

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
 Data File : BF087855.D
 Acq On : 9 Jun 2016 16:31
 Operator : UM/SJ
 Sample : H3399-13 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-32

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-BF060716.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	1.644	3	5	7	rVB	3373845	4238238	50.09%	7.138%
2	1.747	13	14	24	rVB	189814	344724	4.07%	0.581%
3	1.884	24	26	38	rVV	1550132	3417241	40.39%	5.755%
4	2.044	38	40	70	rVB4	86146	459836	5.43%	0.774%
5	4.982	295	297	301	rBV	157473	204890	2.42%	0.345%
6	5.416	332	335	337	rVB	1275264	1700243	20.09%	2.863%
7	6.456	423	426	428	rBV	1475063	1805245	21.34%	3.040%
8	6.582	435	437	440	rVB	1609596	1620531	19.15%	2.729%
9	6.822	456	458	460	rBV	722496	700705	8.28%	1.180%
10	6.970	469	471	474	rVB	1128098	1327152	15.69%	2.235%
11	7.382	504	507	509	rBV	1231819	1067302	12.61%	1.797%
12	8.102	568	570	574	rBV	1054030	997354	11.79%	1.680%
13	9.176	662	664	667	rBV	2003467	1758324	20.78%	2.961%
14	9.576	697	699	701	rBV	117837	164986	1.95%	0.278%
15	9.851	721	723	725	rBV	1061171	991387	11.72%	1.670%
16	10.056	738	741	742	rBV	103025	85391	1.01%	0.144%
17	10.399	769	771	773	rBV	123956	131676	1.56%	0.222%
18	10.639	789	792	794	rBV	961154	1043401	12.33%	1.757%
19	10.765	800	803	806	rBV2	66177	104497	1.24%	0.176%
20	10.936	816	818	820	rBV3	110407	145632	1.72%	0.245%
21	11.131	834	835	838	rVB	106101	110065	1.30%	0.185%
22	11.211	838	842	847	rBV4	65445	204819	2.42%	0.345%
23	11.325	850	852	853	rBV	623094	764389	9.03%	1.287%
24	11.359	853	855	856	rVV	655756	842053	9.95%	1.418%
25	11.405	856	859	860	rVV	256476	251750	2.98%	0.424%
26	11.439	860	862	864	rVB	95753	89932	1.06%	0.151%
27	11.554	869	872	876	rBV2	97386	138490	1.64%	0.233%
28	11.828	894	896	897	rBV	110660	102358	1.21%	0.172%
29	11.862	897	899	900	rVV	172308	199642	2.36%	0.336%
30	11.896	900	902	904	rVB2	187594	177511	2.10%	0.299%
31	11.942	904	906	910	rVB2	185344	267697	3.16%	0.451%
32	12.125	920	922	927	rVB2	86321	131516	1.55%	0.221%
33	12.537	955	958	960	rVB	1167713	1019176	12.05%	1.716%
34	12.765	975	978	980	rBV	886841	1047913	12.38%	1.765%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

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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-BF060716.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.914	989	991	993	rVB	1294322	1355674	16.02%	2.283%
36	13.085	1002	1006	1008	rVB2	123355	186473	2.20%	0.314%
37	13.154	1010	1012	1014	rBV	119437	105548	1.25%	0.178%
38	13.188	1014	1015	1019	rVB4	93781	153985	1.82%	0.259%
39	13.279	1019	1023	1025	rBV2	60397	109109	1.29%	0.184%
40	13.405	1030	1034	1037	rBV	4226748	8461177	100.00%	14.250%
41	13.451	1037	1038	1039	rVV	102380	93008	1.10%	0.157%
42	13.485	1039	1041	1042	rVV	67849	109970	1.30%	0.185%
43	13.508	1042	1043	1045	rVB	106659	91702	1.08%	0.154%
44	13.600	1048	1051	1053	rVB	140612	234523	2.77%	0.395%
45	13.645	1053	1055	1056	rBV2	134663	211525	2.50%	0.356%
46	13.668	1056	1057	1058	rVV	293001	234037	2.77%	0.394%
47	13.691	1058	1059	1061	rVV	332387	445198	5.26%	0.750%
48	13.737	1061	1063	1065	rVV	760080	617630	7.30%	1.040%
49	13.805	1067	1069	1070	rBV	163601	208635	2.47%	0.351%
50	13.874	1073	1075	1078	rVB3	63739	117344	1.39%	0.198%
51	13.954	1078	1082	1089	rBV2	1574714	2666834	31.52%	4.491%
52	14.057	1089	1091	1093	rBV2	104364	121245	1.43%	0.204%
53	14.102	1093	1095	1097	rBV	151706	179572	2.12%	0.302%
54	14.160	1097	1100	1104	rBV3	283093	514753	6.08%	0.867%
55	14.228	1104	1106	1108	rVB	177570	145691	1.72%	0.245%
56	14.320	1111	1114	1115	rBV	800254	841695	9.95%	1.418%
57	14.354	1115	1117	1119	rVB	517219	429154	5.07%	0.723%
58	14.434	1122	1124	1125	rBV2	75567	96516	1.14%	0.163%
59	14.560	1133	1135	1138	rVB	1531891	1523781	18.01%	2.566%
60	14.628	1140	1141	1142	rBV	105630	123446	1.46%	0.208%
61	14.731	1148	1150	1153	rVB2	217049	335211	3.96%	0.565%
62	14.811	1153	1157	1159	rVV2	182025	351967	4.16%	0.593%
63	14.914	1163	1166	1168	rVV	690582	967300	11.43%	1.629%
64	14.960	1168	1170	1174	rVV	659916	1154008	13.64%	1.943%
65	15.051	1176	1178	1185	rVB4	149571	349511	4.13%	0.589%
66	15.200	1187	1191	1193	rVV	1232068	2071171	24.48%	3.488%
67	15.245	1193	1195	1197	rVV	281027	353214	4.17%	0.595%
68	15.303	1197	1200	1203	rVV2	367526	516063	6.10%	0.869%
69	15.371	1203	1206	1211	rVB2	424433	881300	10.42%	1.484%
70	15.451	1211	1213	1216	rVB	91208	119374	1.41%	0.201%
71	15.508	1216	1218	1223	rBV	122199	197495	2.33%	0.333%

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Sampling : 1 Min Area: 3 % of largest Peak
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72	15.623	1223	1228	1231	rBV	285652	728597	8.61%	1.227%
73	15.817	1242	1245	1247	rBV	114638	170082	2.01%	0.286%
74	15.977	1256	1259	1262	rBV	724315	1196178	14.14%	2.014%
75	16.434	1297	1299	1304	rVB2	77379	154691	1.83%	0.261%
76	16.526	1304	1307	1314	rBV	146644	339176	4.01%	0.571%
77	16.720	1321	1324	1332	rVB2	112896	249684	2.95%	0.420%
78	17.028	1348	1351	1357	rVB	212182	507757	6.00%	0.855%
79	17.131	1357	1360	1366	rVB	93178	201551	2.38%	0.339%
80	17.280	1370	1373	1385	rVB5	122801	466584	5.51%	0.786%
81	17.703	1406	1410	1415	rBV	122680	315661	3.73%	0.532%
82	17.806	1416	1419	1428	rVB5	64070	199158	2.35%	0.335%
83	19.200	1536	1541	1549	rVB3	150806	518675	6.13%	0.874%

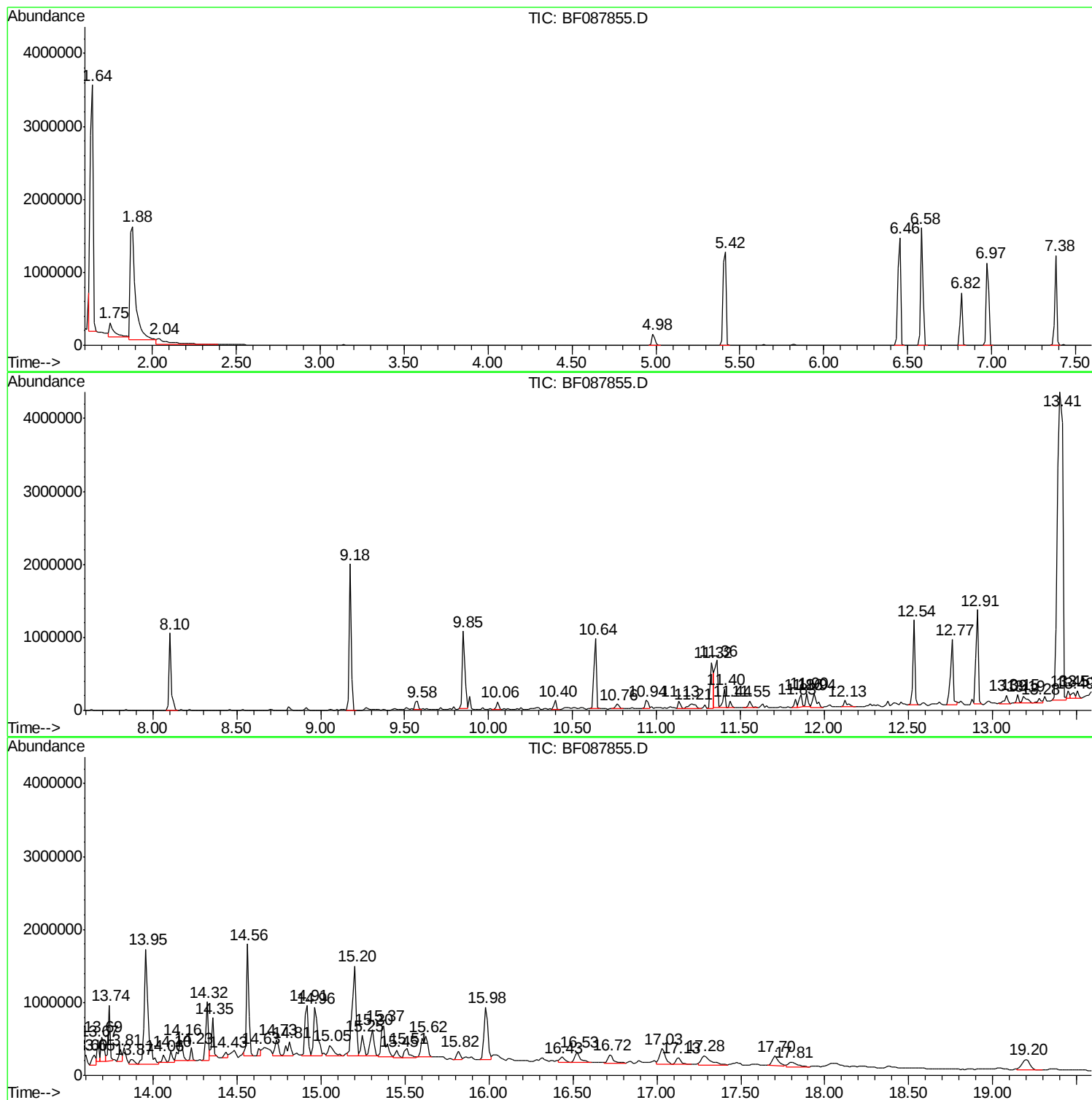
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
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Acq On : 9 Jun 2016 16:31
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Sample : H3399-13 2X
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Instrument :
BNA_F
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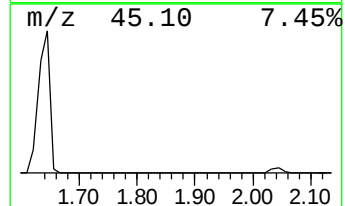
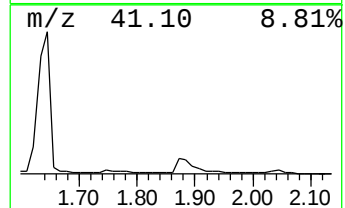
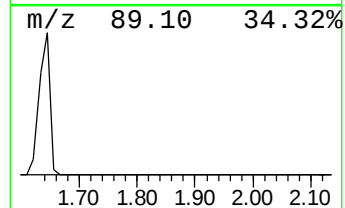
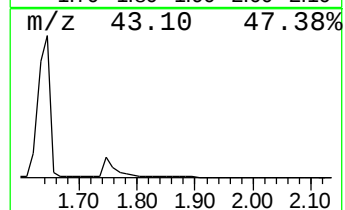
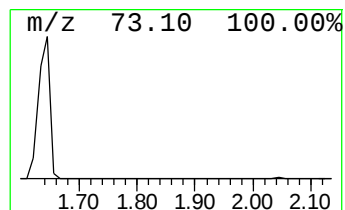
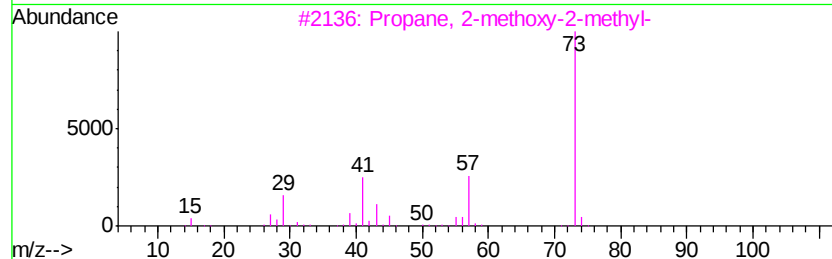
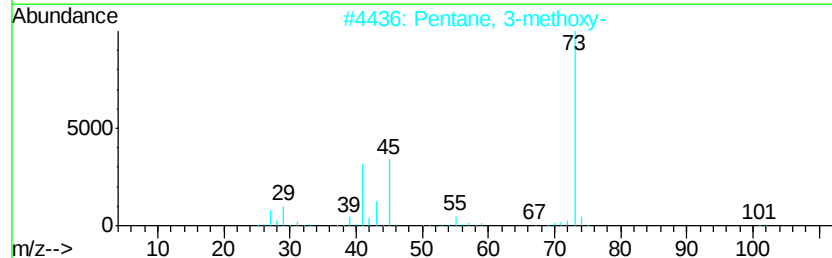
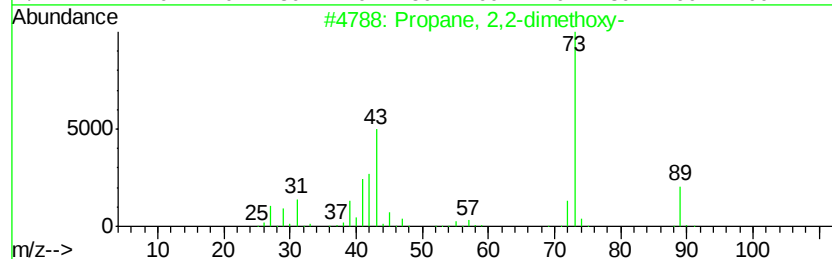
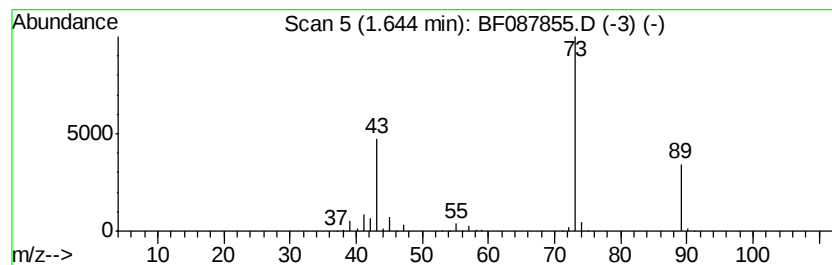
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	120.97 ng	4238240	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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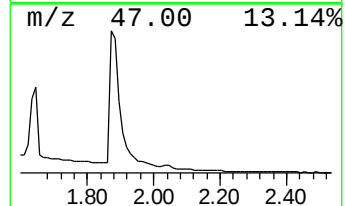
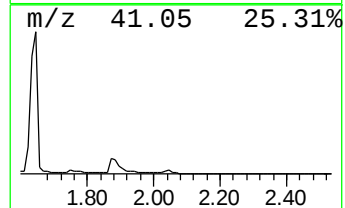
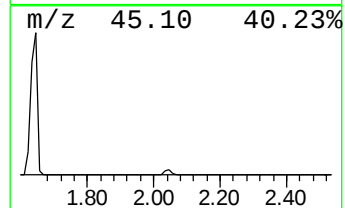
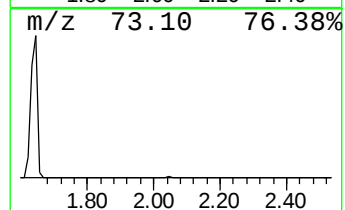
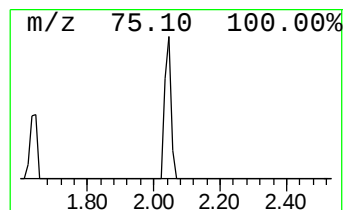
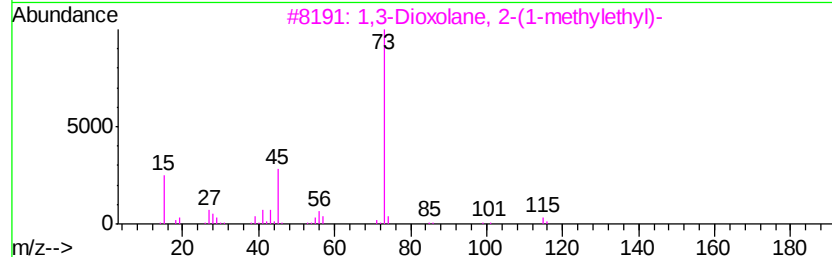
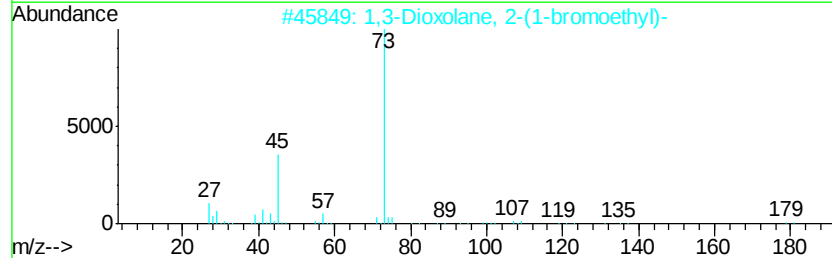
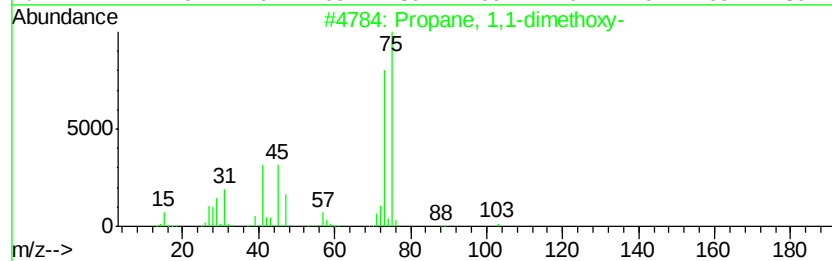
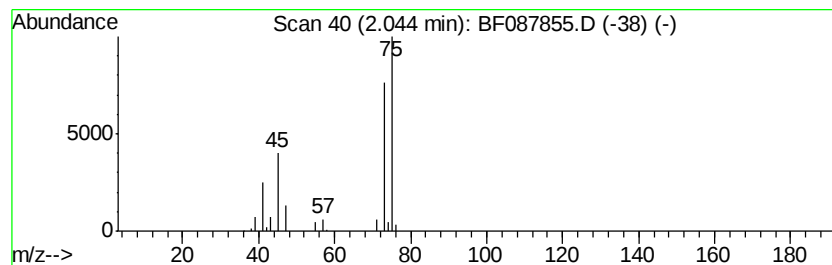
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	13.13 ng	459836	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Glycine	75	C2H5NO2	000056-40-6	7



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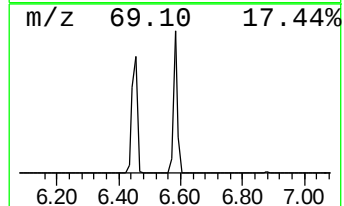
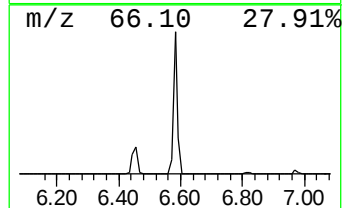
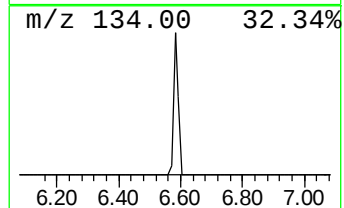
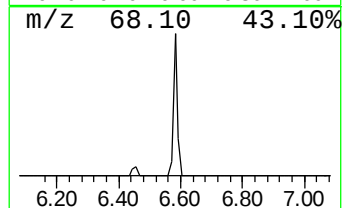
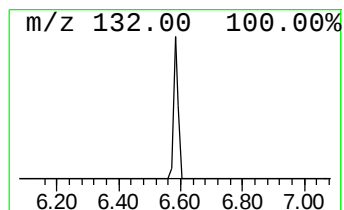
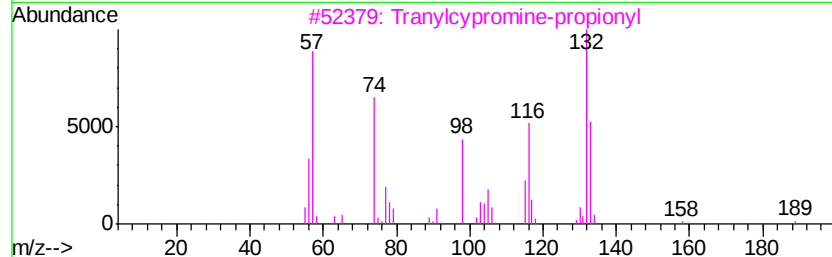
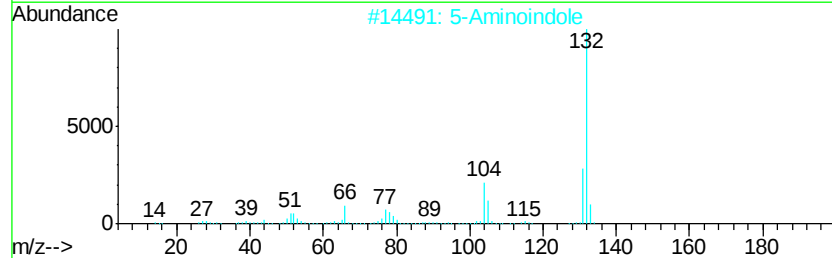
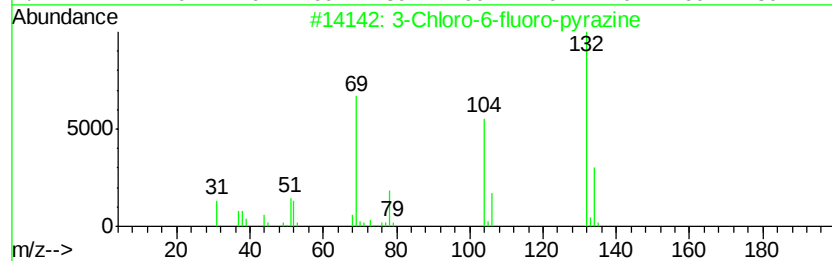
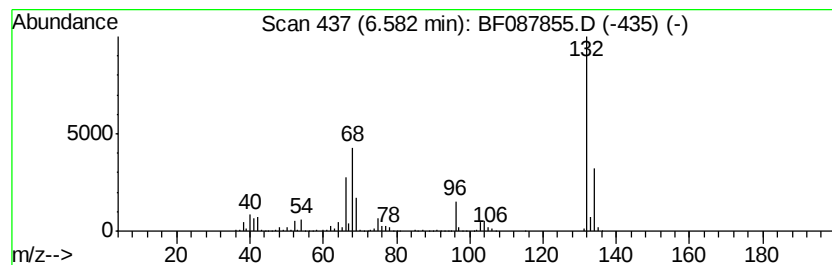
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.58 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	46.25 ng	1620530	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	



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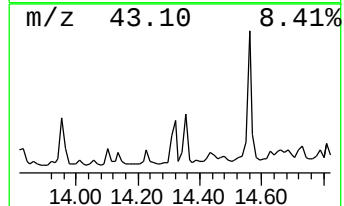
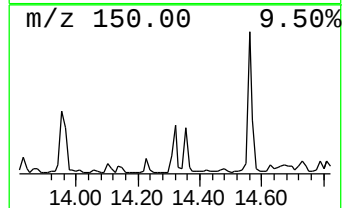
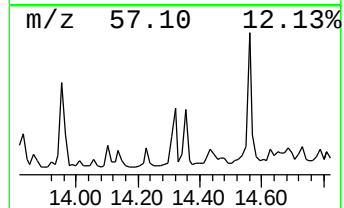
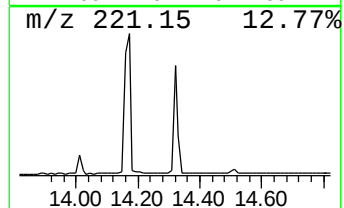
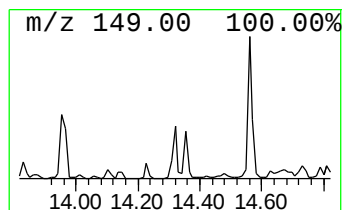
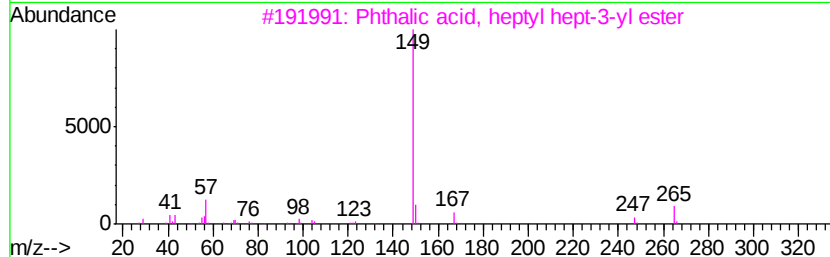
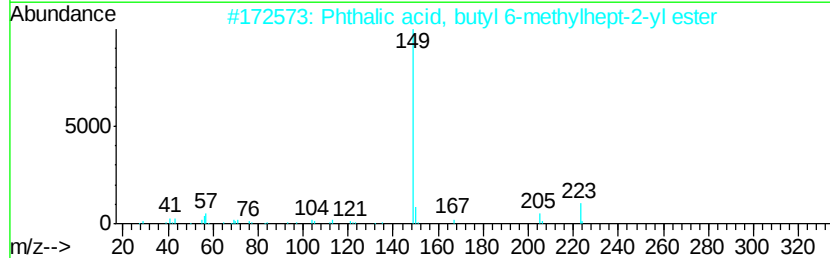
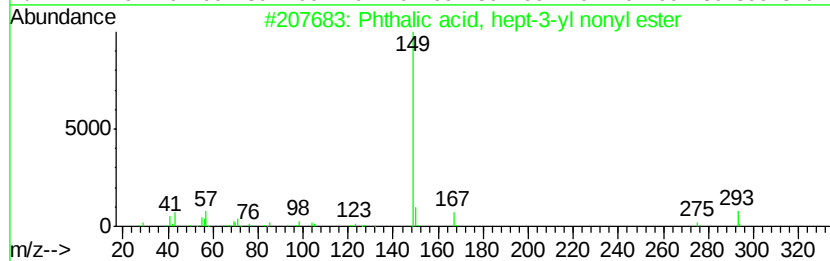
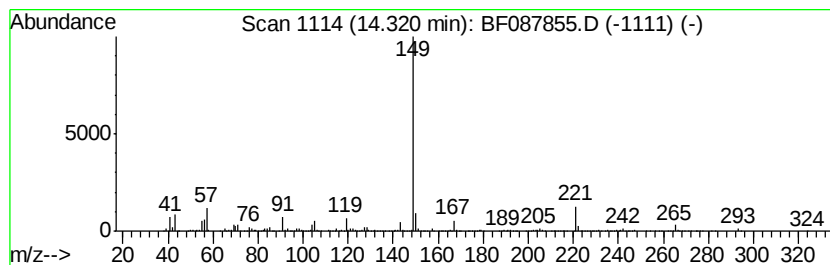
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phthalic acid, hept-3-yl no... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	6.31 ng	841695	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	64
2		Phthalic acid, butyl 6-methylhep...	334	C20H30O4	1000377-95-8	64
3		Phthalic acid, heptyl hept-3-yl ...	362	C22H34O4	1000356-99-1	64
4		Phthalic acid, hexyl 6-methylhep...	362	C22H34O4	1000377-96-0	64
5		Phthalic acid, cyclohexyl isohex...	304	C18H24O4	1000315-34-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

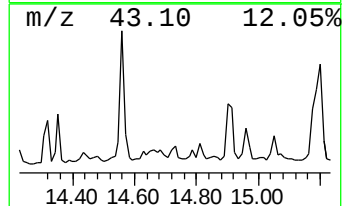
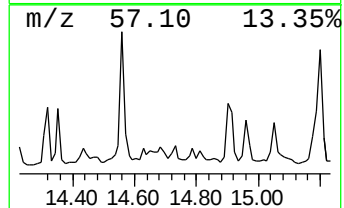
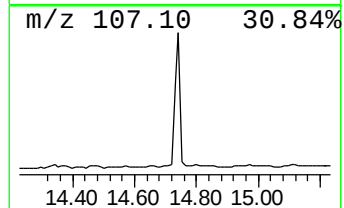
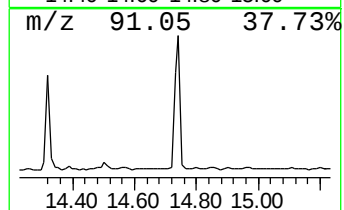
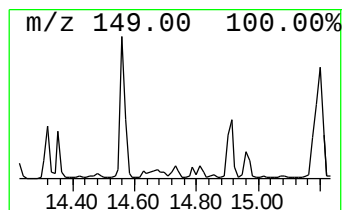
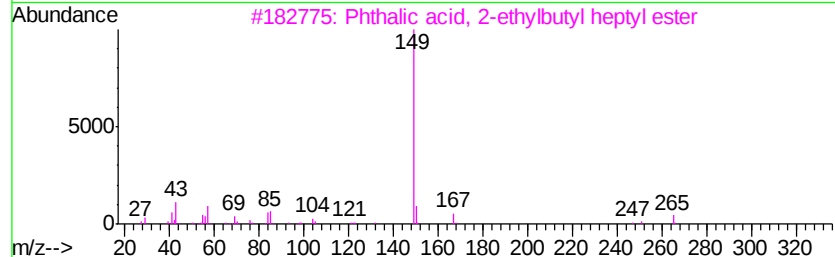
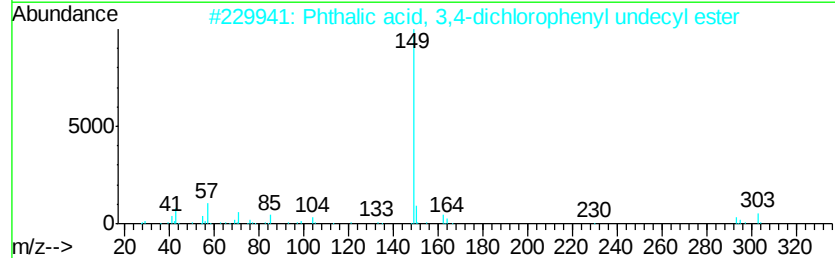
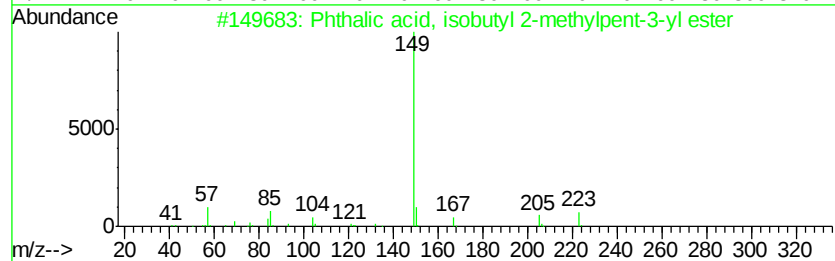
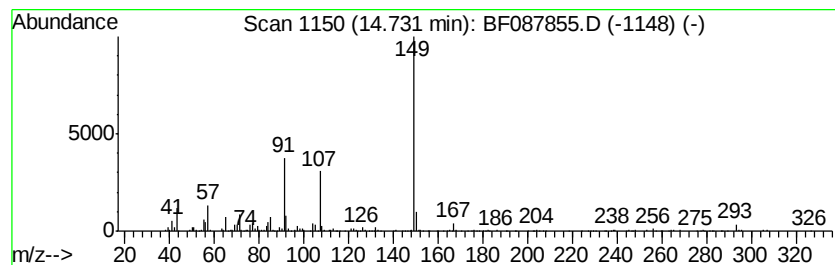
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, isobutyl 2-m... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	7.61 ng	335211	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, isobutyl 2-methyl...	306	C18H26O4	1000356-90-7	72
2		Phthalic acid, 3,4-dichloropheny...	464	C25H30Cl2O4	1000315-28-0	64
3		Phthalic acid, 2-ethylbutyl hept...	348	C21H32O4	1000356-89-2	64
4		Phthalic acid, 2,3-dimethylpheny...	396	C25H32O4	1000357-09-1	64
5		Dibutyl phthalate	278	C16H22O4	000084-74-2	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

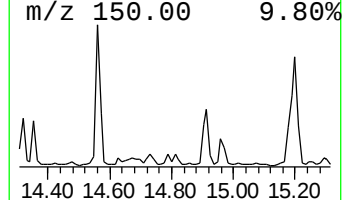
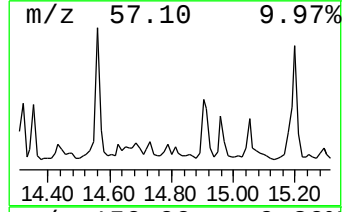
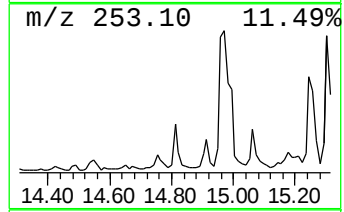
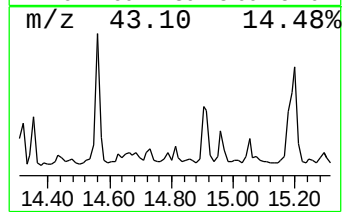
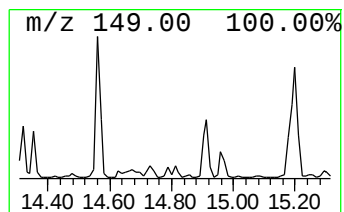
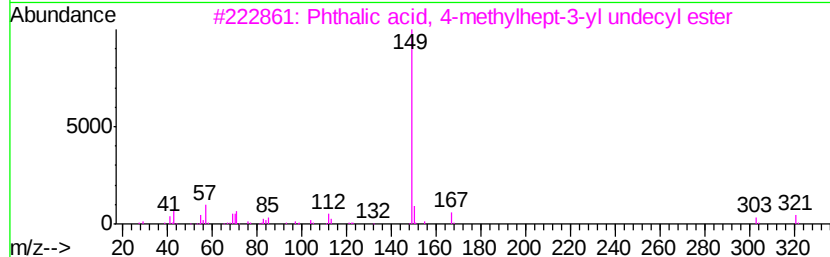
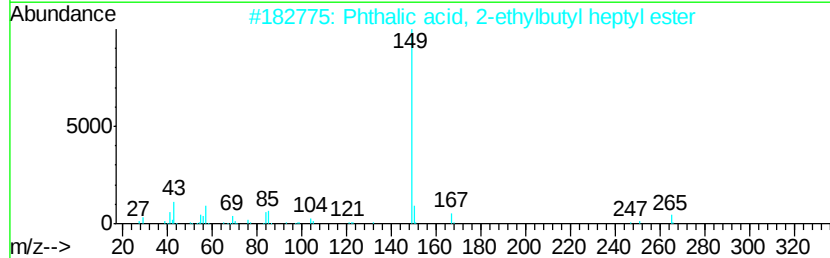
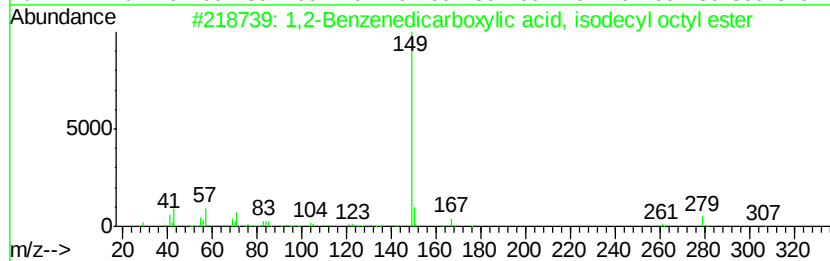
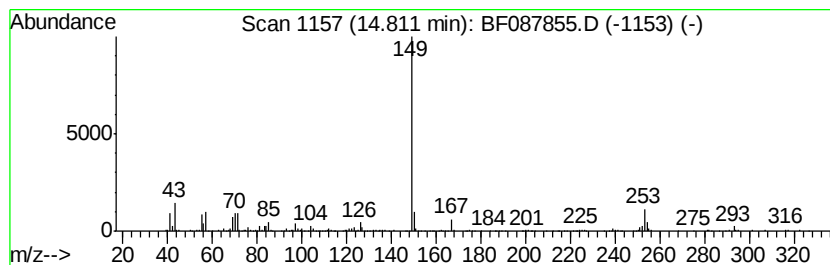
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,2-Benzenedicarboxylic aci... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	7.99 ng	351967	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	68
2		Phthalic acid, 2-ethylbutyl hept...	348	C21H32O4	1000356-89-2	64
3		Phthalic acid, 4-methylhept-3-yl...	432	C27H44O4	1000377-94-6	64
4		Didecyl phthalate	446	C28H46O4	000084-77-5	64
5		Phthalic acid, cycloheptyl propy...	304	C18H24O4	1000322-82-7	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

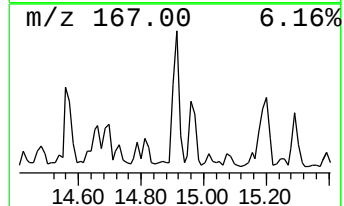
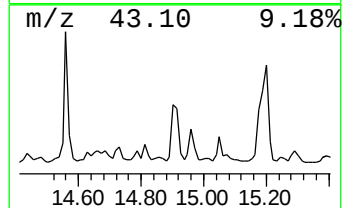
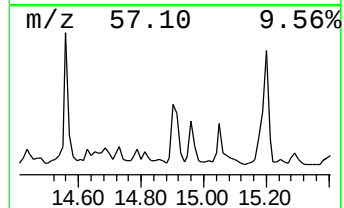
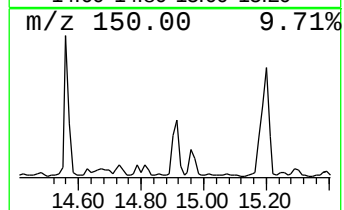
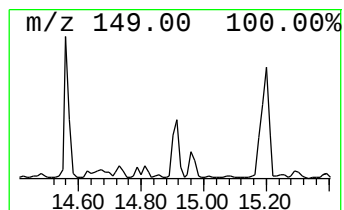
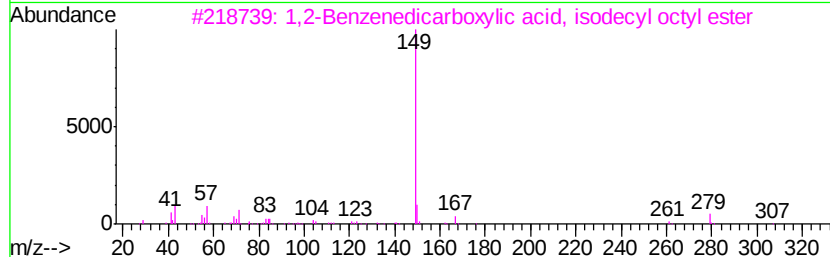
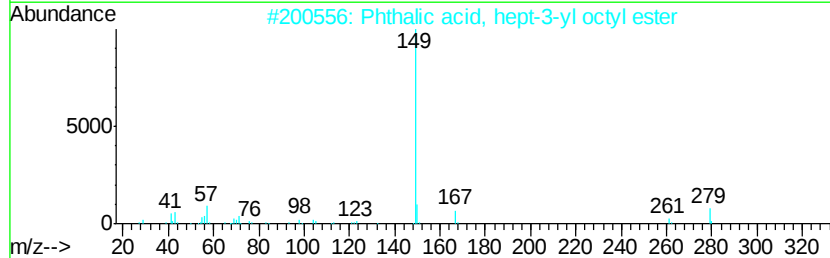
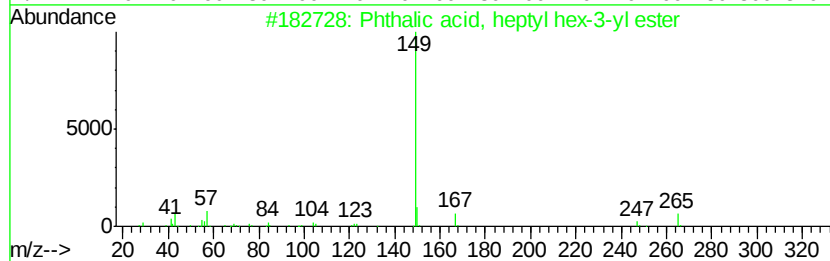
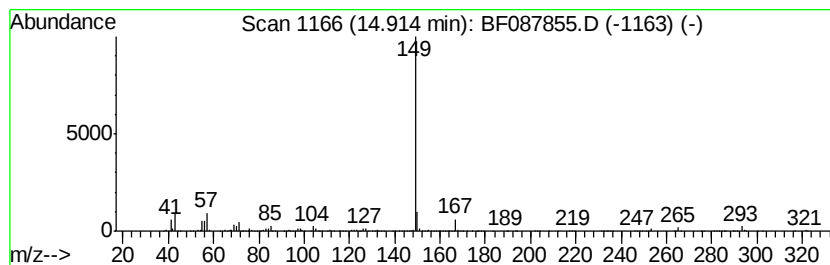
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phthalic acid, heptyl hex-3... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	21.95 ng	967300	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, heptyl hex-3-yl e...	348	C21H32O4	1000356-95-8	86
2		Phthalic acid, hept-3-yl octyl e...	376	C23H36O4	1000356-99-2	80
3		1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	80
4		Phthalic acid, hexyl 6-methylhep...	362	C22H34O4	1000377-96-0	80
5		Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

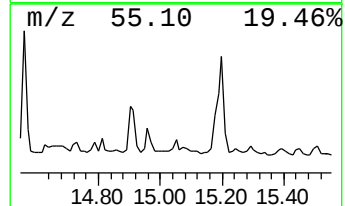
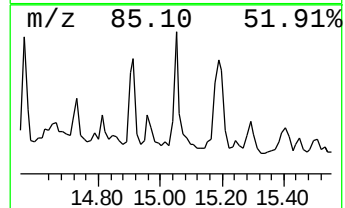
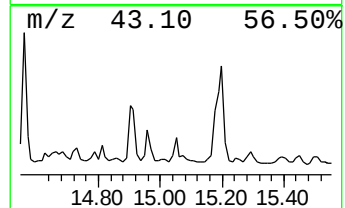
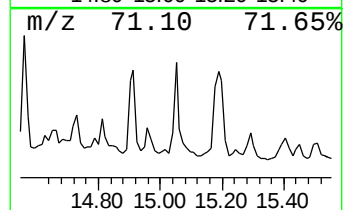
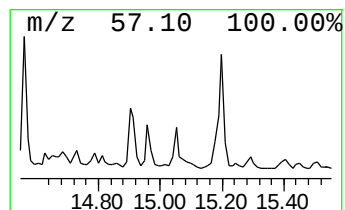
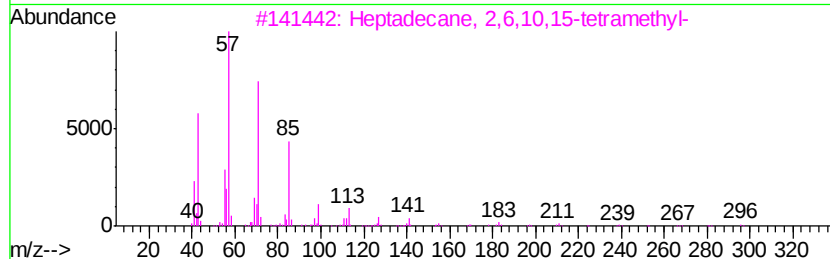
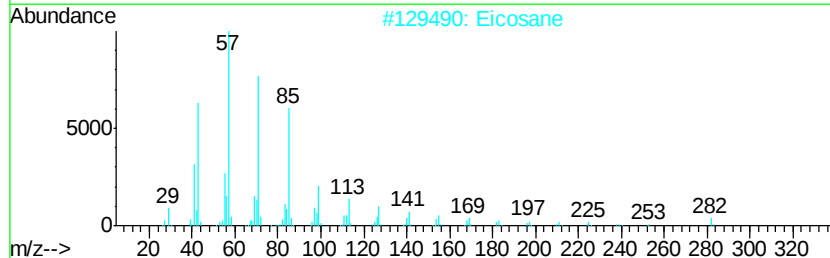
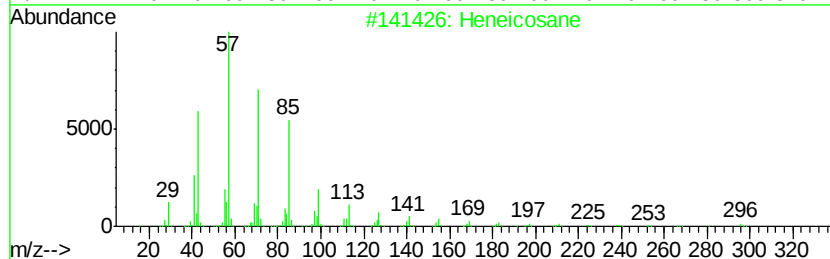
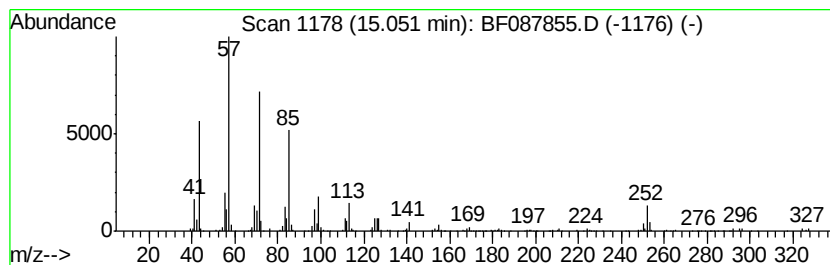
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	7.93 ng	349511	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	99
2		Eicosane	282	C20H42	000112-95-8	93
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4		Pentacosane	352	C25H52	000629-99-2	83
5		Octacosane	394	C28H58	000630-02-4	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

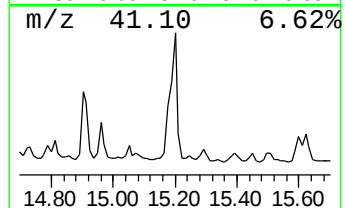
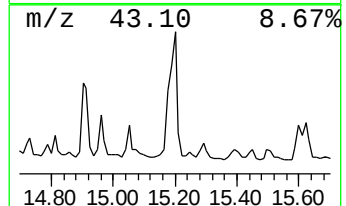
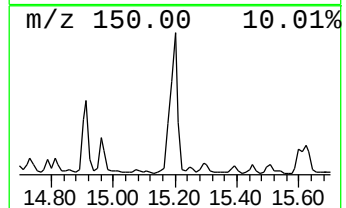
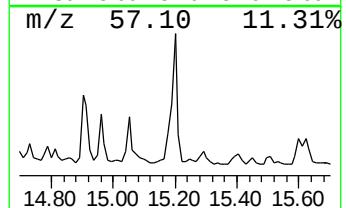
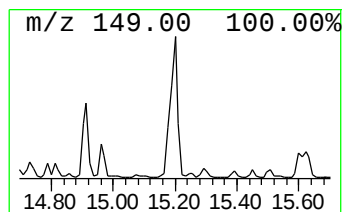
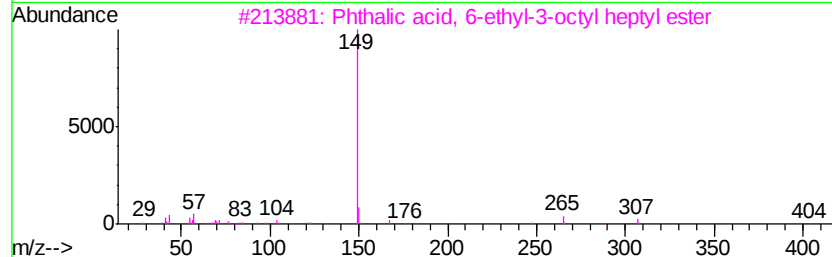
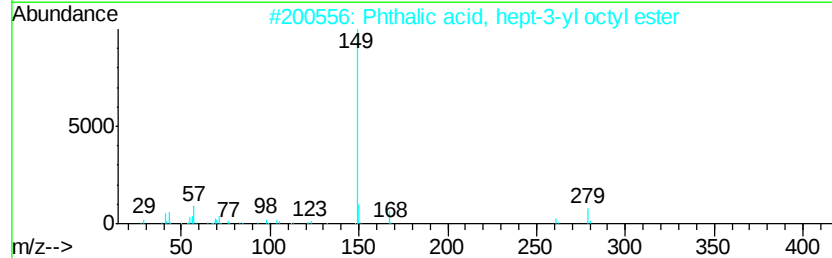
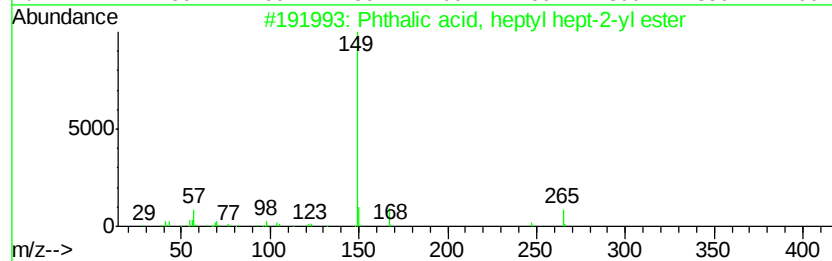
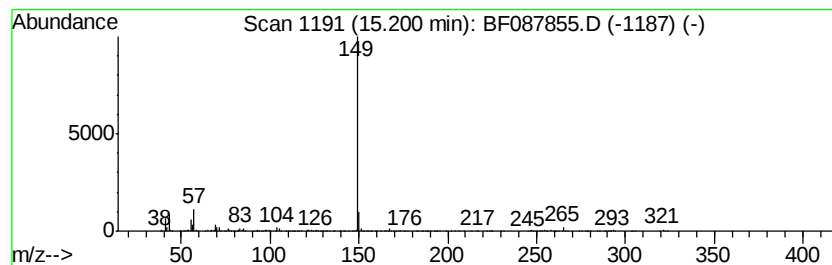
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phthalic acid, heptyl hept-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	47.00 ng	2071170	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, heptyl hept-2-yl ...	362	C22H34O4	1000356-97-4	78
2		Phthalic acid, hept-3-yl octyl e...	376	C23H36O4	1000356-99-2	72
3		Phthalic acid, 6-ethyl-3-octyl h...	404	C25H40O4	1000315-17-7	72
4		Phthalic acid, 5-methylhex-2-yl ...	418	C26H42O4	1000371-08-3	72
5		Phthalic acid, decyl hept-3-yl e...	404	C25H40O4	1000356-99-4	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

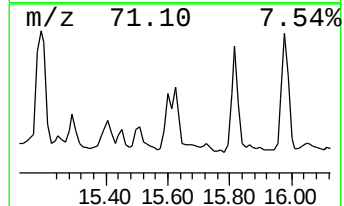
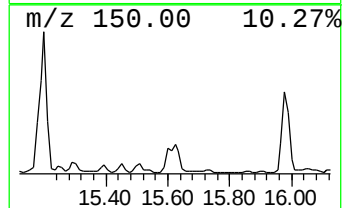
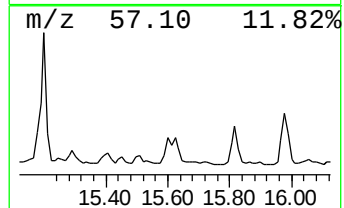
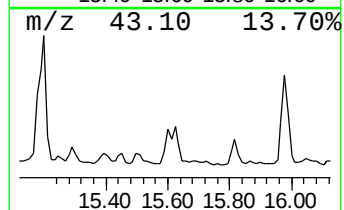
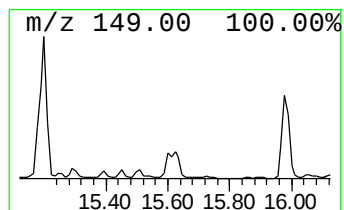
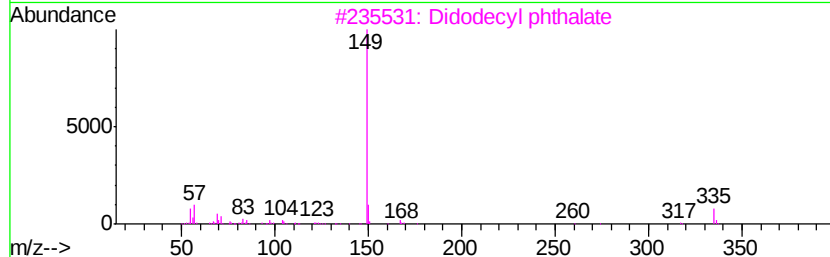
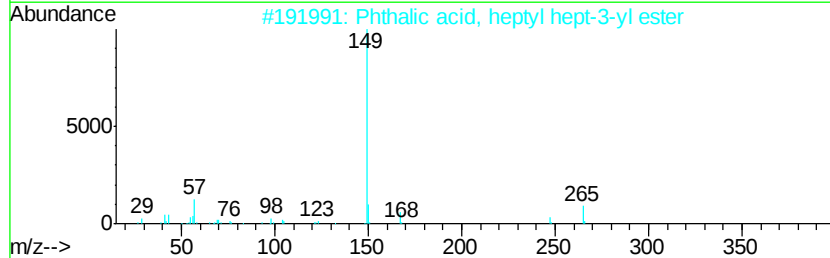
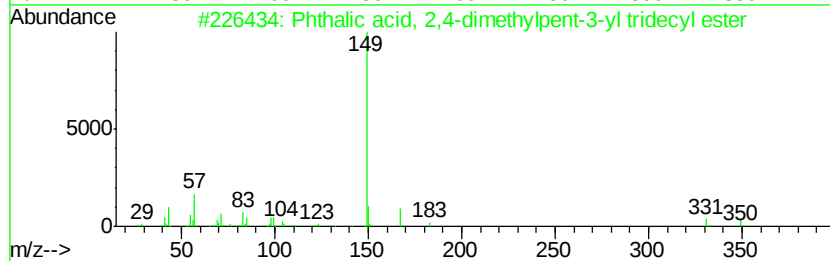
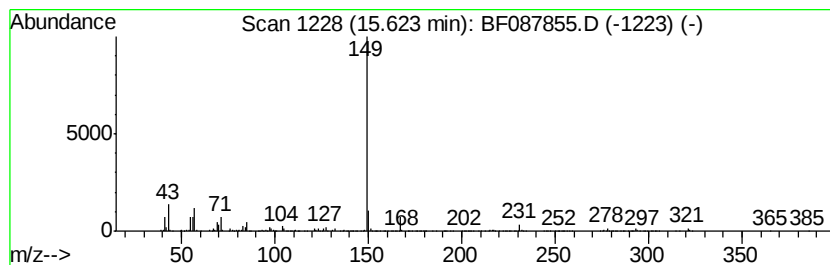
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Phthalic acid, 2,4-dimethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	16.53 ng	728597	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 2,4-dimethylpent-...	446	C28H46O4	1000356-85-2	86
2		Phthalic acid, heptyl hept-3-yl ...	362	C22H34O4	1000356-99-1	80
3		Didodecyl phthalate	502	C32H54O4	002432-90-8	80
4		Phthalic acid, octyl 2-propylpen...	390	C24H38O4	1000377-92-4	80
5		Phthalic acid, dodecyl nonyl ester	460	C29H48O4	1000308-92-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

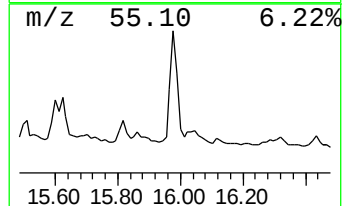
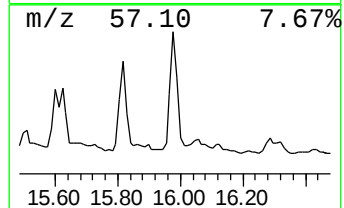
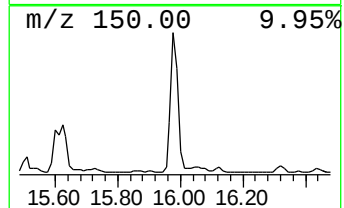
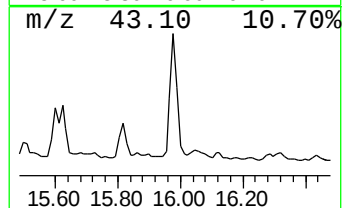
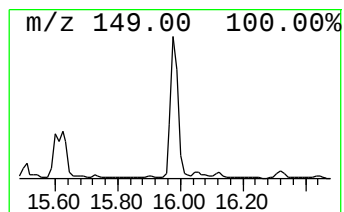
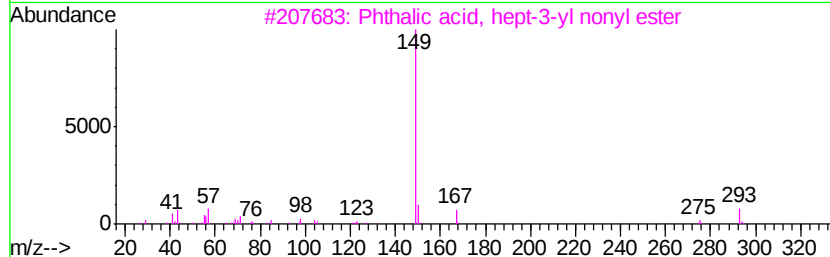
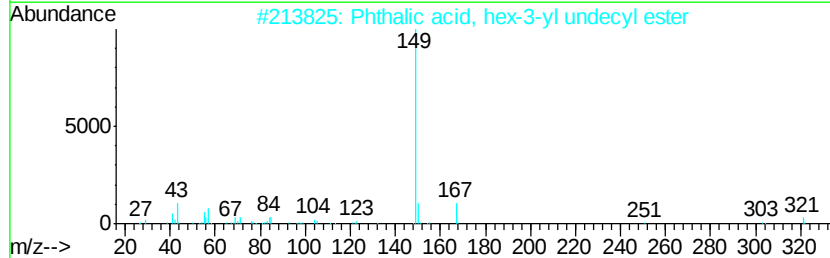
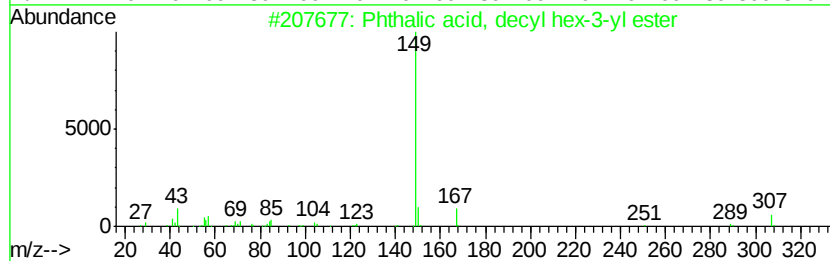
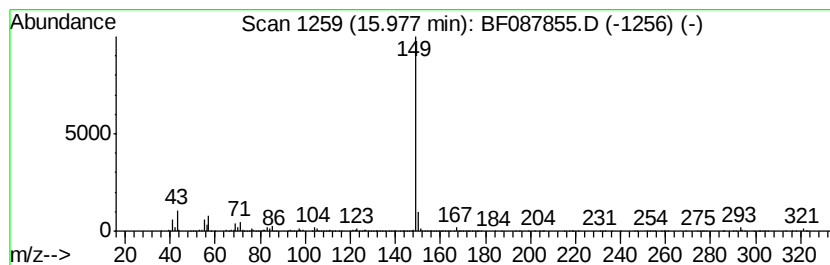
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Phthalic acid, decyl hex-3-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	27.15 ng	1196180	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, decyl hex-3-yl ester	390	C24H38O4	1000356-96-1	80
2		Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	80
3		Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80
4		Phthalic acid, 4-methylpent-2-yl...	376	C23H36O4	1000356-87-9	80
5		1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-32

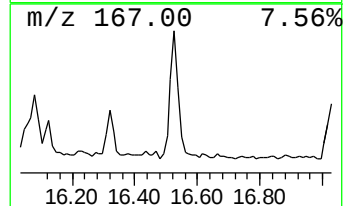
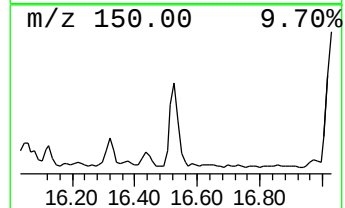
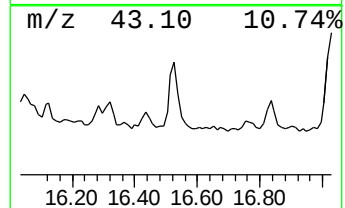
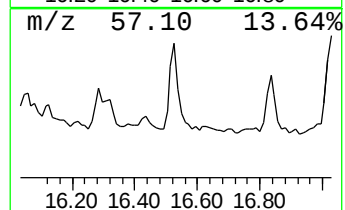
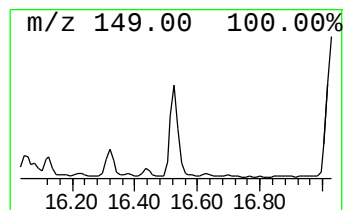
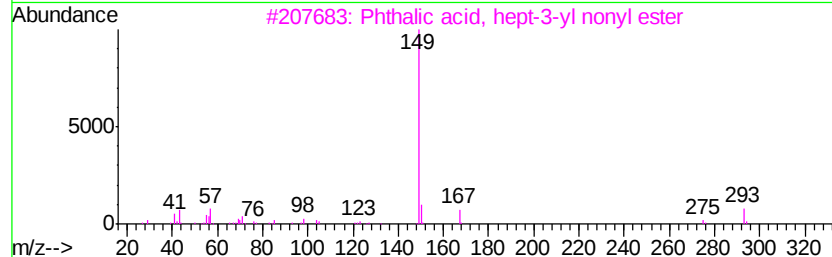
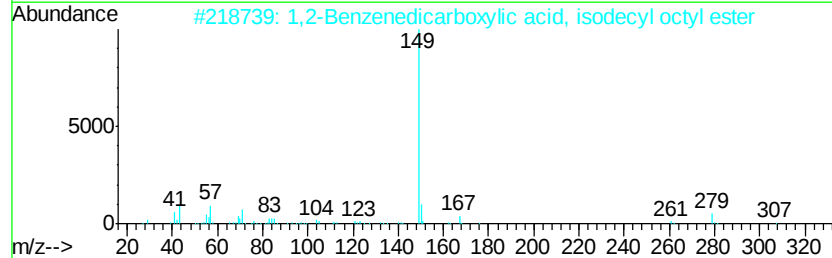
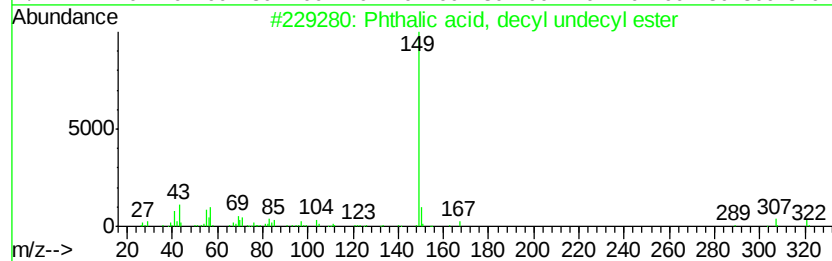
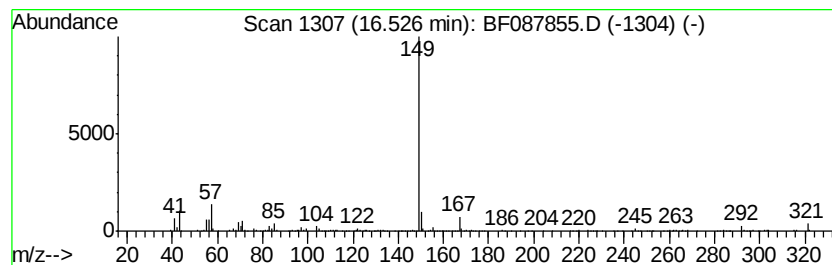
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Phthalic acid, decyl undecyl... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	7.70 ng	339176	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, decyl undecyl ester	460	C29H48O4	1000308-91-9	86
2		1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	80
3		Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80
4		1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	80
5		Phthalic acid, 6-methylhept-2-yl...	432	C27H44O4	1000377-96-5	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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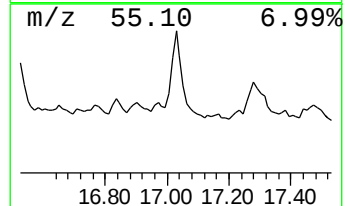
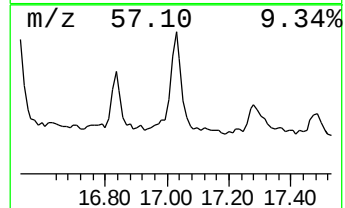
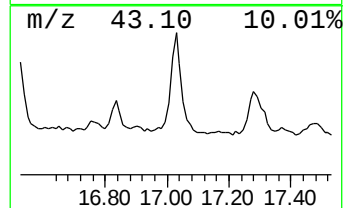
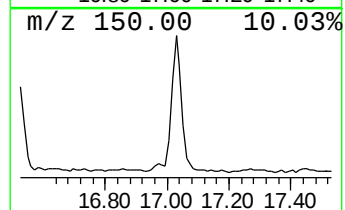
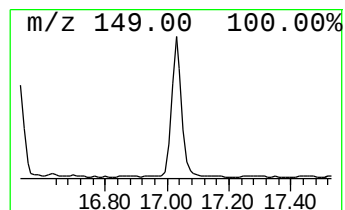
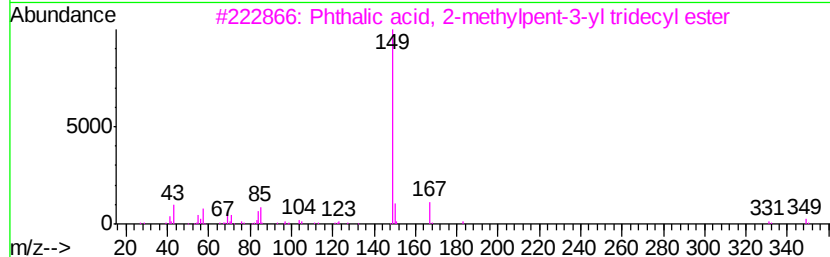
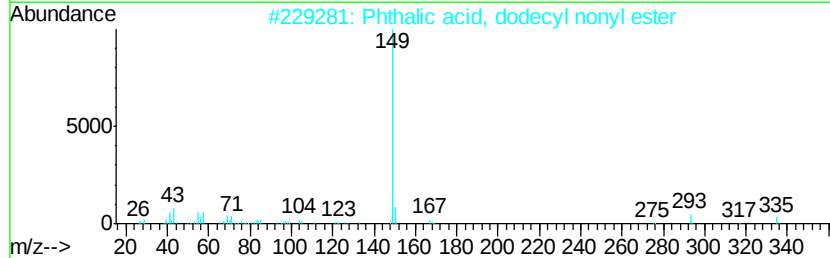
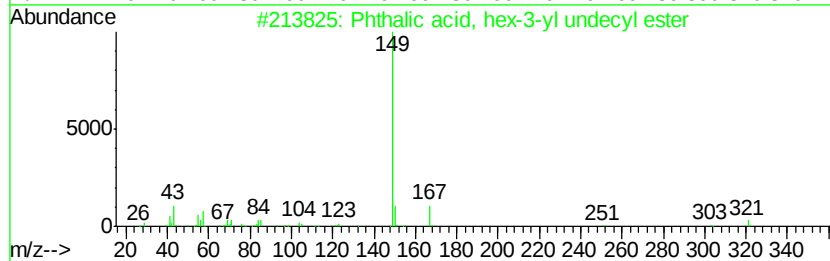
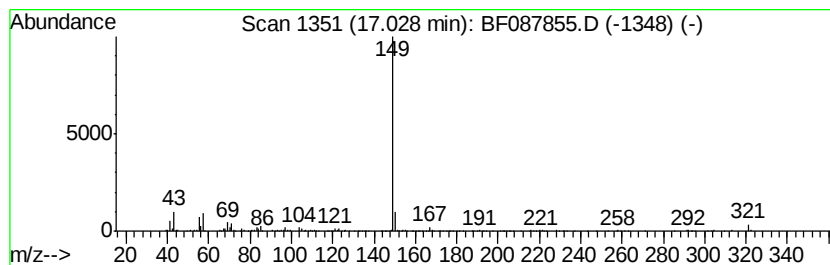
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Phthalic acid, hex-3-yl und... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	11.52 ng	507757	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	86
2		Phthalic acid, dodecyl nonyl ester	460	C29H48O4	1000308-92-6	80
3		Phthalic acid, 2-methylpent-3-yl...	432	C27H44O4	1000356-91-8	80
4		1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	72
5		Phthalic acid, hexyl 2-propylpen...	362	C22H34O4	1000377-92-2	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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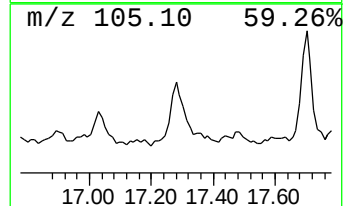
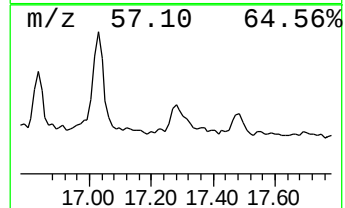
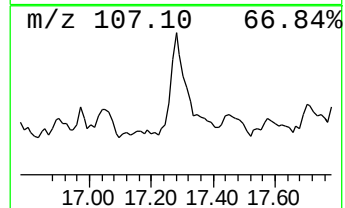
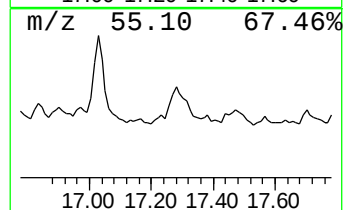
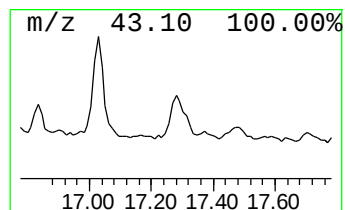
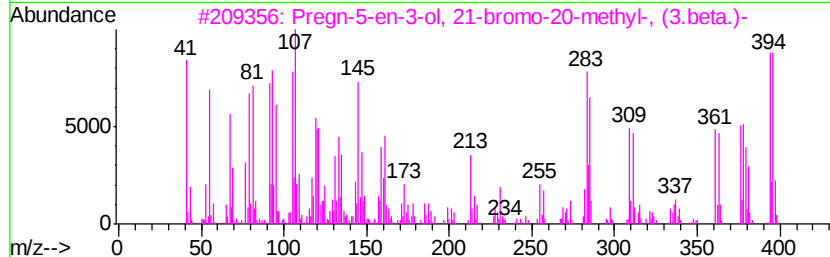
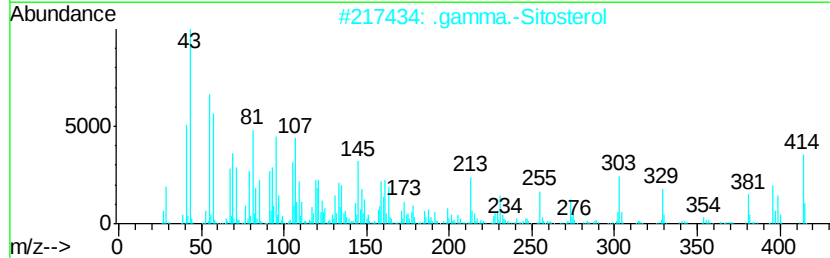
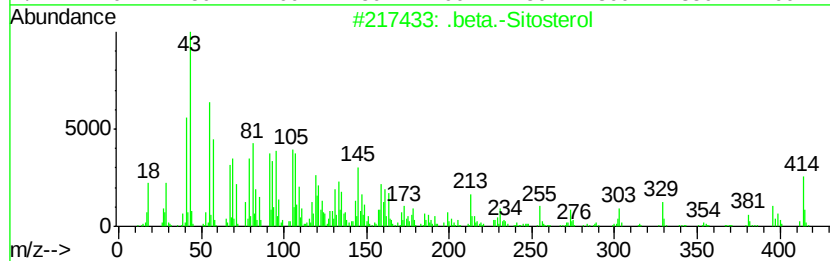
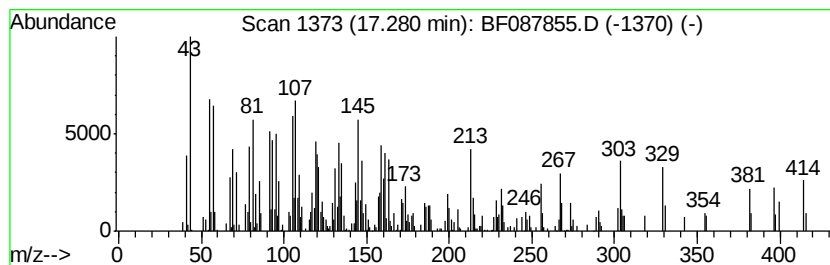
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 .beta.-Sitosterol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	10.59 ng	466584	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol	414	C29H50O	000083-46-5	97
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	60
3		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	25
4		Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	11
5		Norflurazon	303	C12H9ClF3N3O	027314-13-2	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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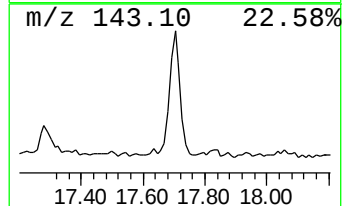
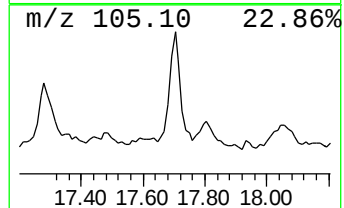
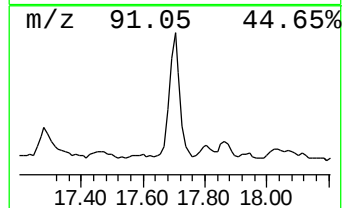
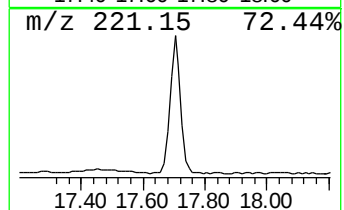
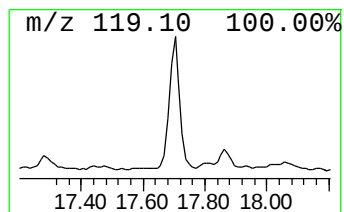
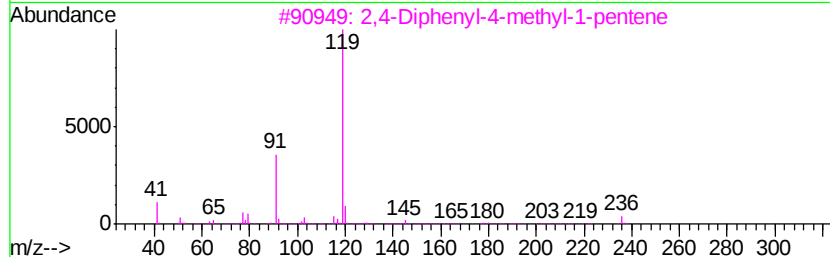
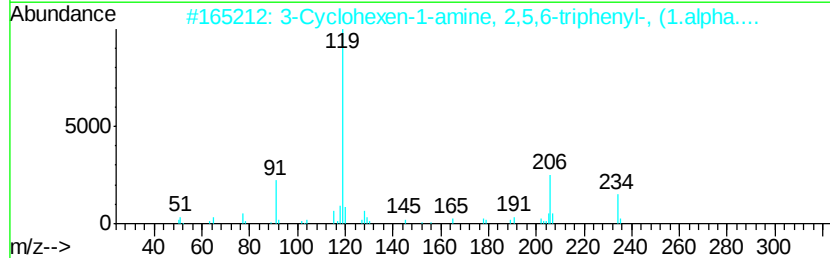
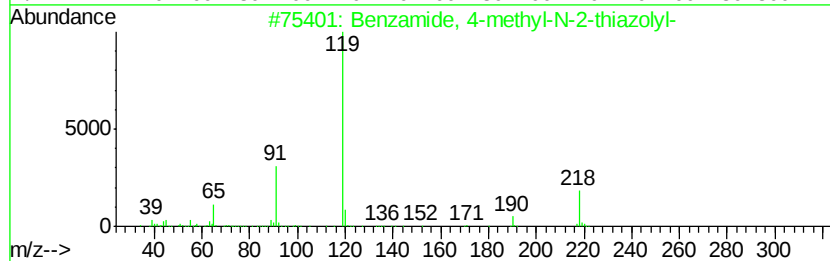
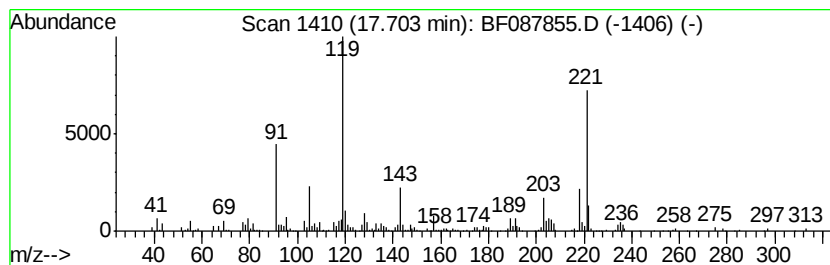
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.70 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	7.16 ng	315661	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzamide, 4-methyl-N-2-thiazolyl-	218	C11H10N2OS	150175-93-2	38
2		3-Cyclohexen-1-amine, 2,5,6-trip...	325	C24H23N	033441-42-8	35
3		2,4-Diphenyl-4-methyl-1-pentene	236	C18H20	1000111-58-0	30
4		Phenyl 2-phenylisopropyl sulfide	228	C15H16S	004148-93-0	27
5		Ethanone, 2-bromo-1-(4-methylphe...	212	C9H9BrO	000619-41-0	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060916\
Data File : BF087855.D
Acq On : 9 Jun 2016 16:31
Operator : UM/SJ
Sample : H3399-13 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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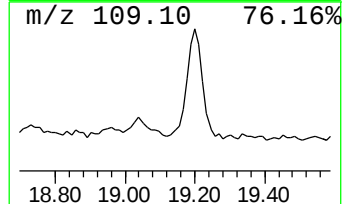
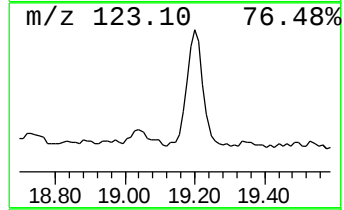
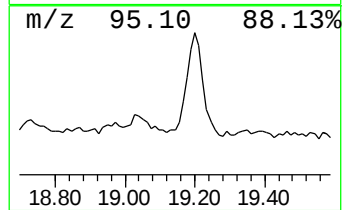
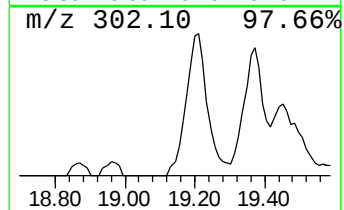
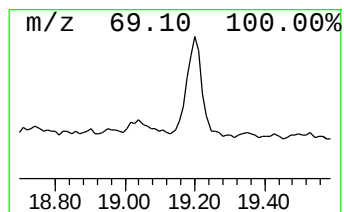
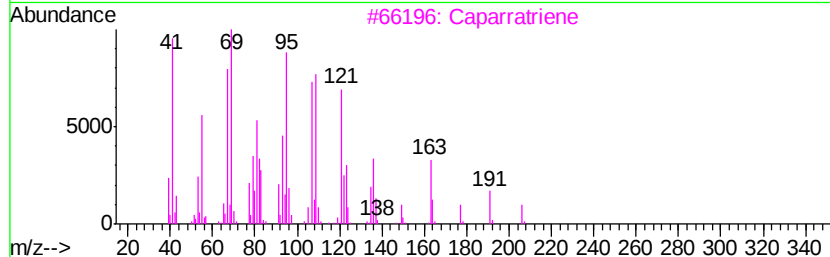
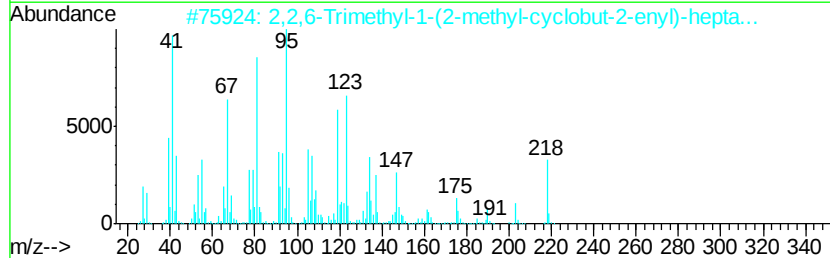
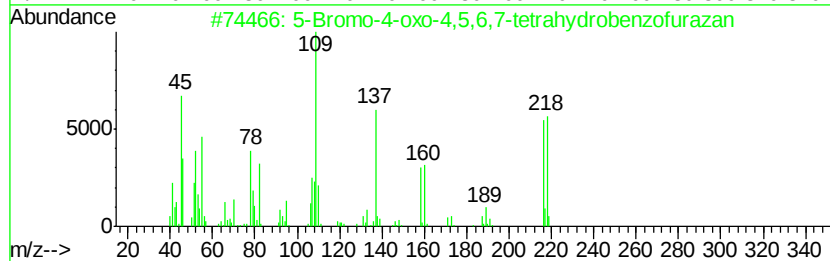
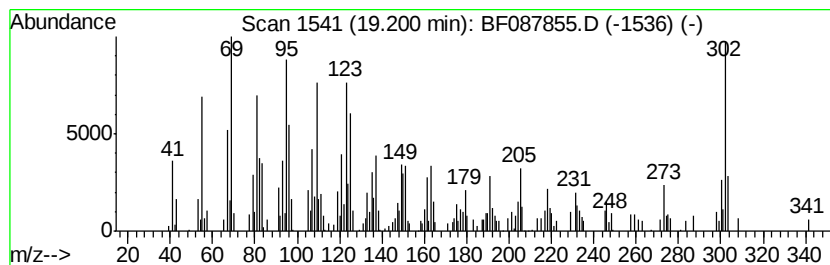
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	11.77 ng	518675	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	50
3		Caparratriene	206	C15H26	1000374-08-7	38
4		Sesquirosefuran	218	C15H22O	039007-93-7	35
5		4-(3-Methylpiperidino)-2-phenylq...	302	C21H22N2	1000326-78-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060916\
 Data File : BF087855.D
 Acq On : 9 Jun 2016 16:31
 Operator : UM/SJ
 Sample : H3399-13 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
Propane, 2,2-dime...	1.64	121.0	ng	4238240	1	6.82	700705	20.0
Propane, 1,1-dime...	2.04	13.1	ng	459836	1	6.82	700705	20.0
unknown6.58	6.58	46.3	ng	1620530	1	6.82	700705	20.0
Phthalic acid, he...	14.32	6.3	ng	841695	5	13.95	2666830	20.0
Phthalic acid, is...	14.73	7.6	ng	335211	6	15.37	881300	20.0
1,2-Benzenedicarb...	14.81	8.0	ng	351967	6	15.37	881300	20.0
Phthalic acid, he...	14.91	21.9	ng	967300	6	15.37	881300	20.0
Heneicosane	15.05	7.9	ng	349511	6	15.37	881300	20.0
Phthalic acid, he...	15.20	47.0	ng	2071170	6	15.37	881300	20.0
Phthalic acid, 2,...	15.62	16.5	ng	728597	6	15.37	881300	20.0
Phthalic acid, de...	15.98	27.1	ng	1196180	6	15.37	881300	20.0
Phthalic acid, de...	16.53	7.7	ng	339176	6	15.37	881300	20.0
Phthalic acid, he...	17.03	11.5	ng	507757	6	15.37	881300	20.0
.beta.-Sitosterol	17.28	10.6	ng	466584	6	15.37	881300	20.0
unknown17.70	17.70	7.2	ng	315661	6	15.37	881300	20.0
5-Bromo-4-oxo-4,5...	19.20	11.8	ng	518675	6	15.37	881300	20.0