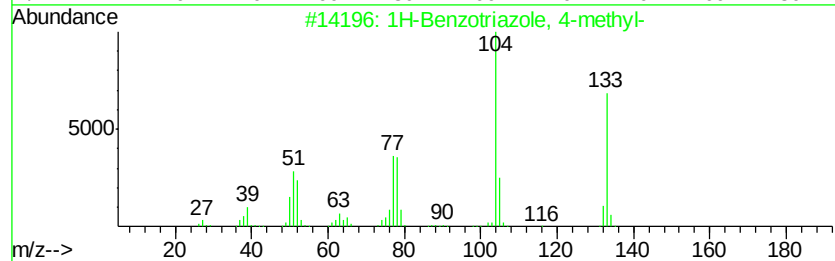
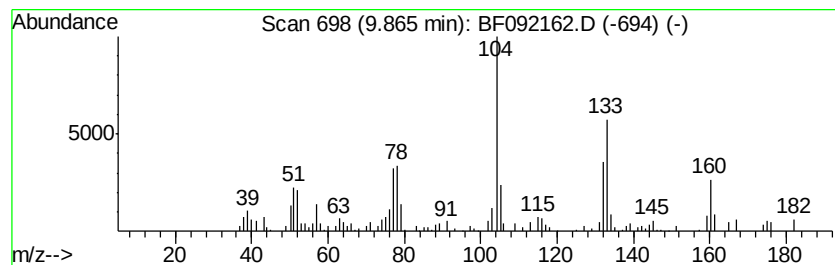
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1H-Benzotriazole, 4-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.86	3.13 ng	183505	Acenaphthene-d10		9.68
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	96
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	91
3	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	62
4	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	58
5	1H-Indol-4-ol	133	C8H7NO	002380-94-1	55



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
Operator : UM/SJ
Sample : I1055-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

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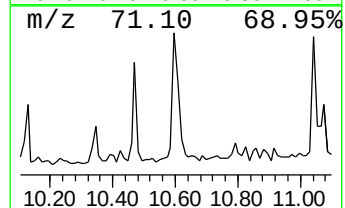
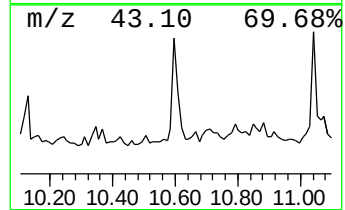
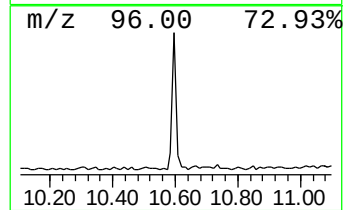
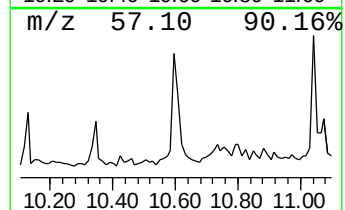
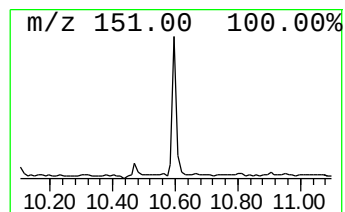
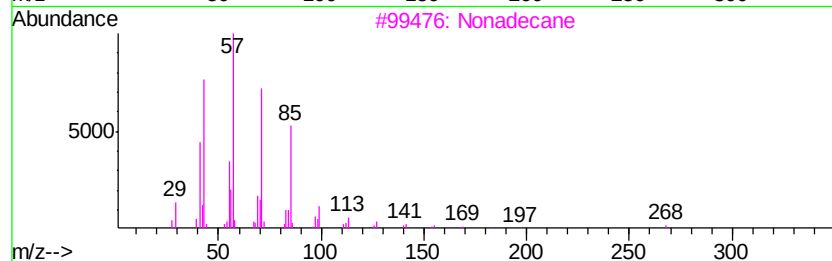
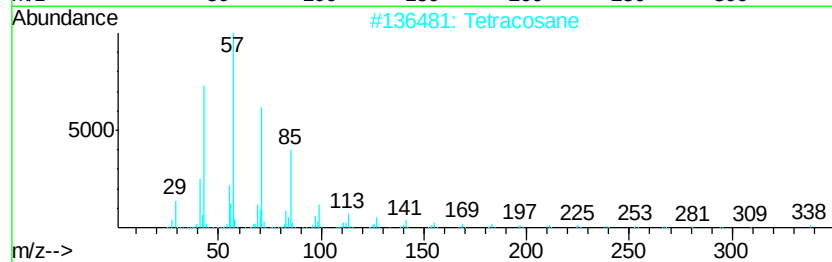
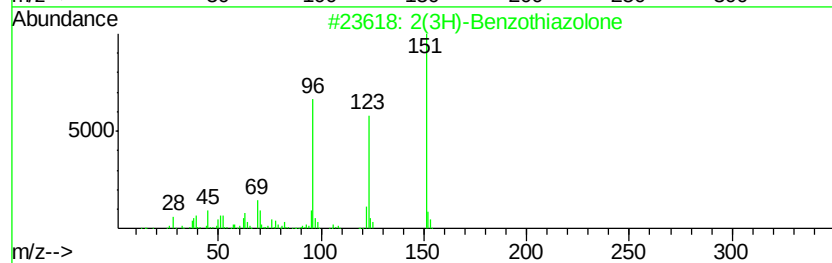
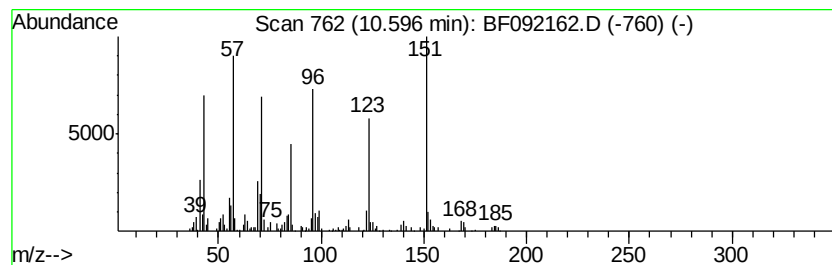
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Benzothiazolone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	4.62 ng	227639	Phenanthrene-d10	11.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	70
2		Tetracosane	338	C24H50	000646-31-1	25
3		Nonadecane	268	C19H40	000629-92-5	25
4		Tridecane	184	C13H28	000629-50-5	25
5		Heptadecane	240	C17H36	000629-78-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
Operator : UM/SJ
Sample : I1055-06
Misc :
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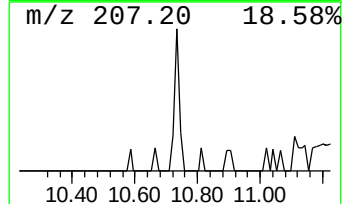
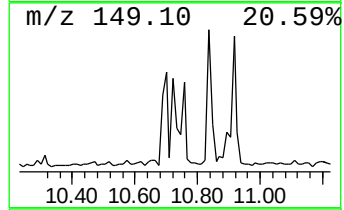
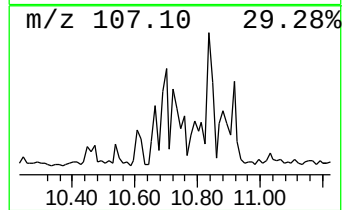
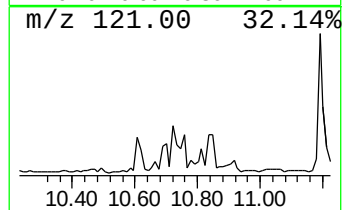
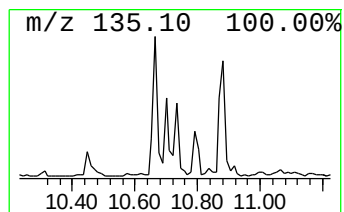
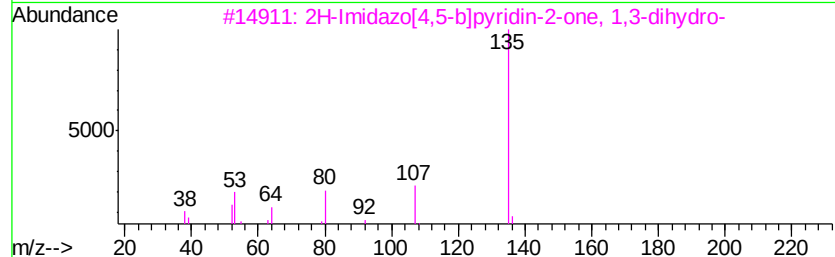
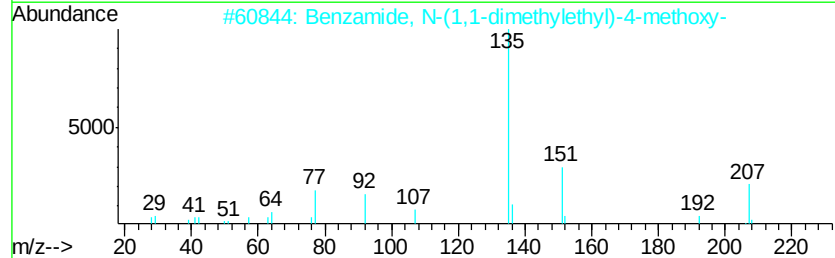
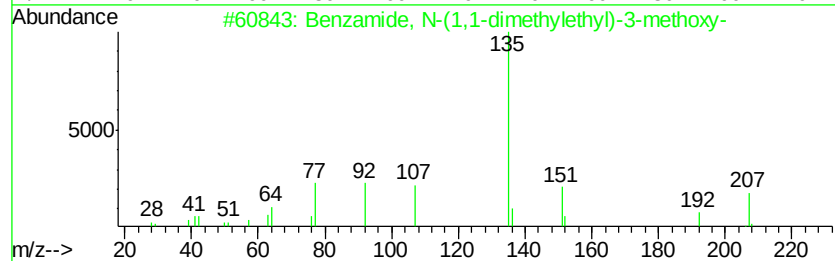
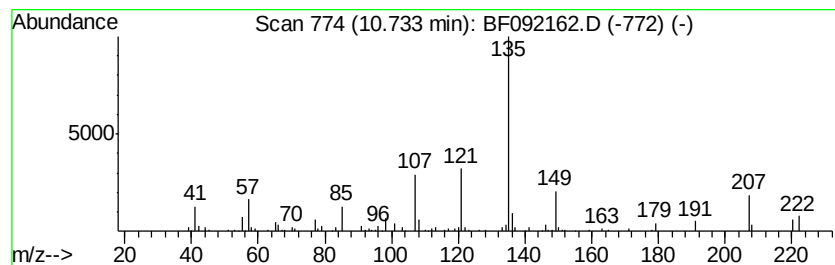
Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzamide, N-(1,1-dimethyle... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.73	2.71 ng	133433	Phenanthrene-d10	11.16		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzamide, N-(1,1-dimethylethyl)...	207	C12H17N02	049834-28-8	53
2		Benzamide, N-(1,1-dimethylethyl)...	207	C12H17N02	019486-73-8	50
3		2H-Imidazo[4,5-b]pyridin-2-one, ...	135	C6H5N3O	016328-62-4	50
4		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	50
5		Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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Sample : I1055-06
Misc :
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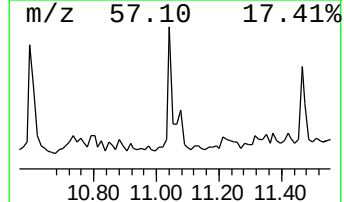
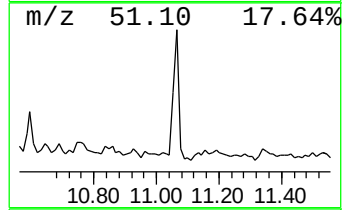
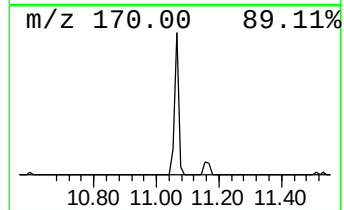
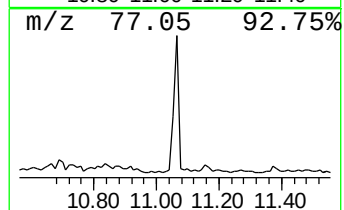
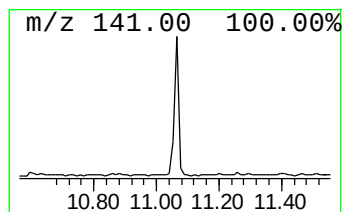
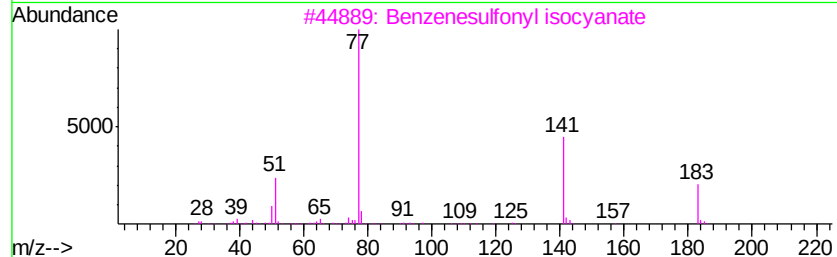
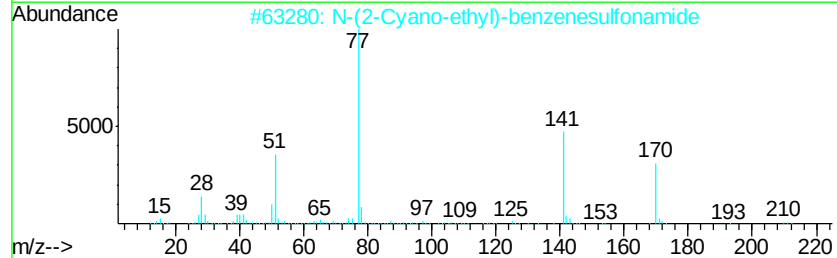
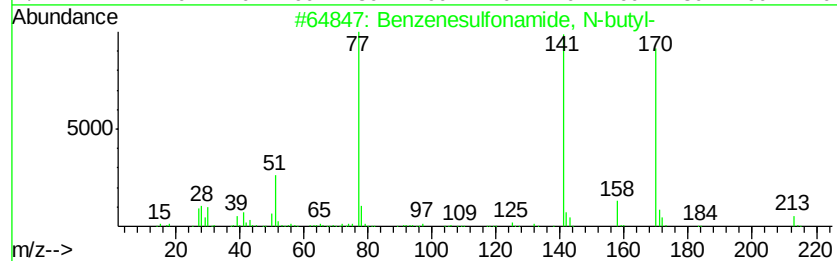
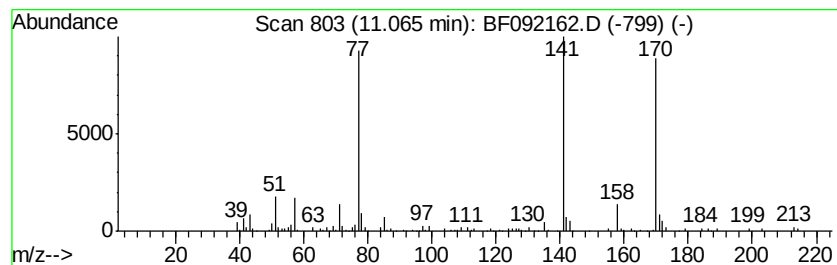
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzenesulfonamide, N-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.06	4.60 ng	226517	Phenanthrene-d10	11.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	91
2	N-(2-Cyano-ethyl)-benzenesulfona...	210	C9H10N2O2S	002619-21-8	78
3	Benzenesulfonyl isocyanate	183	C7H5NO3S	002845-62-7	47
4	p-Chloromandelic acid	186	C8H7ClO3	000492-86-4	43
5	N-(2-Cyanoethyl)-N-methyl-benzen...	224	C10H12N2O2S	218920-78-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
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Misc :
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Instrument :
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ClientSampleId :
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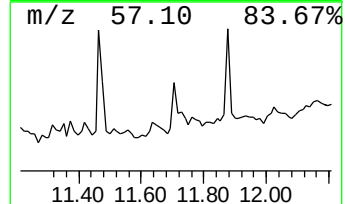
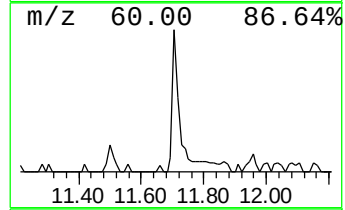
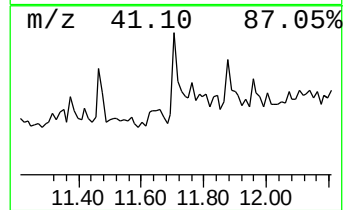
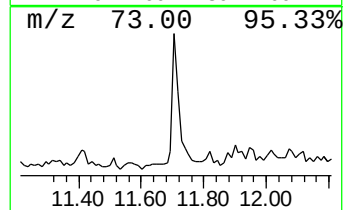
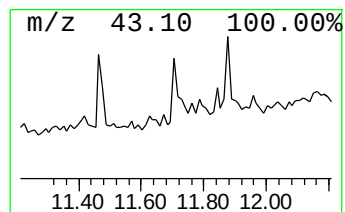
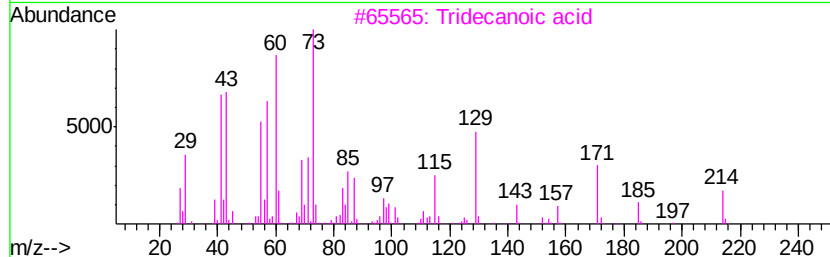
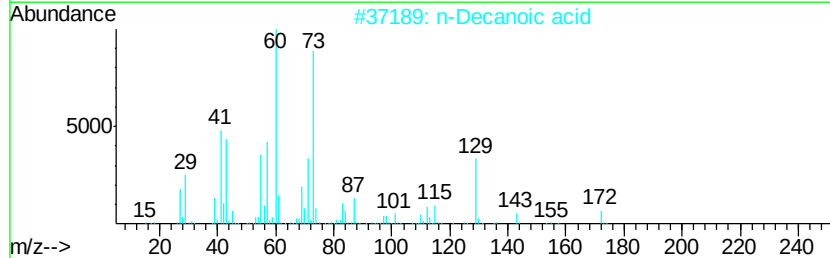
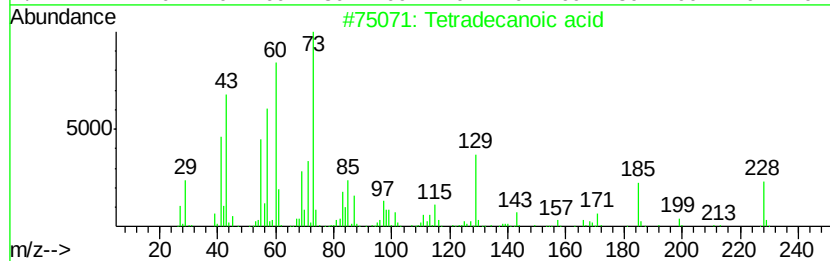
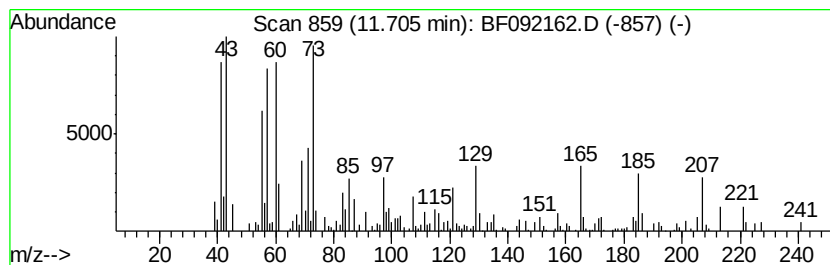
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	4.47 ng	220447	Phenanthrene-d10	11.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2			n-Decanoic acid	172	C10H20O2	000334-48-5	60
3			Tridecanoic acid	214	C13H26O2	000638-53-9	50
4			Undecanoic acid	186	C11H22O2	000112-37-8	46
5			Nonanoic acid	158	C9H18O2	000112-05-0	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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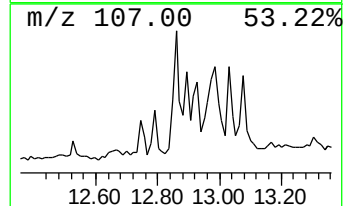
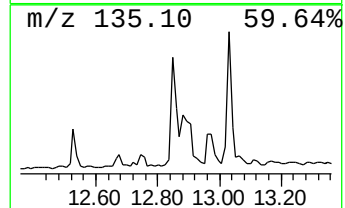
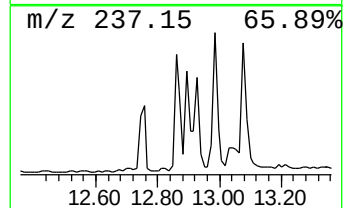
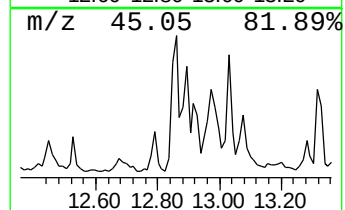
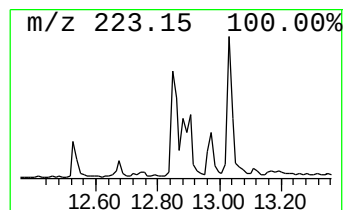
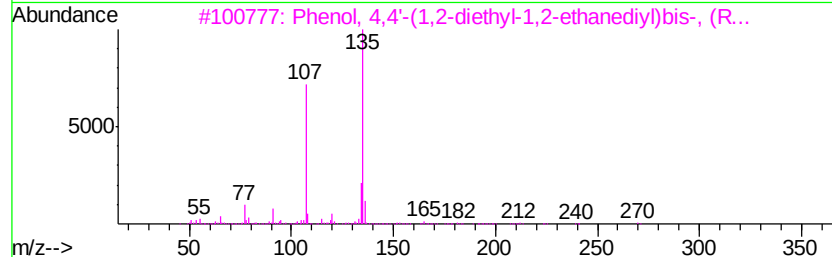
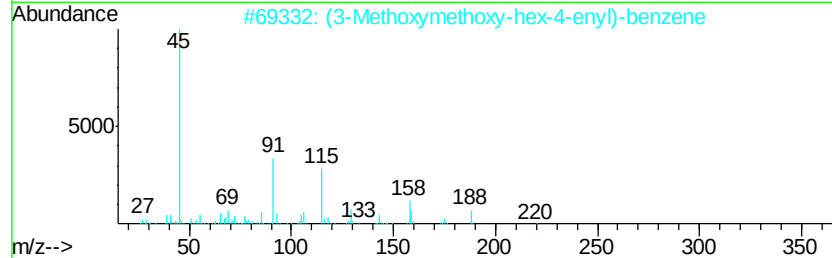
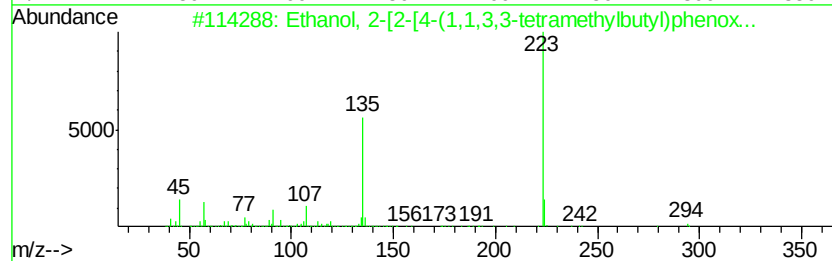
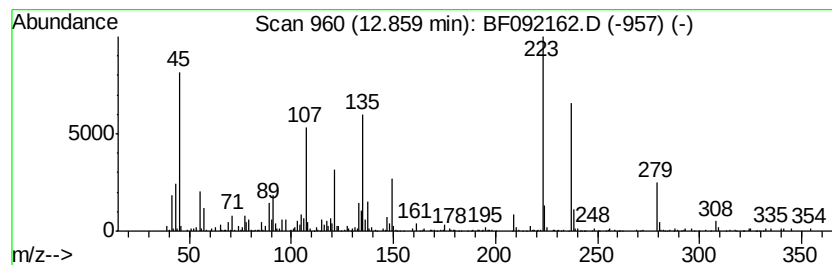
Instrument :
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown12.86 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	11.71 ng	444070	Chrysene-d12	13.80
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294 C18H30O3	002315-61-9	27
2	(3-Methoxymethoxy-hex-4-enyl)-be...	220 C14H20O2	1000185-27-0	15
3	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270 C18H22O2	000084-16-2	14
4	Oxiranecarboxylic acid, 3-phenyl...	192 C11H12O3	002272-55-1	14
5	1-(2-Fluoro-4-nitro-phenyl)-2-me...	238 C12H15FN2O2	1000278-20-9	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
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Sample : I1055-06
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Instrument :
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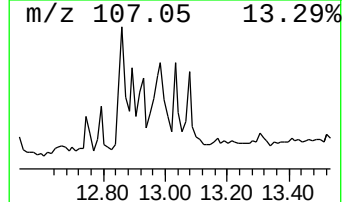
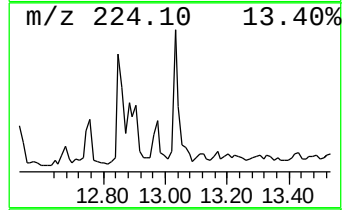
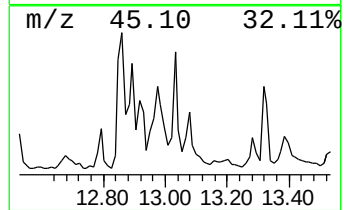
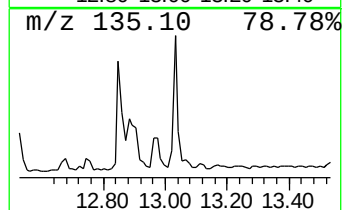
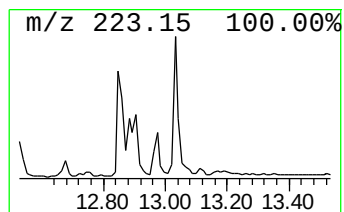
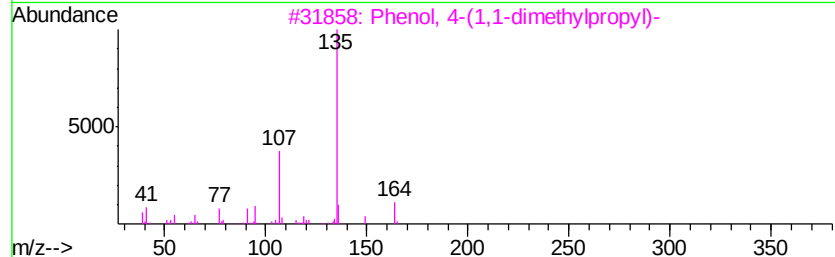
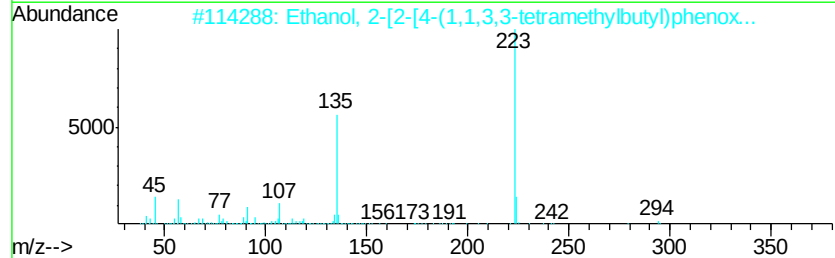
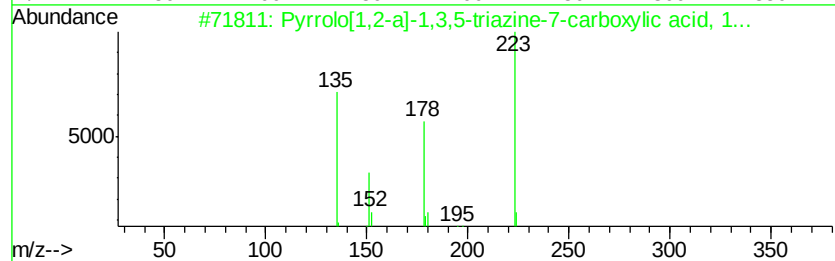
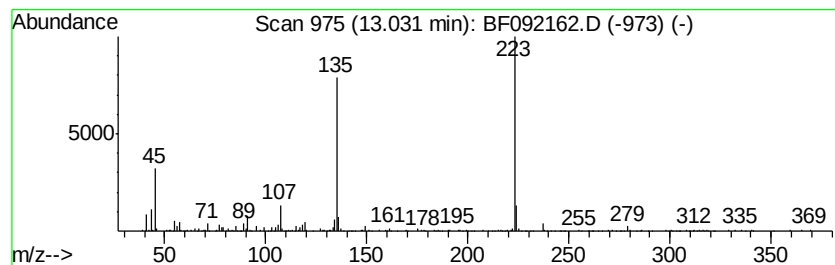
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	4.44 ng	168426	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	58
3		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	35
4		Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	35
5		2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092162.D
Acq On : 10 Jan 2017 2:24
Operator : UM/SJ
Sample : I1055-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-31

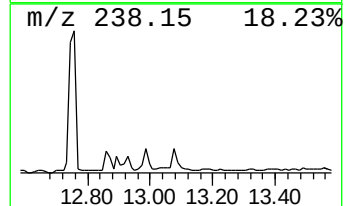
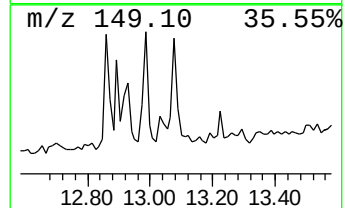
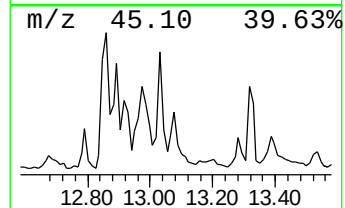
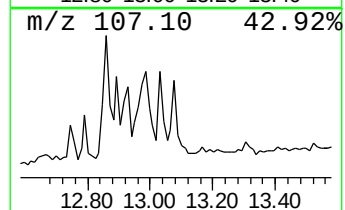
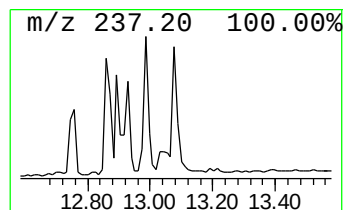
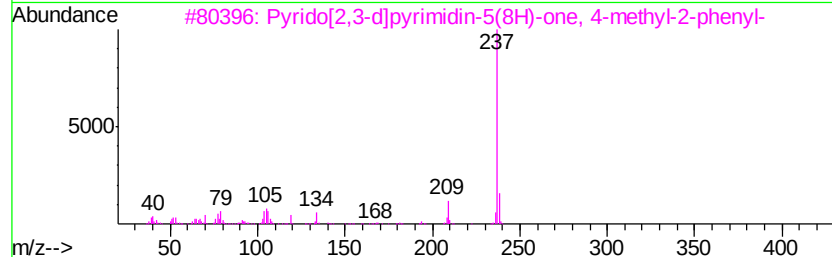
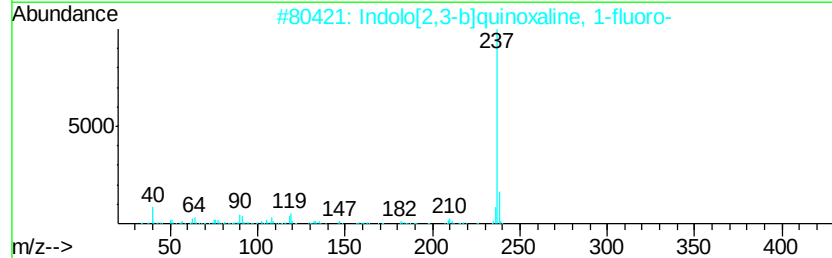
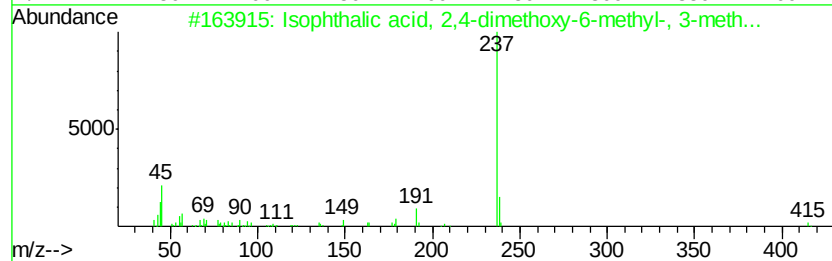
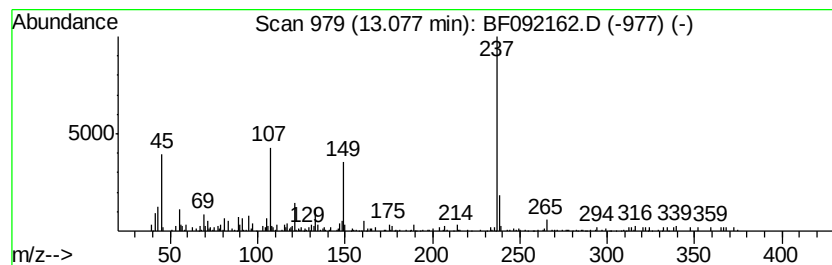
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown13.08 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.08	2.68 ng	101745	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isophthalic acid, 2,4-dimethoxy-...	446	C23H26O9	019314-77-3	38
2		Indolo[2,3-b]quinoxaline, 1-fluoro-	237	C14H8FN3	296244-71-8	27
3		Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	27
4		1-Phenyl-3-(2-pyridyl)-5-pyrazolone	237	C14H11N3O	021683-60-3	27
5		2-Acetylmethylamino-5,5-dimethyl...	252	C12H16N2O2S	1000285-58-5	23



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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Acq On : 10 Jan 2017 2:24
Operator : UM/SJ
Sample : I1055-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-31

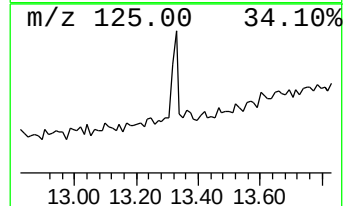
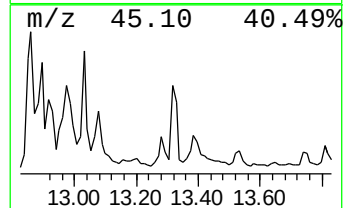
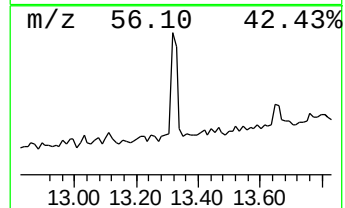
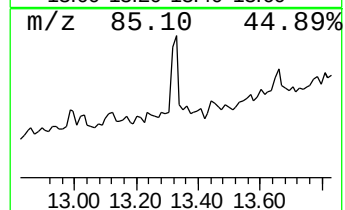
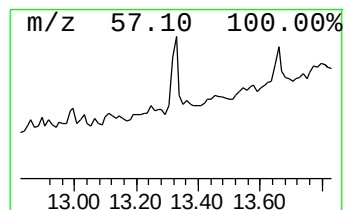
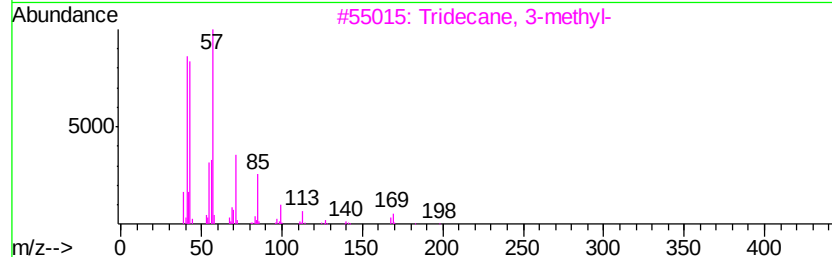
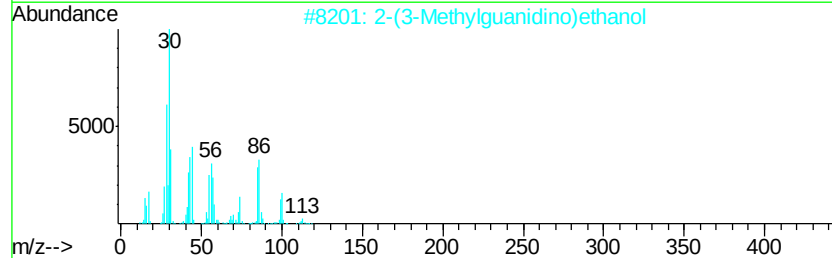
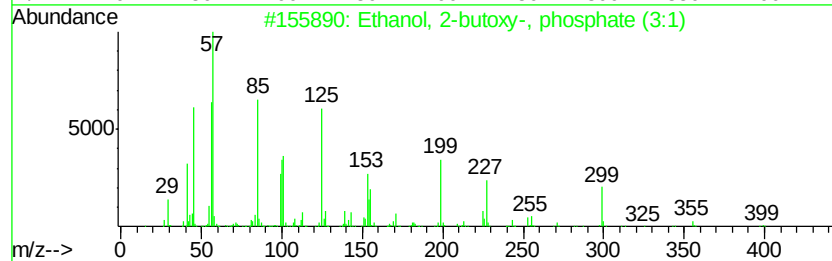
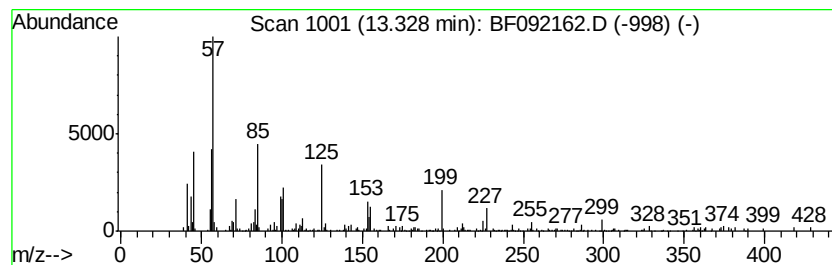
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Ethanol, 2-butoxy-, phospho... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	6.39 ng	242245	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	80
2		2-(3-Methylguanidino)ethanol	117	C4H11N3O	1000242-22-5	27
3		Tridecane, 3-methyl-	198	C14H30	006418-41-3	27
4		Dodecane, 3-methyl-	184	C13H28	017312-57-1	14
5		Pentadecane, 6-methyl-	226	C16H34	010105-38-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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 Acq On : 10 Jan 2017 2:24
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 Sample : I1055-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-31

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Methyl Isobutyl K...	2.66	3.8 ng		155517	1	6.64	809649	20.0
2-Pentanone, 4-hy...	4.76	9.1 ng		367955	1	6.64	809649	20.0
unknown6.41	6.41	68.8 ng		2784390	1	6.64	809649	20.0
Benzene, 1,2,3,4-...	7.42	4.7 ng		261543	2	7.93	1103270	20.0
Benzene, 1,2,4,5-...	7.67	6.6 ng		363703	2	7.93	1103270	20.0
2-Propanol, 1-[1-...	8.16	6.4 ng		355174	2	7.93	1103270	20.0
Benzothiazole	8.21	10.1 ng		557540	2	7.93	1103270	20.0
Naphthalene, 1-me...	8.74	4.0 ng		221323	2	7.93	1103270	20.0
unknown8.94	8.94	3.3 ng		194527	3	9.68	1172380	20.0
Ethanone, 1-[4-(1...	9.13	2.8 ng		166365	3	9.68	1172380	20.0
1H-Benzotriazole,...	9.86	3.1 ng		183505	3	9.68	1172380	20.0
2(3H)-Benzothiazo...	10.60	4.6 ng		227639	4	11.16	985589	20.0
Benzamide, N-(1,1...	10.73	2.7 ng		133433	4	11.16	985589	20.0
Benzenesulfonamid...	11.06	4.6 ng		226517	4	11.16	985589	20.0
Tetradecanoic acid	11.71	4.5 ng		220447	4	11.16	985589	20.0
unknown12.86	12.86	11.7 ng		444070	5	13.80	758629	20.0
Pyrrolo[1,2-a]-1,...	13.03	4.4 ng		168426	5	13.80	758629	20.0
unknown13.08	13.08	2.7 ng		101745	5	13.80	758629	20.0
Ethanol, 2-butoxy...	13.33	6.4 ng		242245	5	13.80	758629	20.0