

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
 Data File : BF092081.D
 Acq On : 4 Jan 2017 21:22
 Operator : UM/SJ
 Sample : I1004-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-30

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	1.978	6	8	29	rVB3	34646	247147	2.98%	0.185%
2	2.618	61	64	66	rBV	56995	90474	1.09%	0.068%
3	4.801	251	255	259	rBV	719744	1032918	12.46%	0.775%
4	5.190	287	289	291	rBV	67950	84085	1.01%	0.063%
5	5.258	293	295	298	rBV	2883935	3828837	46.19%	2.874%
6	5.407	305	308	312	rVB3	84099	216277	2.61%	0.162%
7	5.476	312	314	319	rBV5	87449	235674	2.84%	0.177%
8	5.544	319	320	323	rVB	110185	110689	1.34%	0.083%
9	5.647	326	329	331	rBV2	76016	154576	1.86%	0.116%
10	5.681	331	332	336	rVB3	71682	104900	1.27%	0.079%
11	5.807	339	343	345	rBV	477542	590242	7.12%	0.443%
12	5.898	348	351	354	rVB3	115771	240035	2.90%	0.180%
13	5.956	354	356	362	rBV3	65727	160256	1.93%	0.120%
14	6.081	364	367	368	rBV2	79557	144557	1.74%	0.108%
15	6.104	368	369	372	rVB	437627	514869	6.21%	0.386%
16	6.173	372	375	381	rBV2	227348	413529	4.99%	0.310%
17	6.264	381	383	384	rBV	150737	207802	2.51%	0.156%
18	6.321	386	388	393	rVB	2043495	2930057	35.34%	2.199%
19	6.436	395	398	401	rVB	5509517	5771992	69.63%	4.332%
20	6.516	403	405	406	rVB2	94627	129261	1.56%	0.097%
21	6.539	406	407	410	rVB3	96518	136316	1.64%	0.102%
22	6.619	410	414	416	rBV2	467741	776703	9.37%	0.583%
23	6.664	416	418	421	rVV	1131968	1617189	19.51%	1.214%
24	6.813	429	431	436	rBV2	3842676	6595416	79.56%	4.950%
25	6.916	438	440	442	rVB	1074903	945638	11.41%	0.710%
26	7.007	445	448	451	rBV3	947177	1533836	18.50%	1.151%
27	7.053	451	452	455	rBV3	331732	538683	6.50%	0.404%
28	7.110	455	457	458	rBV	382116	377033	4.55%	0.283%
29	7.156	458	461	462	rBV2	196672	262502	3.17%	0.197%
30	7.236	462	468	471	rBV2	4868785	7881669	95.08%	5.916%
31	7.281	471	472	473	rVV	142729	110601	1.33%	0.083%
32	7.316	473	475	477	rVB	597841	618402	7.46%	0.464%
33	7.361	477	479	483	rVB3	334545	793919	9.58%	0.596%
34	7.441	483	486	487	rBV	2111492	2214704	26.72%	1.662%

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35	7.464	487	488	490	rVB2	436432	436957	5.27%	0.328%
36	7.533	492	494	495	rBV	258196	262686	3.17%	0.197%
37	7.556	495	496	498	rBV	243751	364026	4.39%	0.273%
38	7.613	498	501	505	rVB3	780905	2330892	28.12%	1.749%
39	7.693	505	508	509	rBV	881439	1320971	15.93%	0.991%
40	7.727	509	511	512	rVB2	370163	416998	5.03%	0.313%
41	7.773	512	515	518	rBV3	554371	1256253	15.15%	0.943%
42	7.830	518	520	522	rBV2	254160	479104	5.78%	0.360%
43	7.899	524	526	527	rBV2	324693	617457	7.45%	0.463%
44	7.944	527	530	534	rVV3	2712215	4996955	60.28%	3.751%
45	8.002	534	535	538	rVB3	953488	942877	11.37%	0.708%
46	8.047	538	539	540	rVB	292504	200511	2.42%	0.150%
47	8.082	540	542	543	rBV2	182189	254960	3.08%	0.191%
48	8.116	543	545	546	rBV	407518	587298	7.08%	0.441%
49	8.150	546	548	549	rVB2	626685	647127	7.81%	0.486%
50	8.196	549	552	553	rBV	1063549	1211351	14.61%	0.909%
51	8.230	553	555	558	rVB4	683257	1329978	16.04%	0.998%
52	8.276	558	559	560	rBV	170997	228969	2.76%	0.172%
53	8.333	560	564	567	rBV4	786884	1310653	15.81%	0.984%
54	8.413	567	571	574	rBV5	1073246	3306900	39.89%	2.482%
55	8.482	574	577	579	rVV	1493894	2478059	29.89%	1.860%
56	8.550	581	583	584	rVV	331238	486426	5.87%	0.365%
57	8.573	584	585	586	rVV	592998	582712	7.03%	0.437%
58	8.607	586	588	590	rVV3	815386	1174631	14.17%	0.882%
59	8.642	590	591	594	rVB3	624585	795023	9.59%	0.597%
60	8.699	594	596	597	rBV2	398393	639599	7.72%	0.480%
61	8.733	597	599	600	rVV	1669765	1928782	23.27%	1.448%
62	8.767	600	602	603	rVV	1730269	2662870	32.12%	1.999%
63	8.847	606	609	610	rVV3	392629	794727	9.59%	0.596%
64	8.870	610	611	613	rVV2	473429	919275	11.09%	0.690%
65	8.973	616	620	622	rVV5	1217452	2857096	34.46%	2.144%
66	9.030	622	625	631	rVB	5576681	8289928	100.00%	6.222%
67	9.213	637	641	644	rBV6	571798	1578065	19.04%	1.184%
68	9.362	652	654	655	rBV2	646304	1125932	13.58%	0.845%
69	9.476	662	664	666	rVB2	403590	397201	4.79%	0.298%
70	9.556	670	671	674	rBV2	516688	744562	8.98%	0.559%
71	9.693	680	683	685	rBV2	2276101	3682347	44.42%	2.764%

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72	9.727	685	686	688 rBV2	366946	401770	4.85%	0.302%
73	9.785	688	691	692 rBV3	537086	861155	10.39%	0.646%
74	9.819	692	694	695 rBV	328309	388517	4.69%	0.292%
75	9.876	697	699	700 rBV2	531251	692087	8.35%	0.519%
76	9.979	706	708	710 rVB2	799869	1115932	13.46%	0.838%
77	10.025	710	712	713 rBV	874400	1125491	13.58%	0.845%
78	10.059	713	715	716 rVV2	941653	1417045	17.09%	1.064%
79	10.116	716	720	724 rVV6	1557949	4485419	54.11%	3.367%
80	10.185	724	726	730 rVV3	936287	1743977	21.04%	1.309%
81	10.447	746	749	751 rBV	1244073	2756264	33.25%	2.069%
82	10.493	751	753	757 rVB3	2734891	4389276	52.95%	3.294%
83	10.619	762	764	766 rBV3	529749	655033	7.90%	0.492%
84	10.699	769	771	774 rBV4	573498	1611475	19.44%	1.210%
85	10.848	783	784	788 rVB3	879670	1093461	13.19%	0.821%
86	10.928	788	791	794 rVB3	501413	833561	10.06%	0.626%
87	11.065	799	803	805 rVB3	1207220	1921276	23.18%	1.442%
88	11.179	811	813	816 rVB	1693049	1685917	20.34%	1.265%
89	11.236	816	818	820 rBV2	289925	435739	5.26%	0.327%
90	11.739	861	862	866 rVB2	709164	1103723	13.31%	0.828%
91	12.516	928	930	932 rBV	712531	714928	8.62%	0.537%
92	12.768	949	952	954 rBV	5122232	5344703	64.47%	4.012%
93	13.659	1028	1030	1034 rVB2	147995	220772	2.66%	0.166%
94	13.808	1040	1043	1045 rBV	1261723	1477708	17.83%	1.109%
95	14.654	1115	1117	1119 rVB	119192	151207	1.82%	0.113%
96	15.179	1160	1163	1165 rBV	943832	1213447	14.64%	0.911%
97	15.431	1183	1185	1189 rVB3	62942	142635	1.72%	0.107%

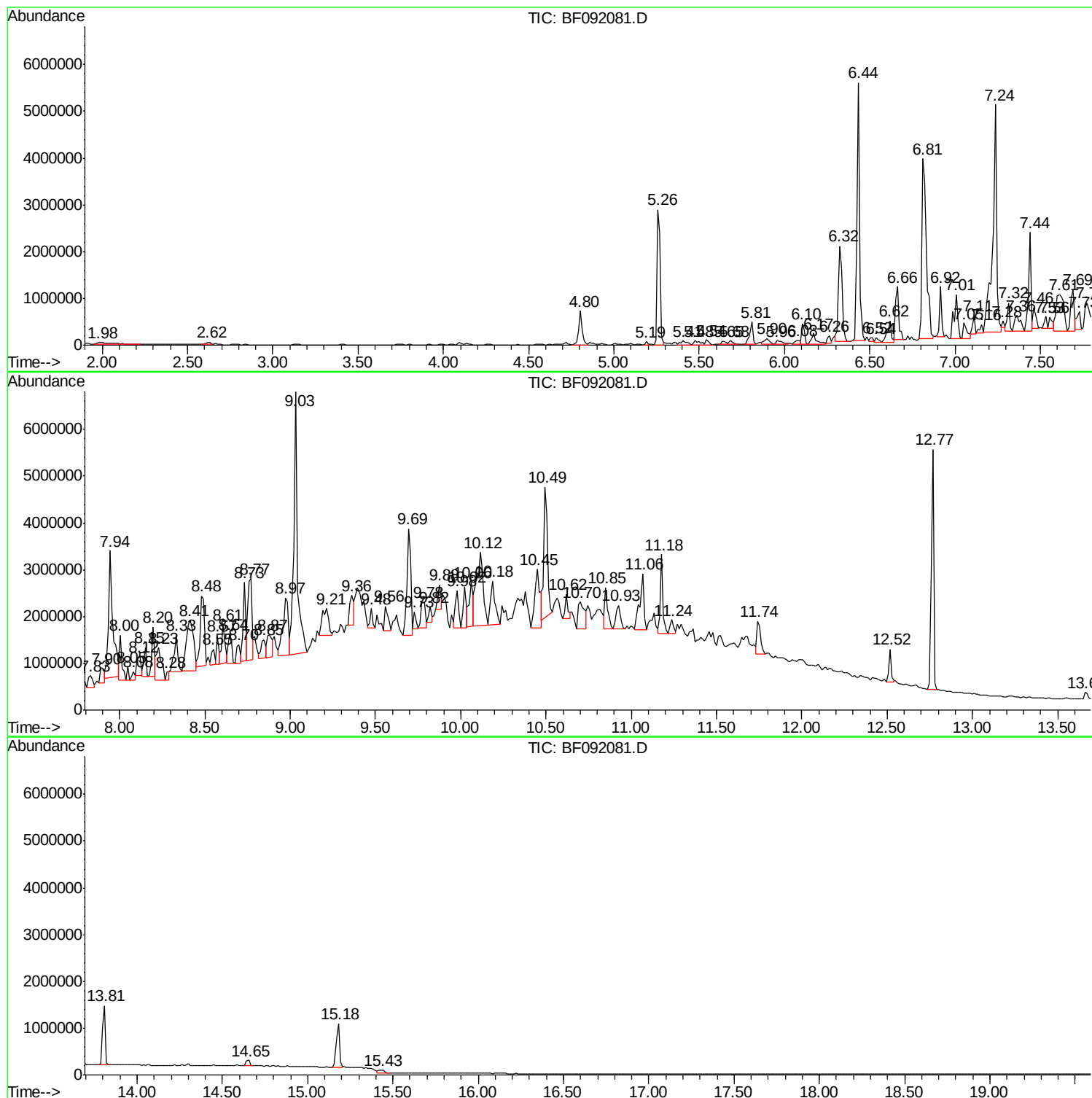
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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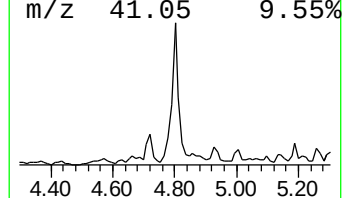
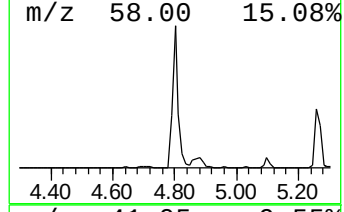
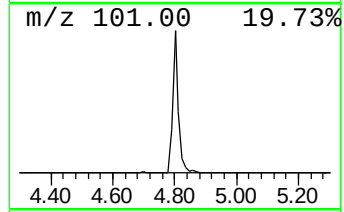
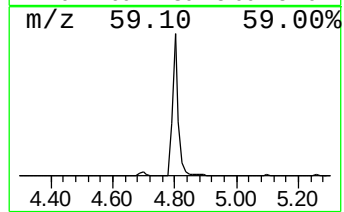
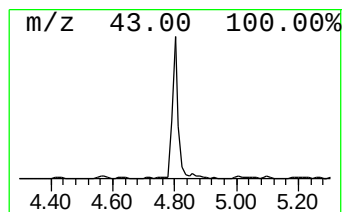
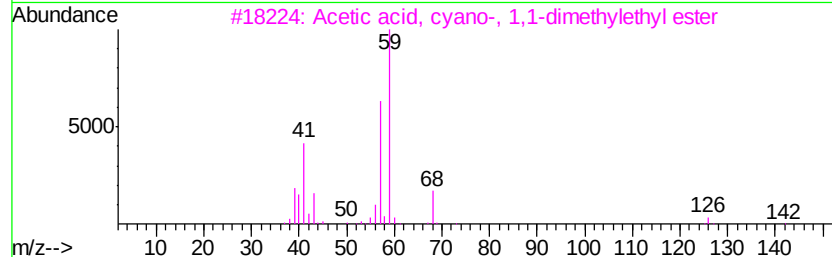
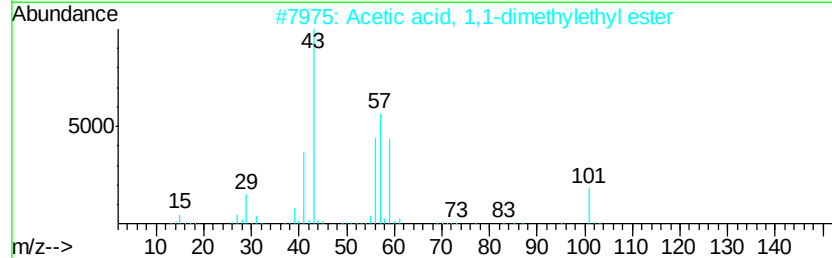
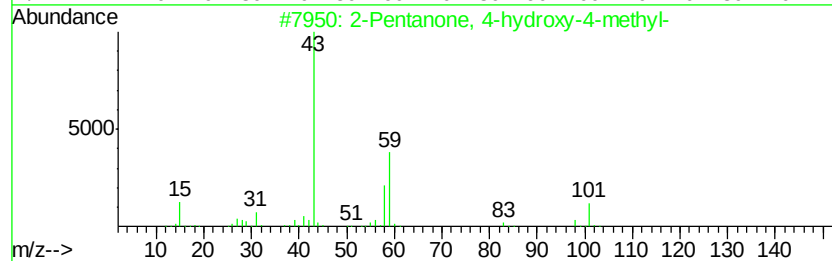
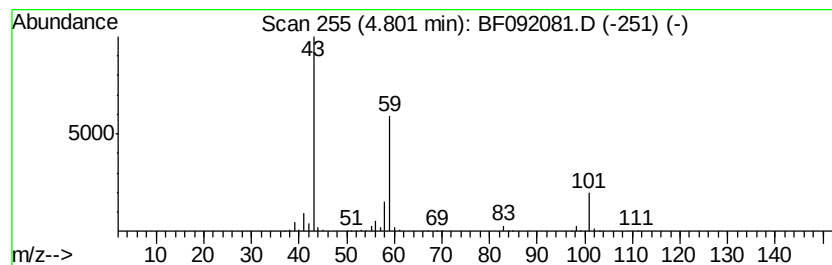
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	12.77 ng	1032920	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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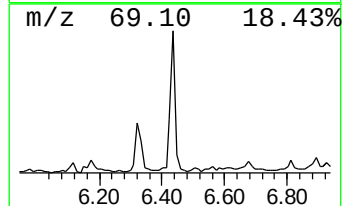
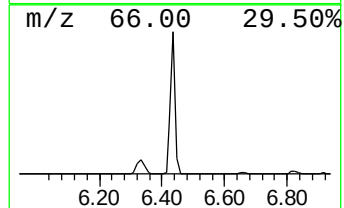
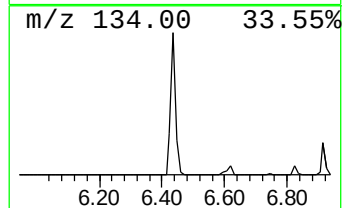
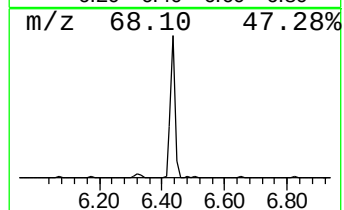
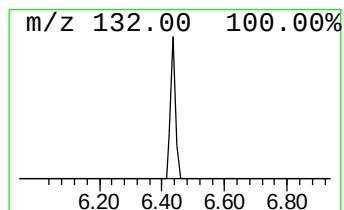
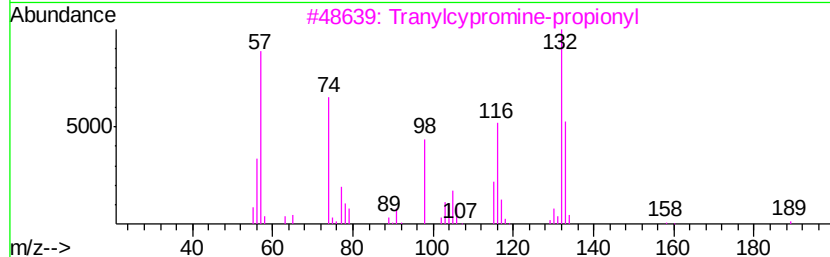
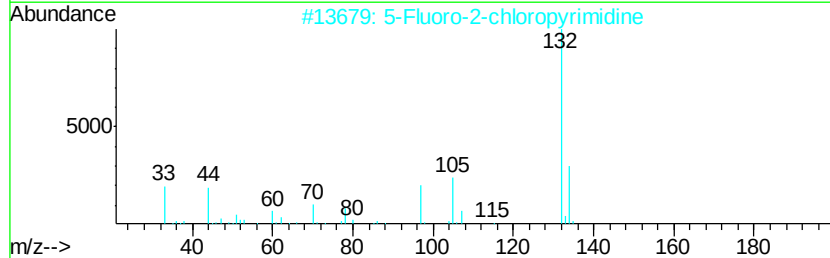
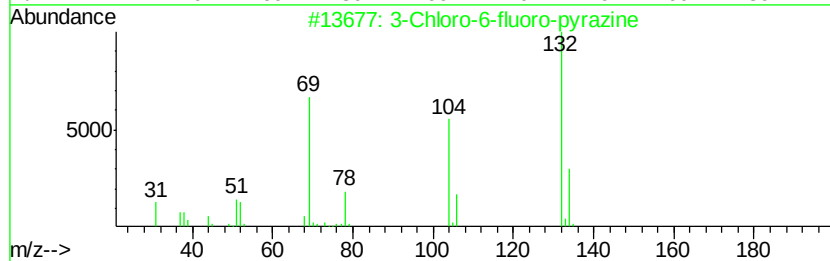
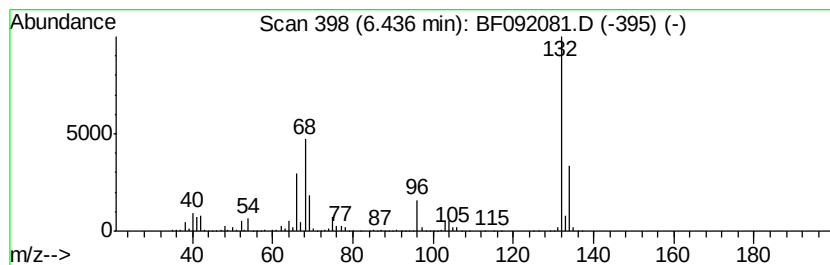
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	71.38 ng	5771990	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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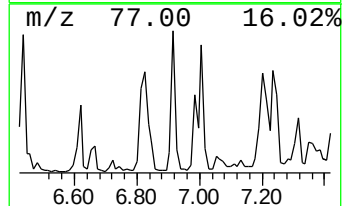
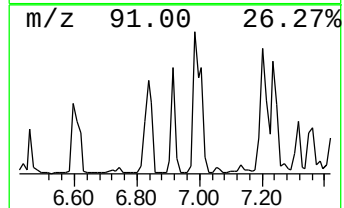
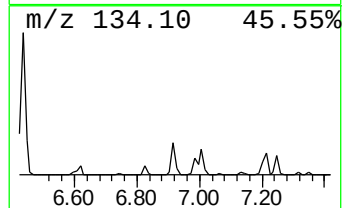
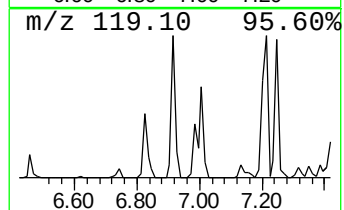
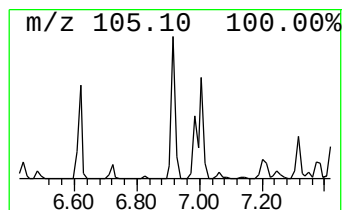
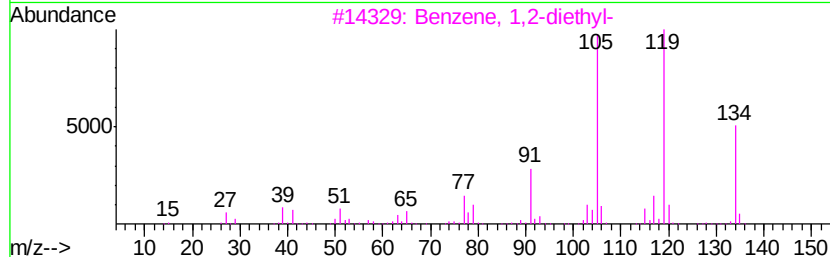
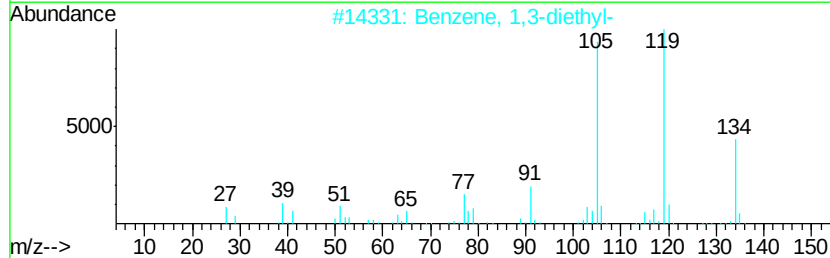
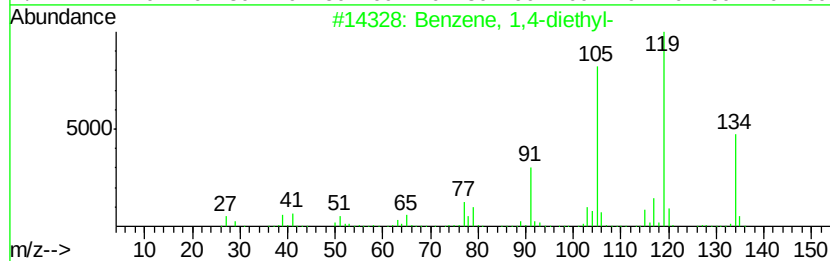
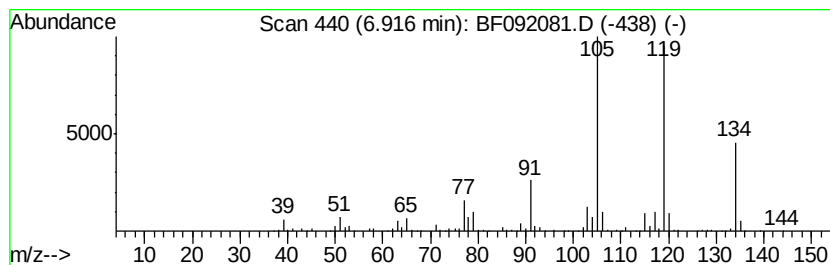
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,4-diethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	11.69 ng	945638	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
3		Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	94
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	83



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MW-30

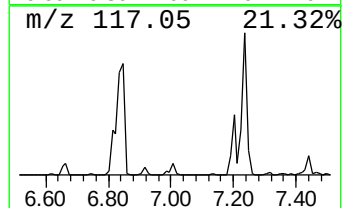
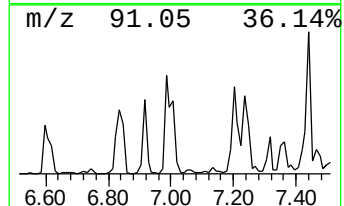
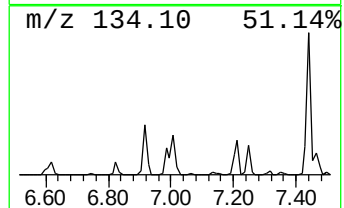
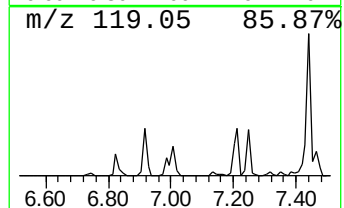
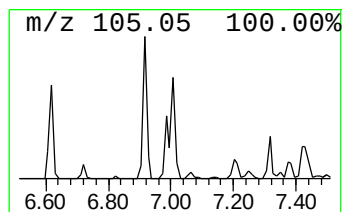
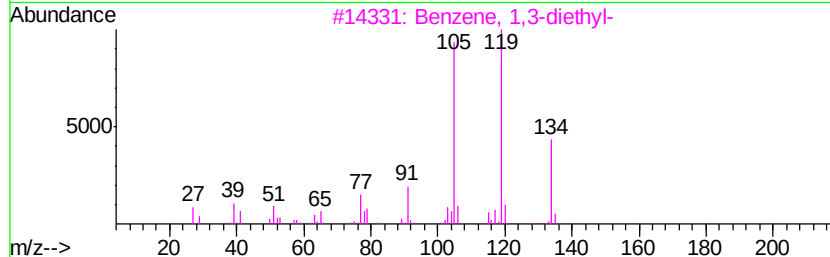
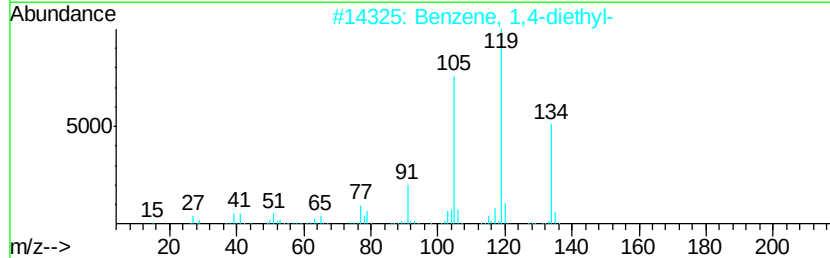
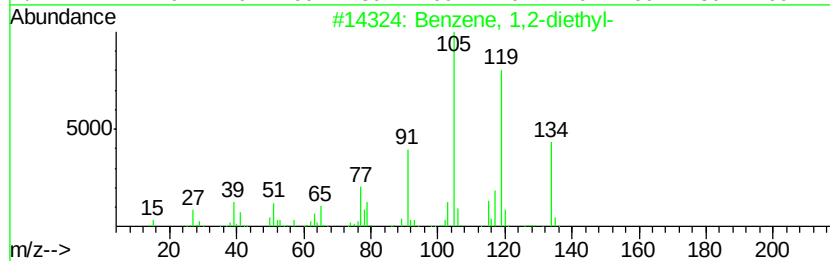
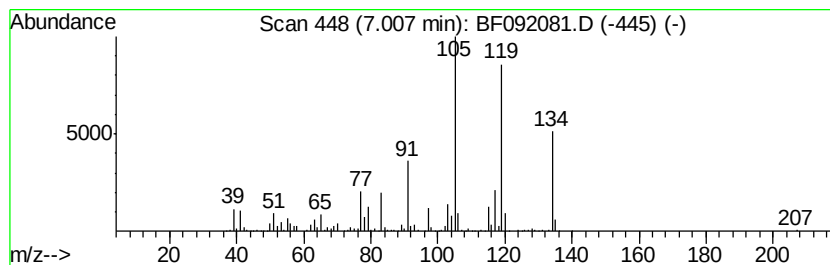
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.01	18.97 ng	1533840	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	95
2		Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	81
3		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	76
4		1,3,8-p-Menthatriene	134	C10H14	021195-59-5	62
5		Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

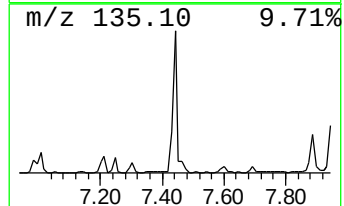
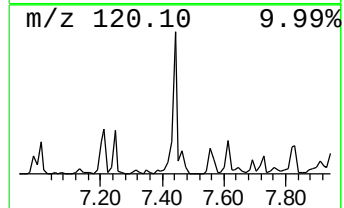
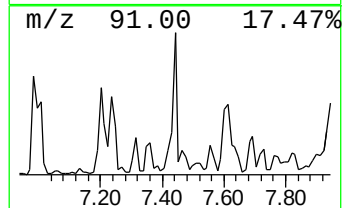
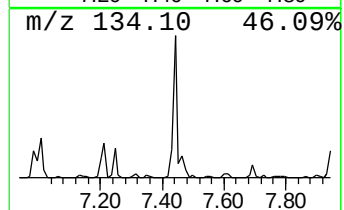
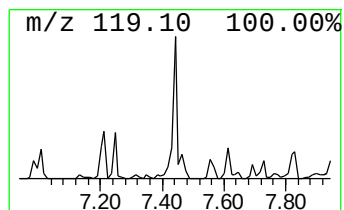
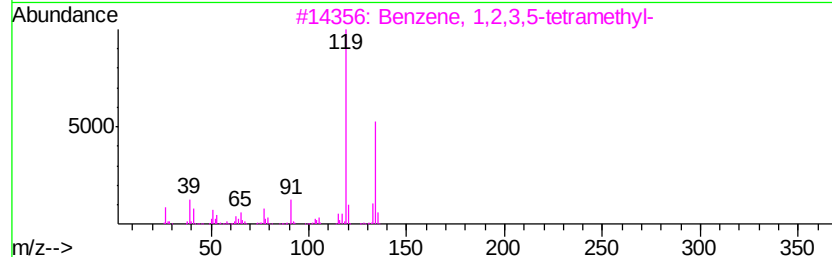
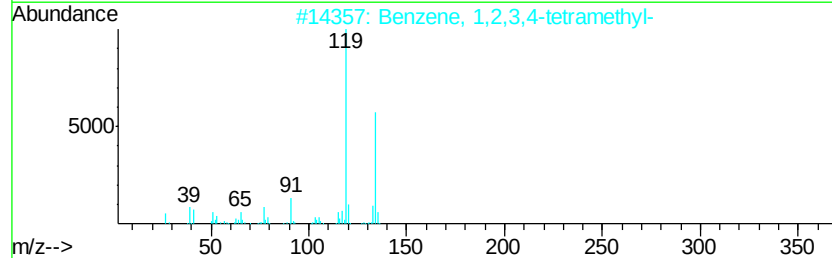
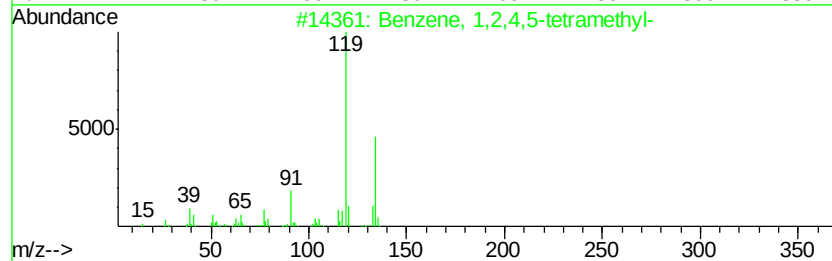
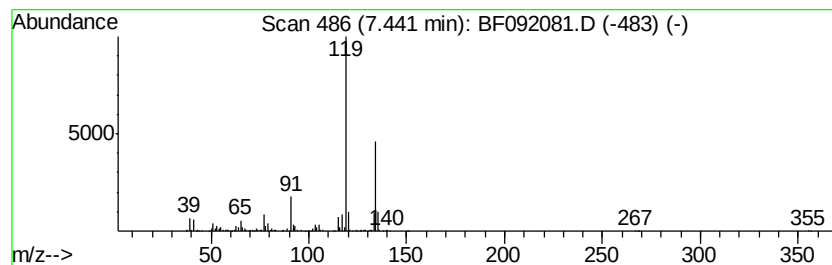
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	8.86 ng	2214700	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

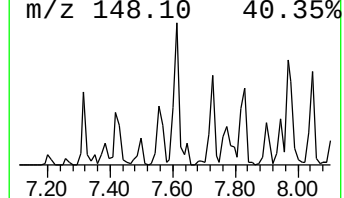
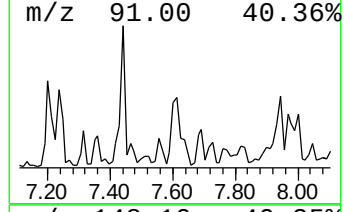
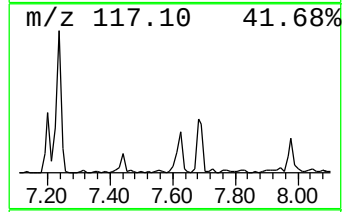
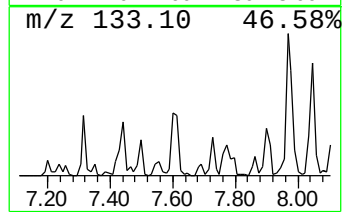
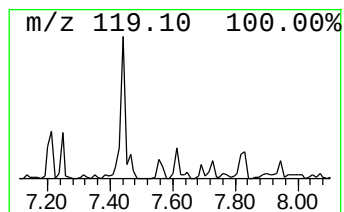
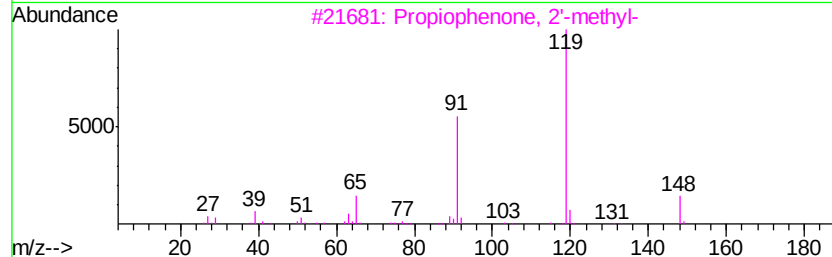
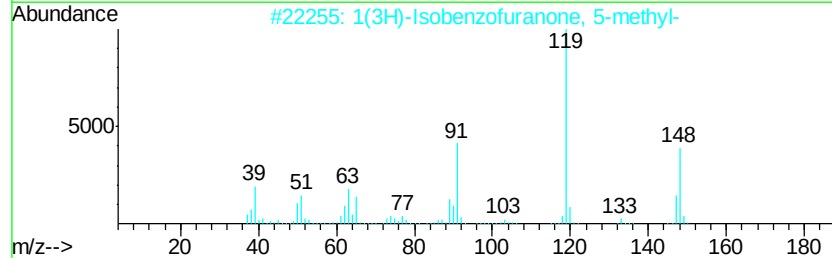
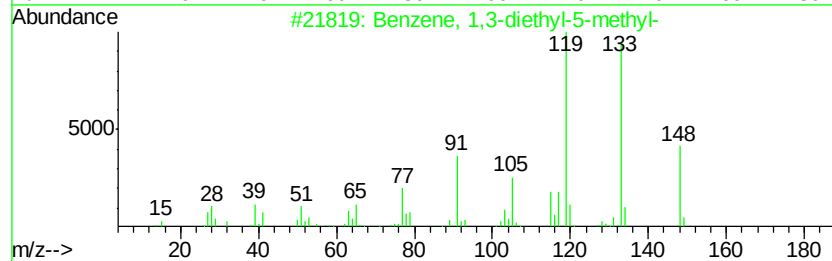
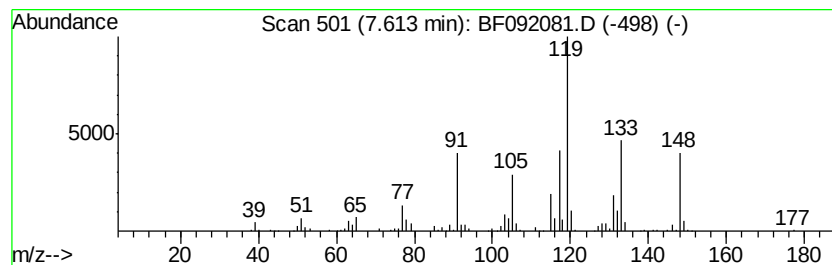
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,3-diethyl-5-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	9.33 ng	2330890	Napthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	58
2		1(3H)-Isobenzofuranone, 5-methyl-	148	C9H8O2	054120-64-8	43
3		Propiophenone, 2'-methyl-	148	C10H12O	002040-14-4	43
4		Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	43
5		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

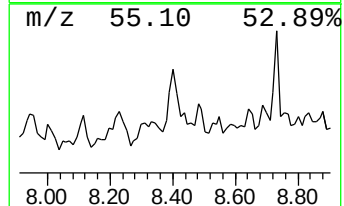
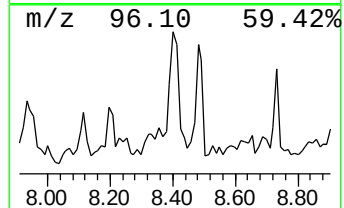
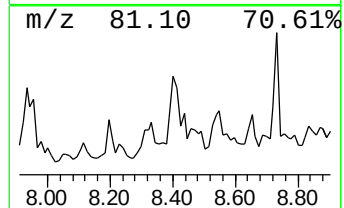
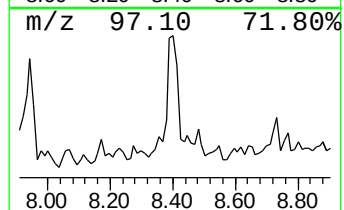
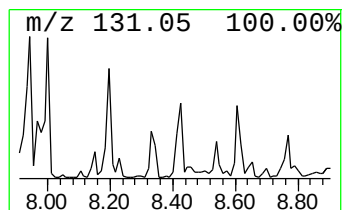
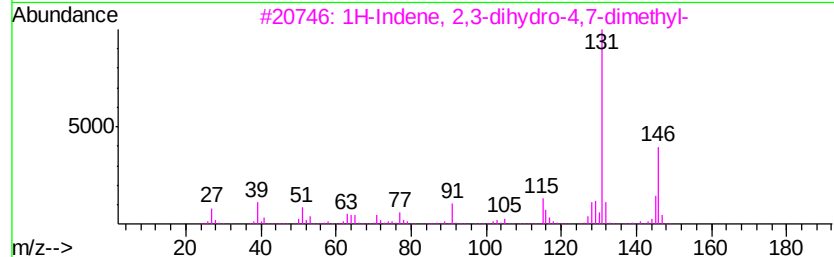
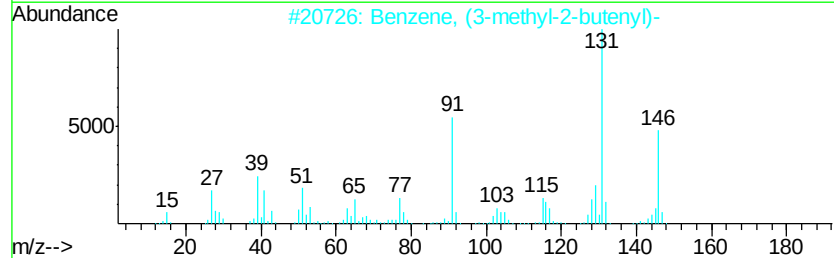
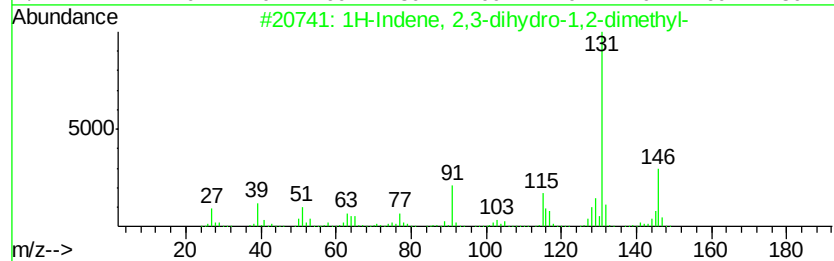
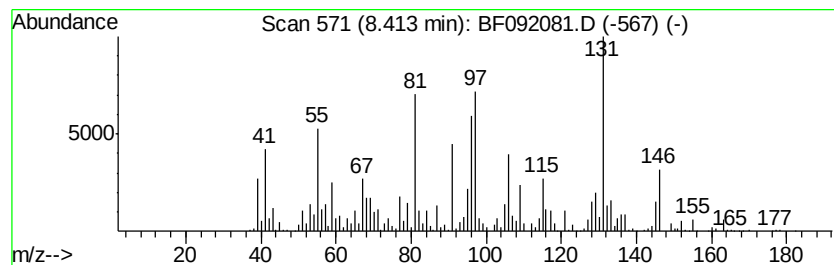
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	13.24 ng	3306900	Napthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	55
2		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	42
3		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	38
4		.alpha.,.beta.,.beta.-Trimethyls...	146	C11H14	000769-57-3	38
5		1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-30

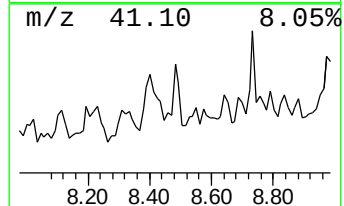
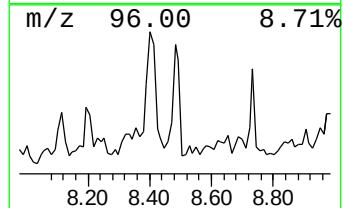
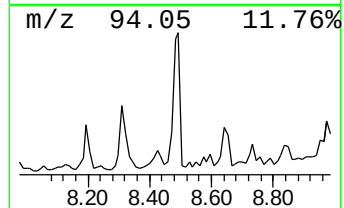
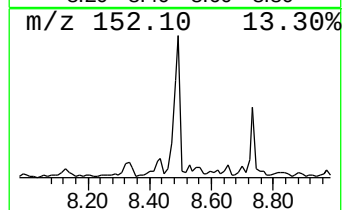
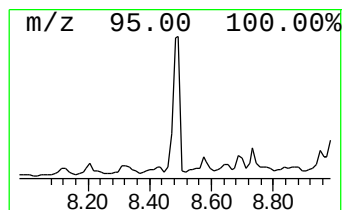
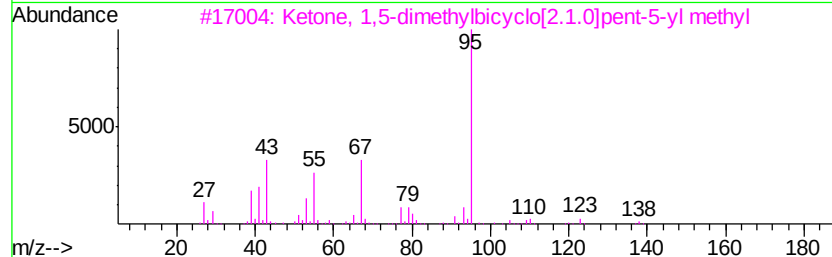
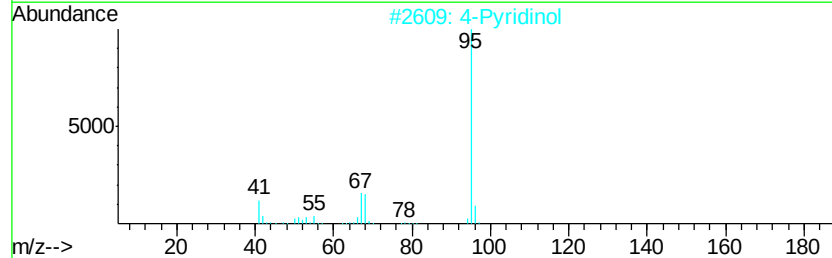
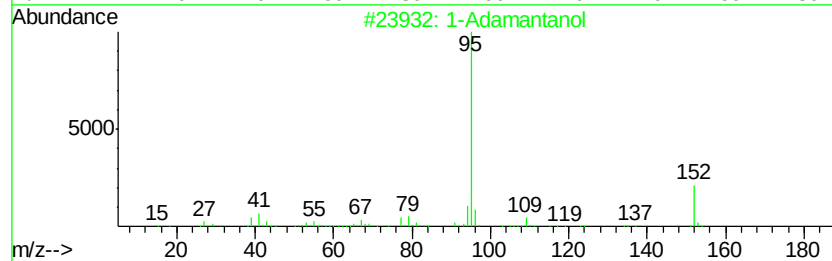
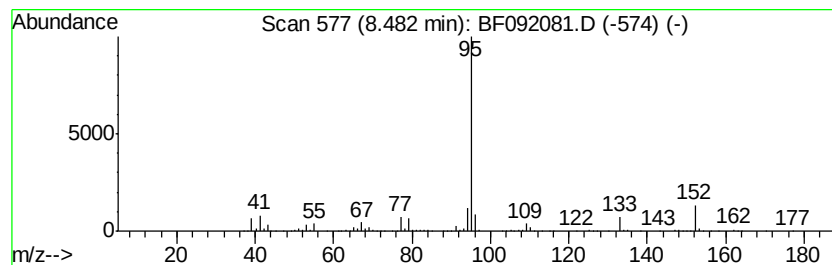
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Adamantanol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	9.92 ng	2478060	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Adamantanol	152	C10H16O	000768-95-6	91
2		4-Pyridinol	95	C5H5NO	000626-64-2	40
3		Ketone, 1,5-dimethylbicyclo[2.1....	138	C9H14O	024081-57-0	38
4		1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	38
5		Cyclopentene, 1,4-dimethyl-5-(1-...	138	C10H18	061142-33-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

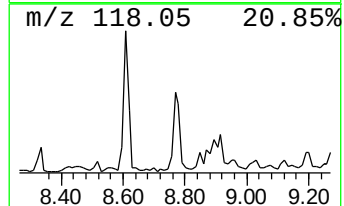
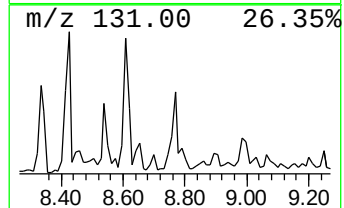
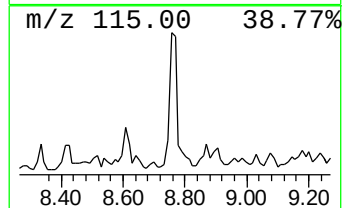
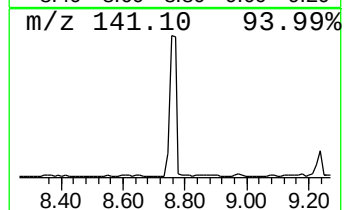
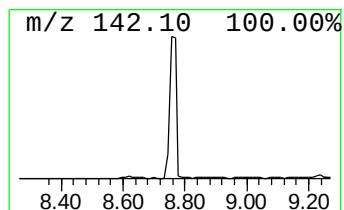
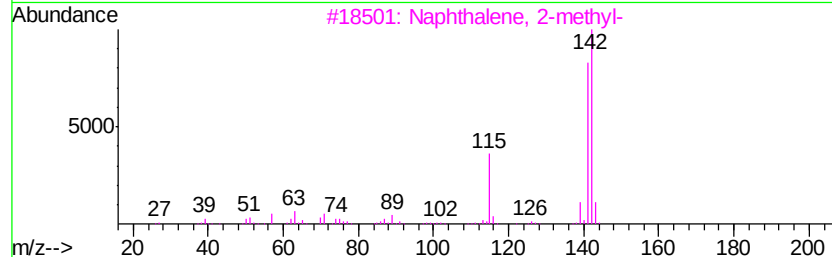
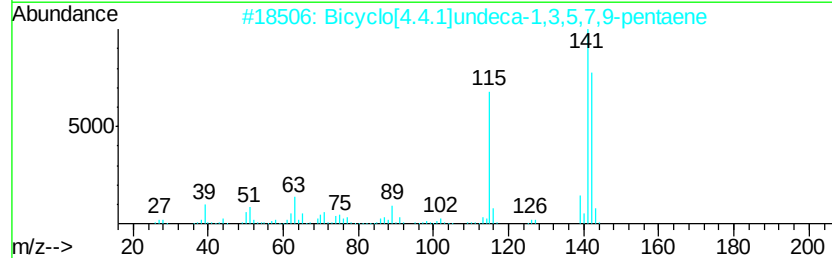
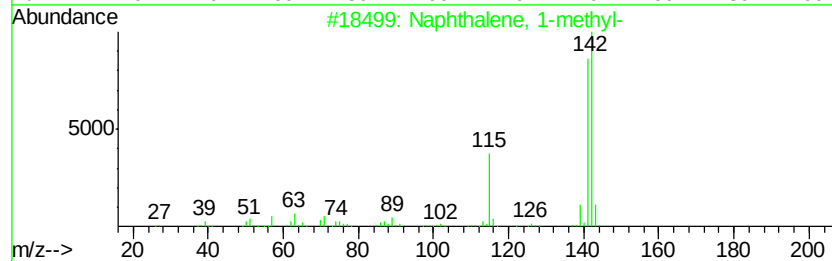
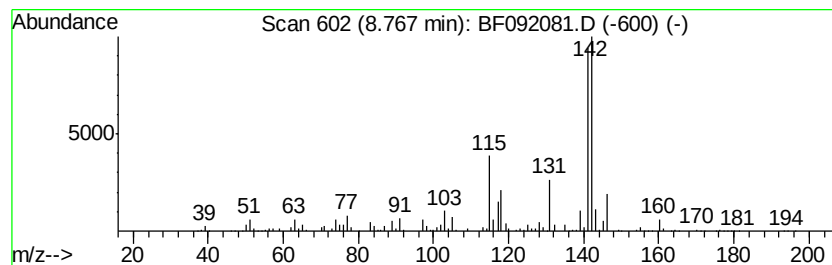
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	10.66 ng	2662870	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	70
2		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	62
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	60
4		Benzocycloheptatriene	142	C11H10	000264-09-5	58
5		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
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Acq On : 4 Jan 2017 21:22
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Sample : I1004-04
Misc :
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Instrument :
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ClientSampled :
MW-30

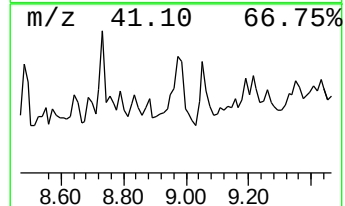
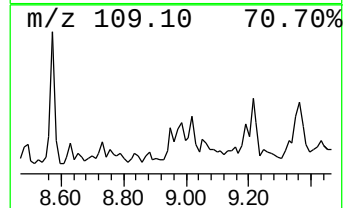
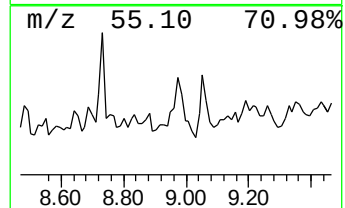
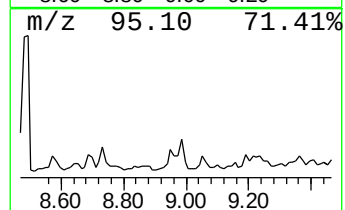
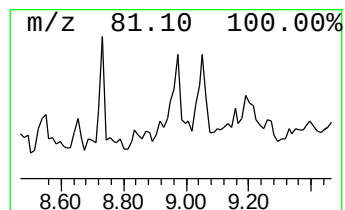
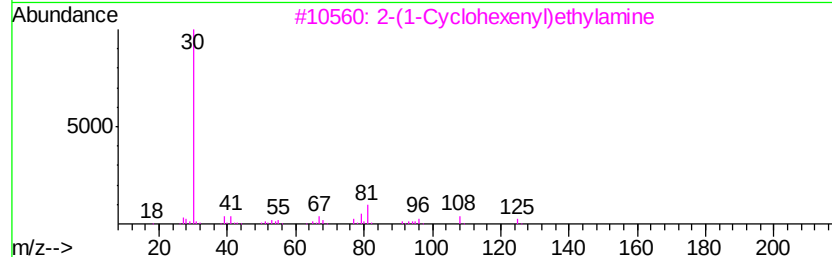
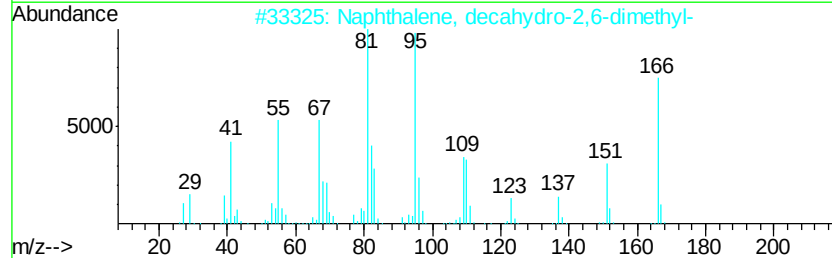
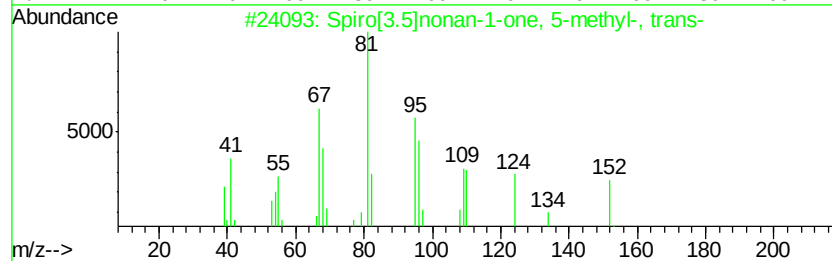
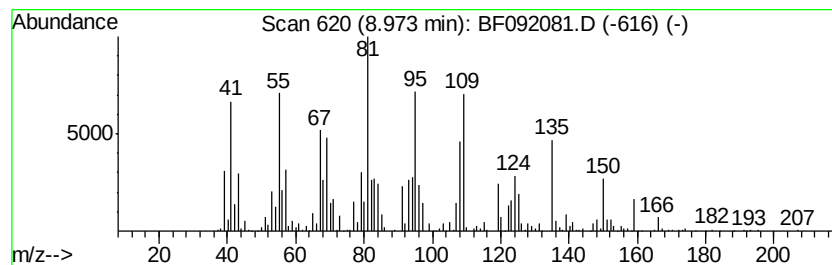
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.97 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	15.52 ng	2857100	Acenaphthene-d10	9.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro[3.5]nonan-1-one, 5-methyl-...	152	C10H16O	065147-56-0	45
2			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	41
3			2-(1-Cyclohexenyl)ethylamine	125	C8H15N	003399-73-3	38
4			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	30
5			Cyclohexene, 4-propyl-	124	C9H16	013487-64-4	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

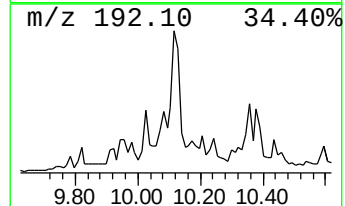
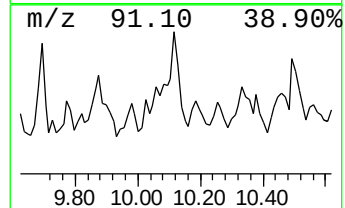
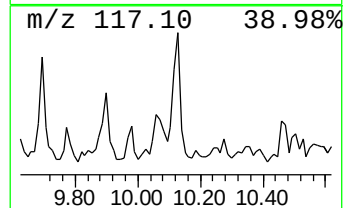
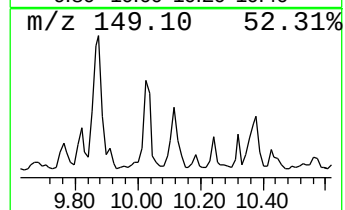
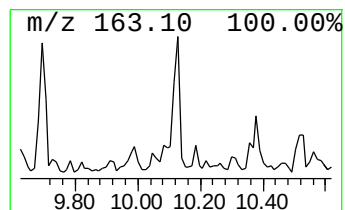
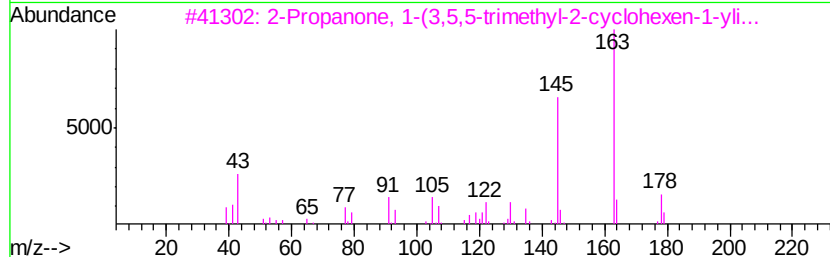
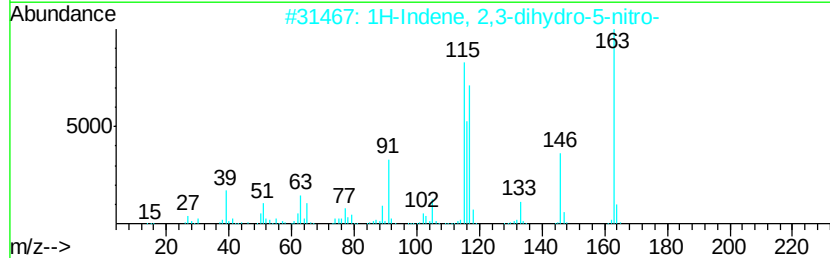
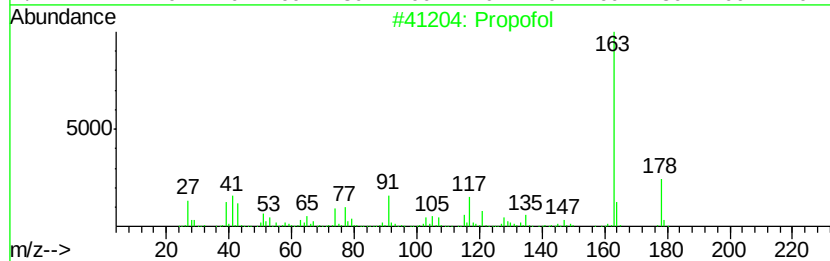
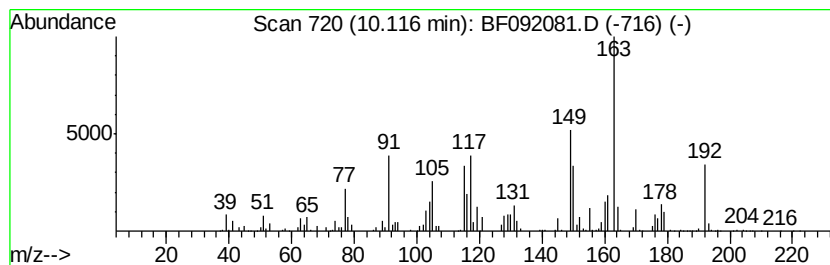
Instrument :
BNA_F
ClientSampleId :
MW-30

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 unknown10.12 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	24.36 ng	4485420	Acenaphthene-d10	9.70
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Propofol		178 C12H18O	002078-54-8 46
2	1H-Indene, 2,3-dihydro-5-nitro-		163 C9H9NO2	007436-07-9 38
3	2-Propanone, 1-(3,5,5-trimethyl-...		178 C12H18O	016695-72-0 35
4	Silane, (4-ethylphenyl)trimethyl-		178 C11H18Si	017988-50-0 30
5	3-Methyl-p-anisaldehyde		150 C9H10O2	032723-67-4 25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

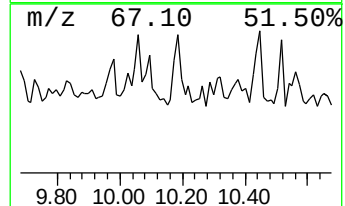
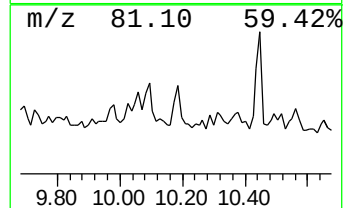
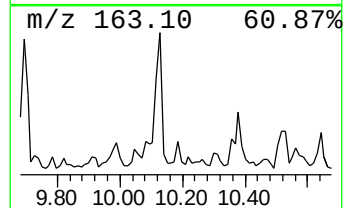
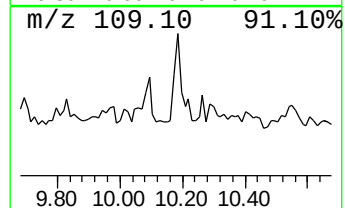
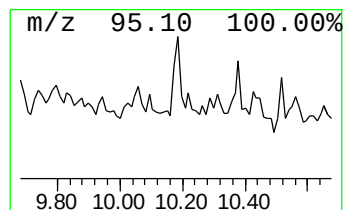
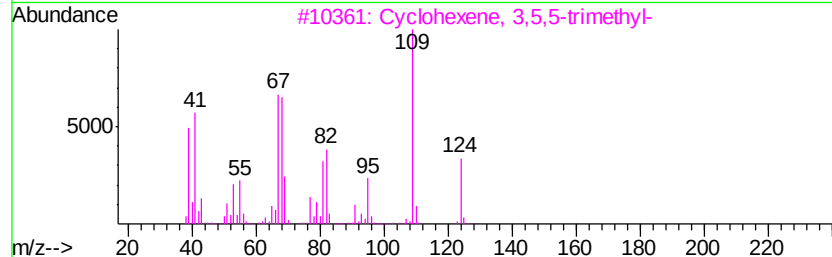
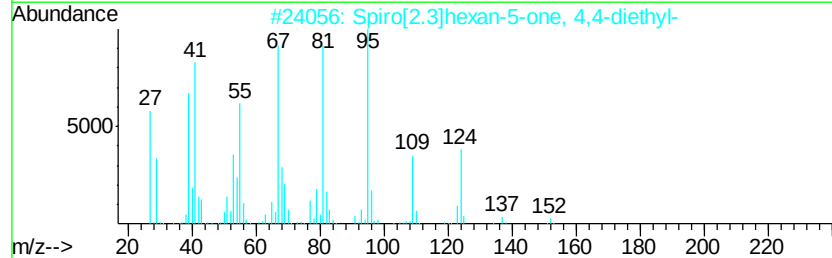
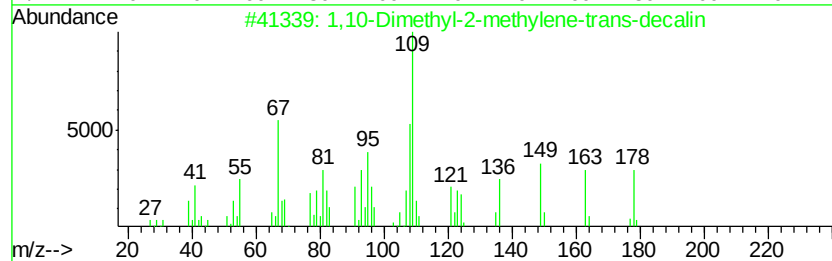
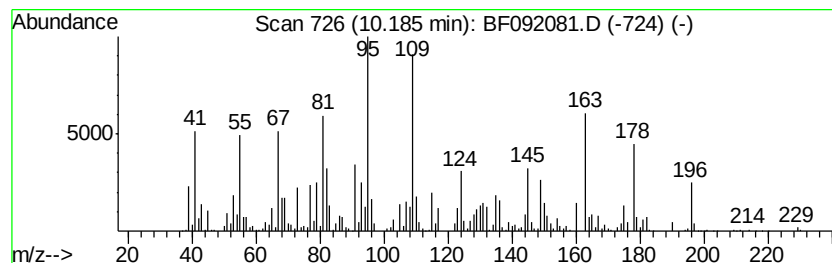
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown10.18 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	9.47 ng	1743980	Acenaphthene-d10	9.70
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,10-Dimethyl-2-methylene-trans-...	178 C13H22	1000103-97-8	43
2	Spiro[2.3]hexan-5-one, 4,4-diethyl-	152 C10H16O	1000154-16-2	42
3	Cyclohexene, 3,5,5-trimethyl-	124 C9H16	000933-12-0	30
4	Pentaleno[1,2-b]oxirene, octahyd...	124 C8H12O	055449-71-3	25
5	Norbornane, 2-isobutyl-	152 C11H20	018127-14-5	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

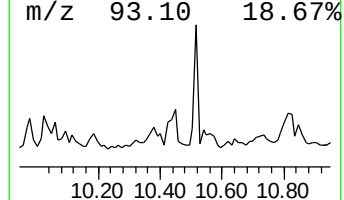
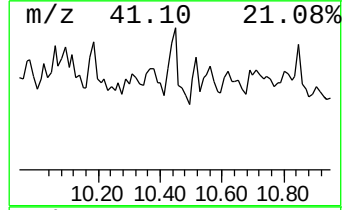
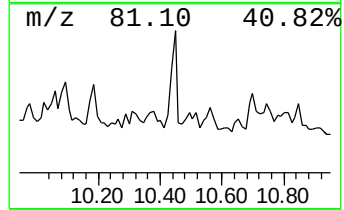
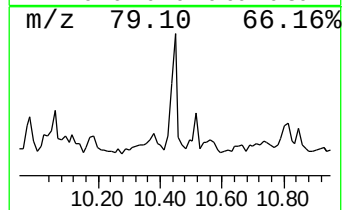
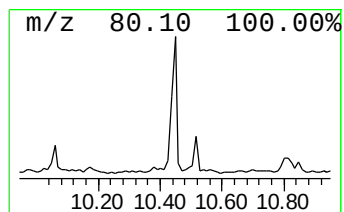
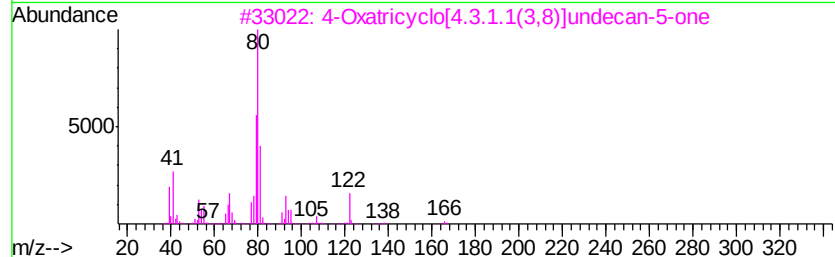
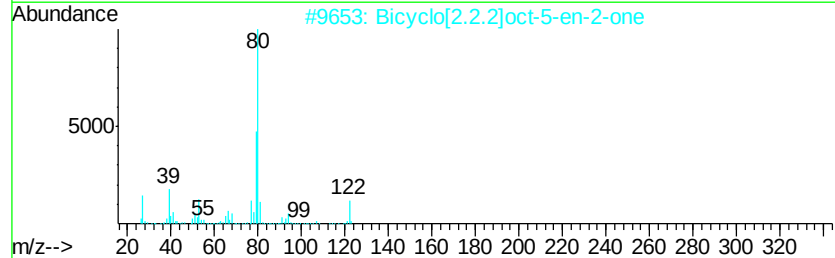
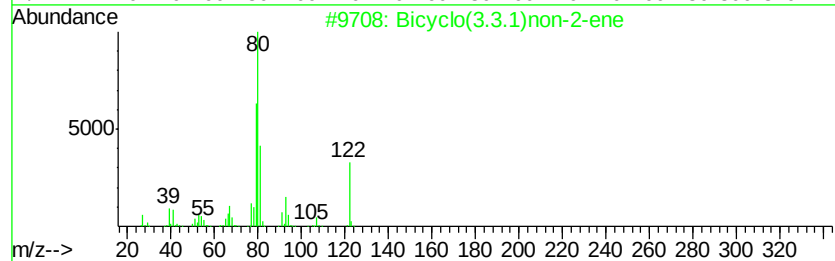
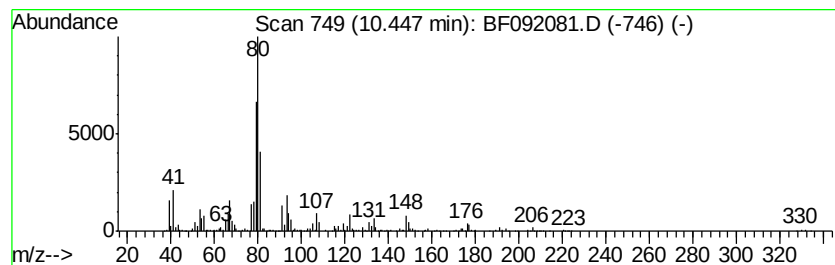
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Bicyclo(3.3.1)non-2-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	32.70 ng	2756260	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo(3.3.1)non-2-ene	122	C9H14	006671-66-5	90
2		Bicyclo[2.2.2]oct-5-en-2-one	122	C8H10O	002220-40-8	86
3		4-Oxatricyclo[4.3.1.1(3,8)]undec...	166	C10H14O2	021898-84-0	78
4		2-Hexen-4-yne, (Z)-	80	C6H8	030626-48-3	72
5		2-Hexen-4-yne, (E)-	80	C6H8	033625-96-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

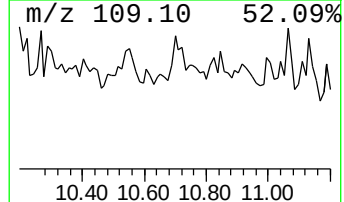
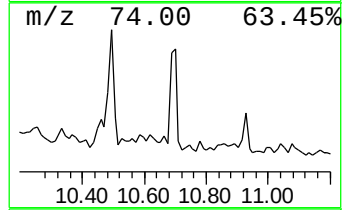
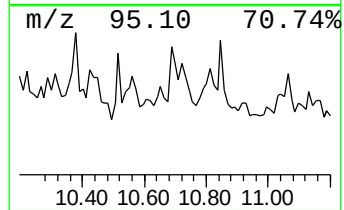
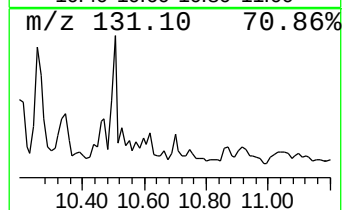
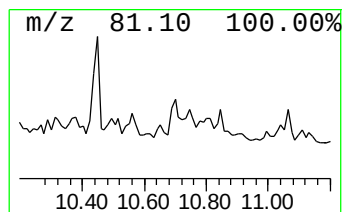
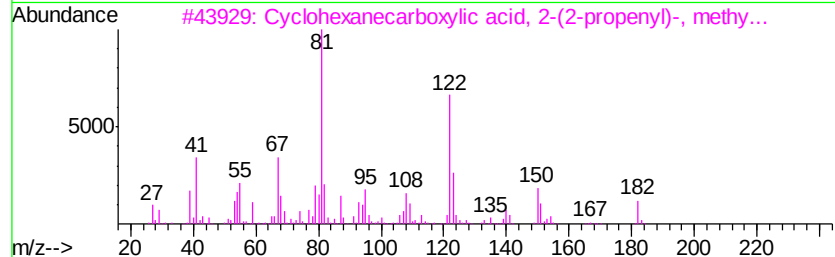
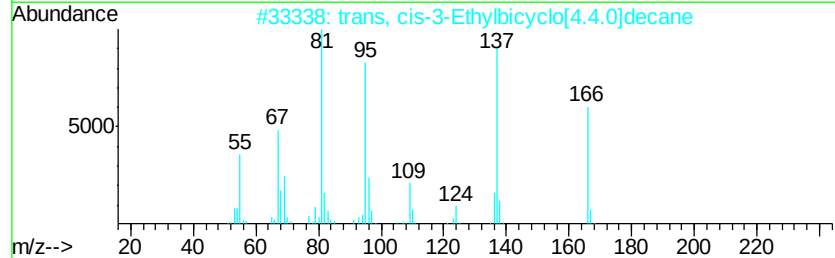
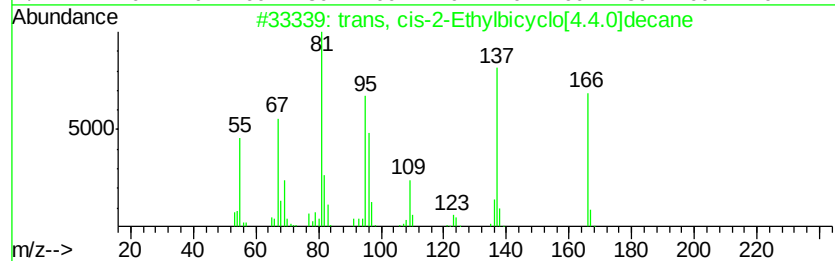
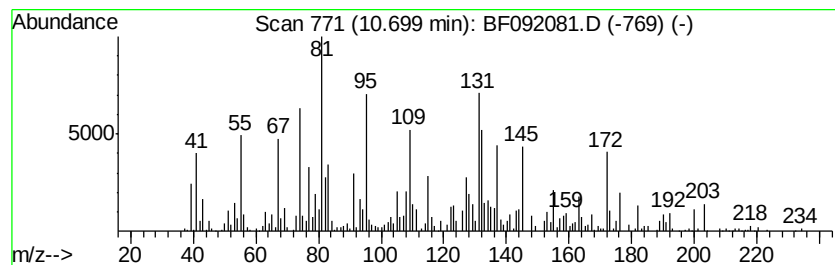
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown10.70 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	19.12 ng	1611480	Phenanthrene-d10	11.18
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	trans, cis-2-Ethylbicyclo[4.4.0]...	166 C12H22	066660-39-7	35
2	trans, cis-3-Ethylbicyclo[4.4.0]...	166 C12H22	066660-43-3	27
3	Cyclohexanecarboxylic acid, 2-(2...	182 C11H18O2	084694-72-4	15
4	Benzofuran, 2-methyl-	132 C9H8O	004265-25-2	15
5	4,5,6,7-Tetrahydro-3-indolinone	137 C8H11NO	058074-25-2	15



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

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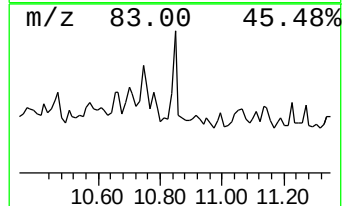
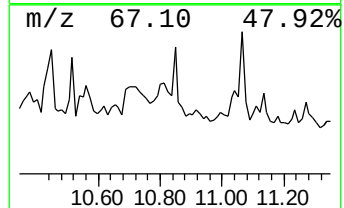
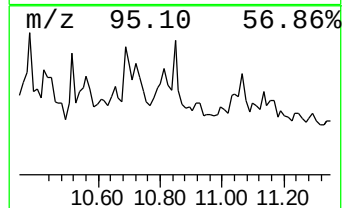
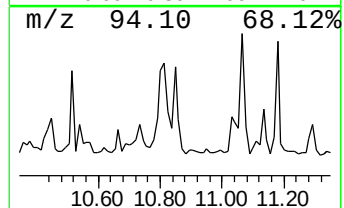
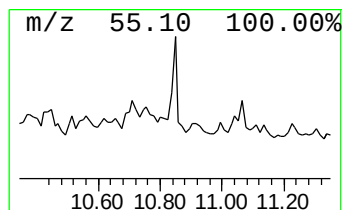
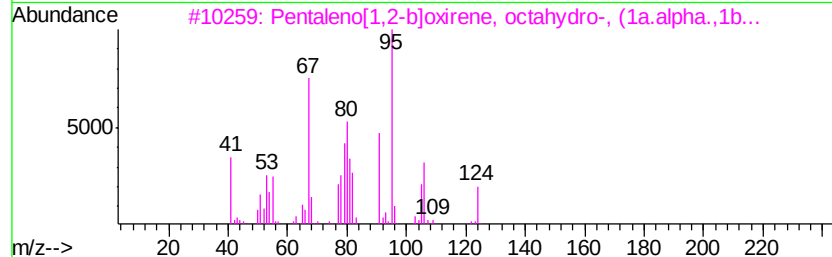
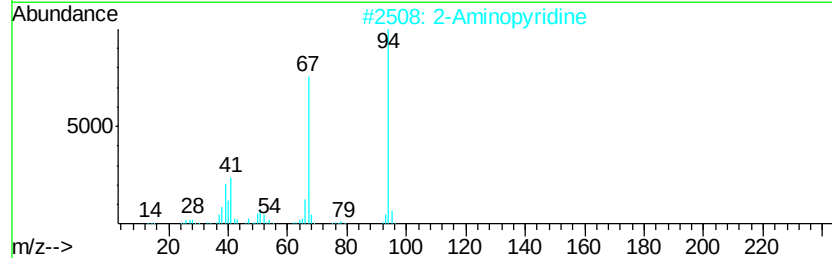
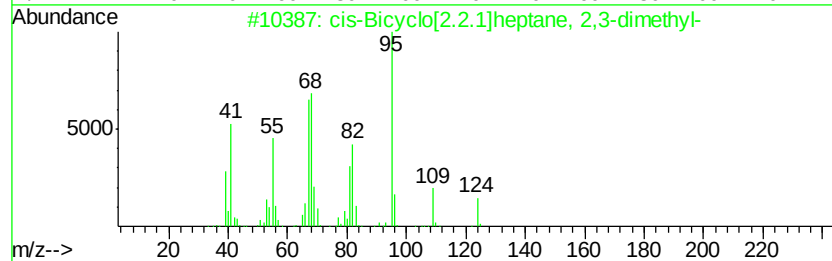
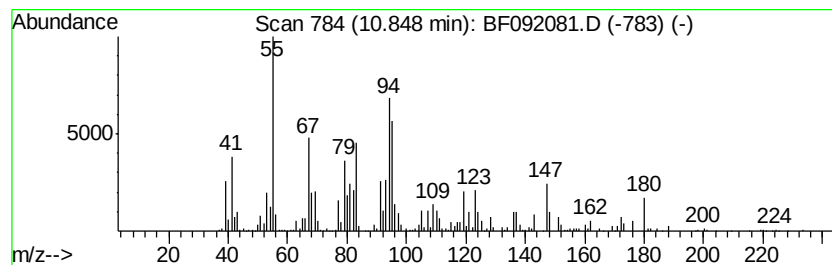
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown10.85 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	12.97 ng	1093460	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-Bicyclo[2.2.1]heptane, 2,3-d...	124	C9H16	1000262-02-5	30
2		2-Aminopyridine	94	C5H6N2	000504-29-0	22
3		Pentaleno[1,2-b]oxirene, octahyd...	124	C8H12O	055449-70-2	20
4		2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	18
5		2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

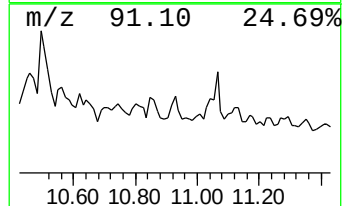
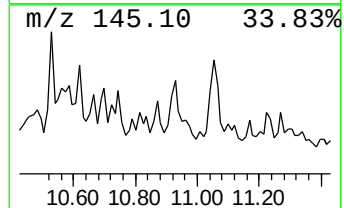
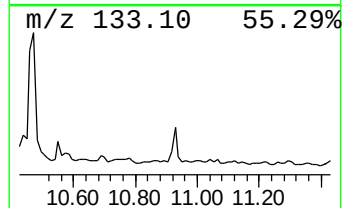
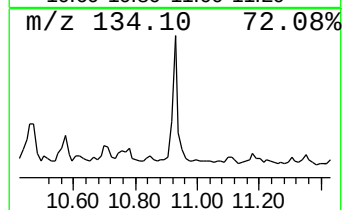
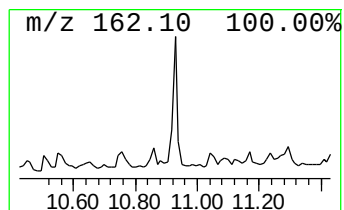
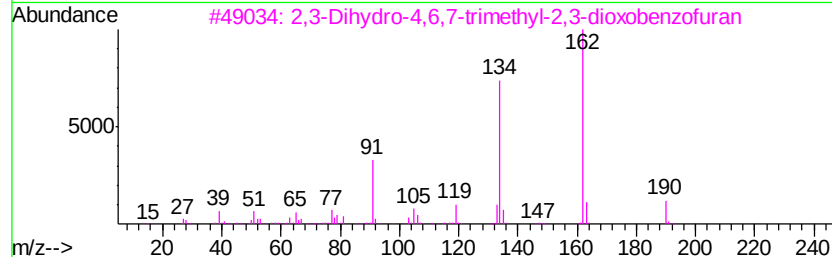
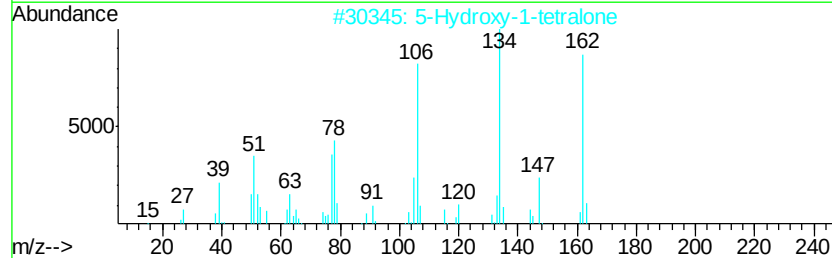
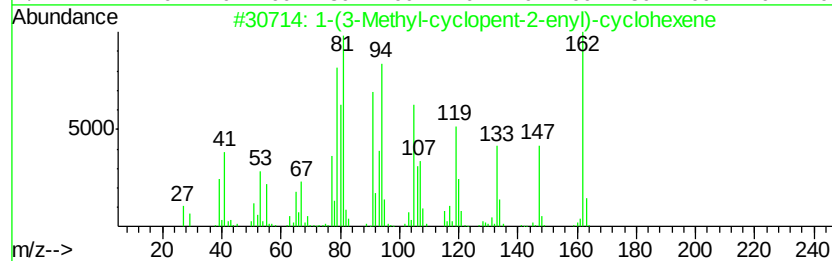
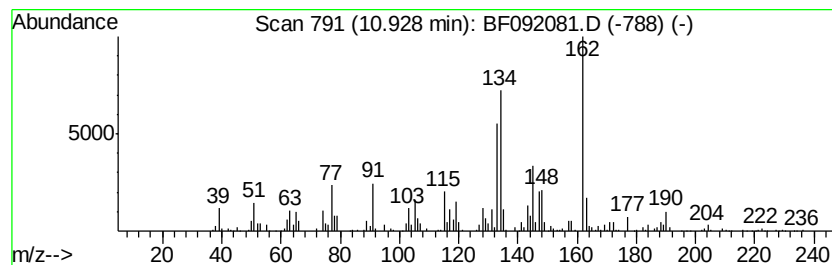
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 1-(3-Methyl-cyclopent-2-eny... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.93	9.89 ng	833561	Phenanthrene-d10	11.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Methyl-cyclopent-2-enyl)-cv...	162	C12H18	1000185-30-7	55
2	5-Hydroxy-1-tetralone	162	C10H10O2	028315-93-7	49
3	2,3-Dihydro-4,6,7-trimethyl-2,3-...	190	C11H10O3	031297-33-3	46
4	2H-1-Benzopyran-2-one, 3,4-dihyd...	162	C10H10O2	000092-47-7	46
5	2H-1-Benzopyran-2-one, 7-hydroxy-	162	C9H6O3	000093-35-6	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
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Misc :
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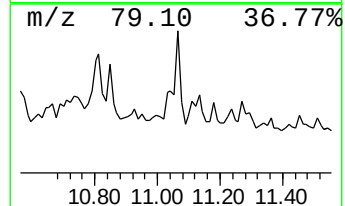
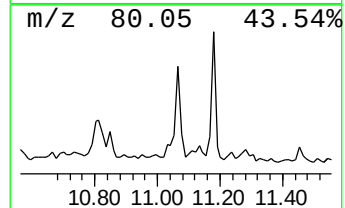
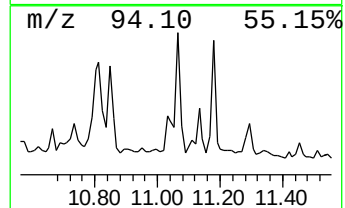
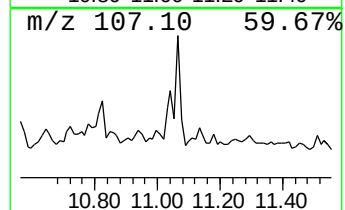
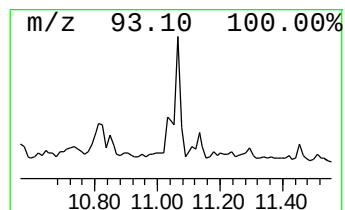
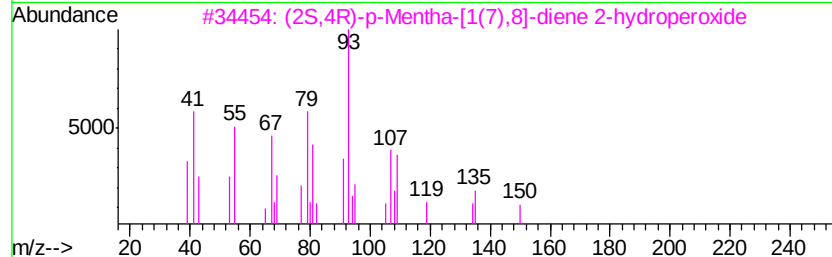
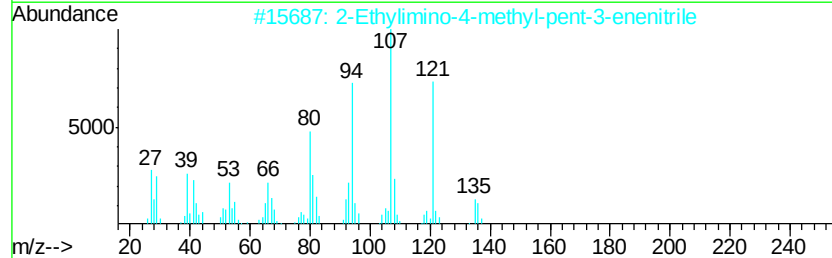
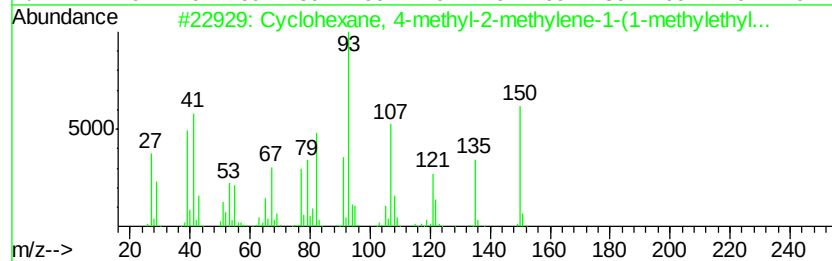
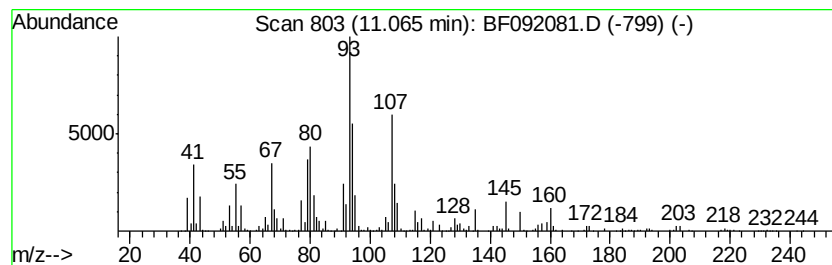
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown11.06 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	22.79 ng	1921280	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 4-methyl-2-methylen...	150	C11H18	056763-62-3	43
2		2-Ethylimino-4-methyl-pent-3-ene...	136	C8H12N2	1000189-21-6	38
3		(2S,4R)-p-Mentha-[1(7),8]-diene ...	168	C10H16O2	1000292-74-4	38
4		1-Isopropenyl-3-propenylcyclopent...	150	C11H18	1000192-81-2	38
5		Spiro[2.4]heptane, 1,2,4,5-tetra...	164	C12H20	074792-98-6	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

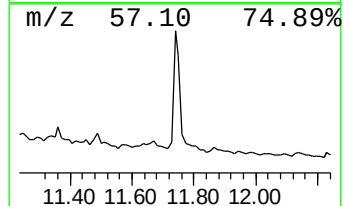
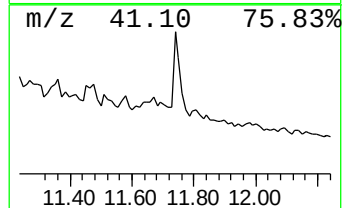
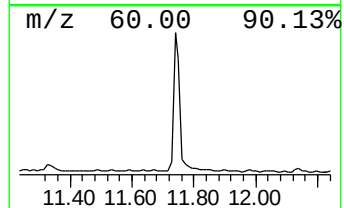
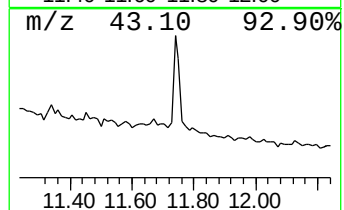
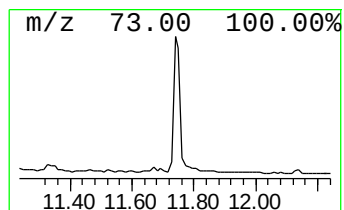
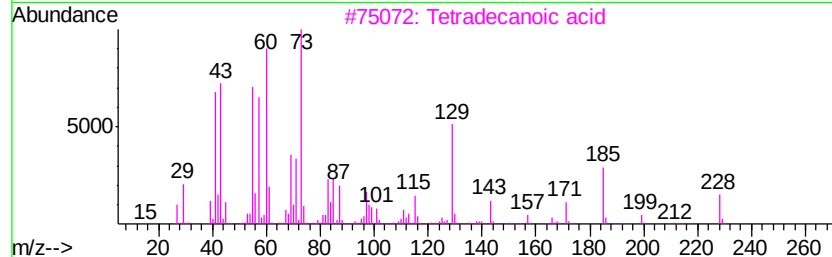
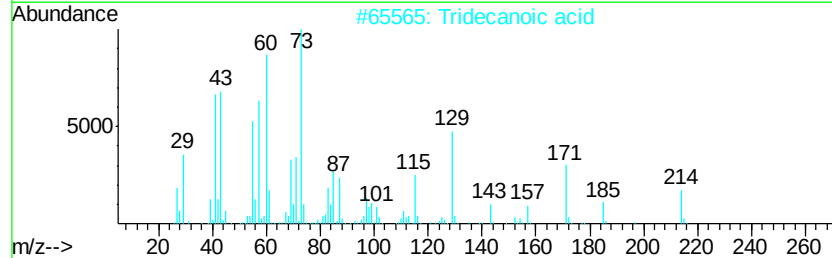
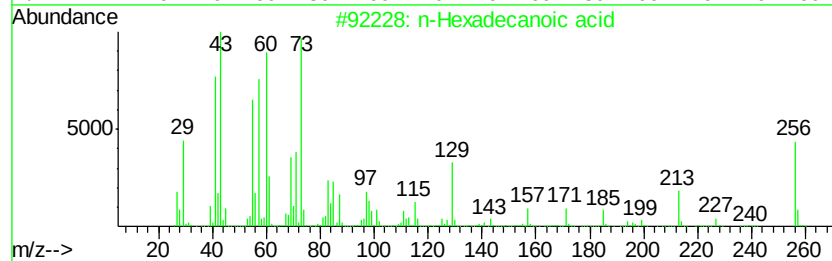
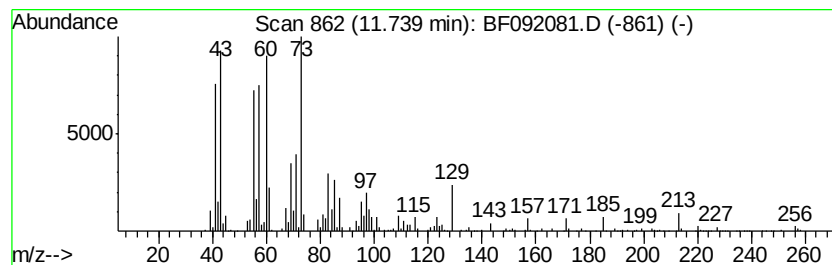
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	13.09 ng	1103720	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		Decane, 2-methyl-	156	C11H24	006975-98-0	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
Data File : BF092081.D
Acq On : 4 Jan 2017 21:22
Operator : UM/SJ
Sample : I1004-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

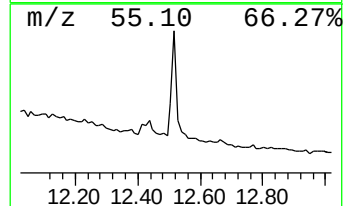
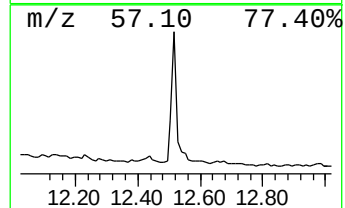
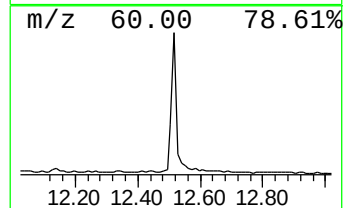
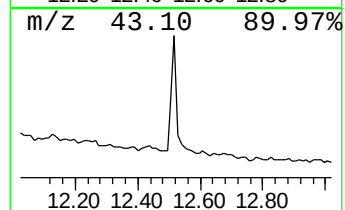
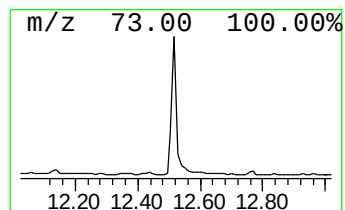
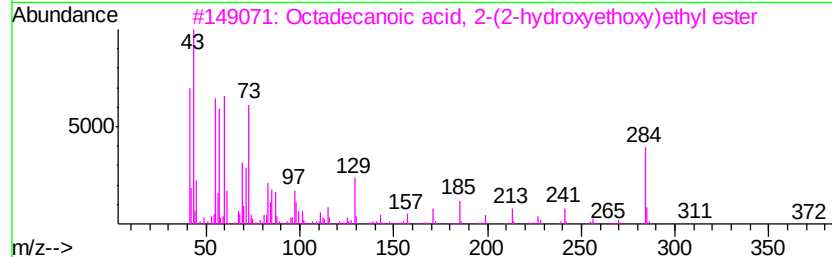
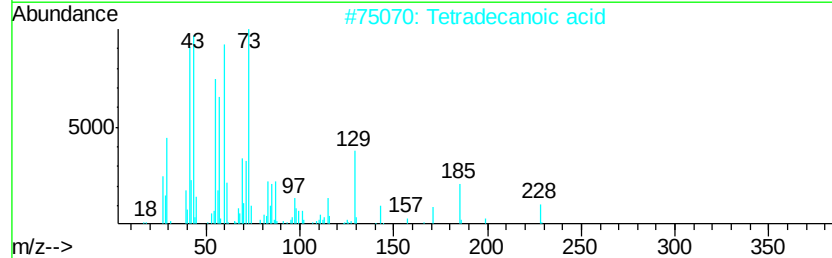
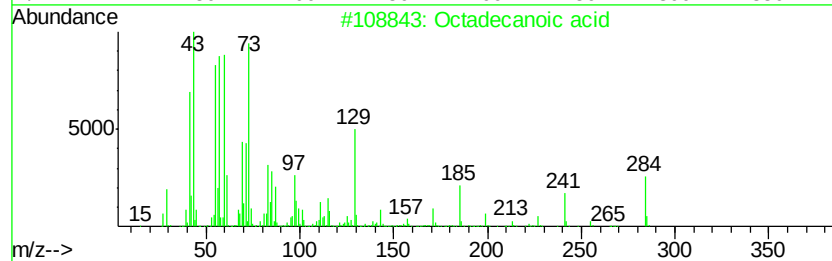
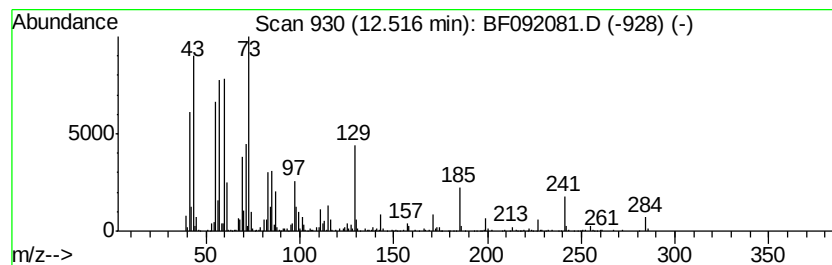
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	9.68 ng	714928	Chrysene-d12	13.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
 Data File : BF092081.D
 Acq On : 4 Jan 2017 21:22
 Operator : UM/SJ
 Sample : I1004-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-30

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
2-Pentanone, 4-hy...	4.80	12.8	ng	1032920	1	6.66	1617190	20.0
unknown6.44	6.44	71.4	ng	5771990	1	6.66	1617190	20.0
Benzene, 1,4-diet...	6.92	11.7	ng	945638	1	6.66	1617190	20.0
Benzene, 1,2-diet...	7.01	19.0	ng	1533840	1	6.66	1617190	20.0
Benzene, 1,2,4,5-...	7.44	8.9	ng	2214700	2	7.94	4996960	20.0
Benzene, 1,3-diet...	7.61	9.3	ng	2330890	2	7.94	4996960	20.0
1H-Indene, 2,3-di...	8.41	13.2	ng	3306900	2	7.94	4996960	20.0
1-Adamantanol	8.48	9.9	ng	2478060	2	7.94	4996960	20.0
Naphthalene, 1-me...	8.77	10.7	ng	2662870	2	7.94	4996960	20.0
unknown8.97	8.97	15.5	ng	2857100	3	9.70	3682350	20.0
unknown10.12	10.12	24.4	ng	4485420	3	9.70	3682350	20.0
unknown10.18	10.18	9.5	ng	1743980	3	9.70	3682350	20.0
Bicyclo(3.3.1)non...	10.45	32.7	ng	2756260	4	11.18	1685920	20.0
unknown10.70	10.70	19.1	ng	1611480	4	11.18	1685920	20.0
unknown10.85	10.85	13.0	ng	1093460	4	11.18	1685920	20.0
1-(3-Methyl-cyclo...	10.93	9.9	ng	833561	4	11.18	1685920	20.0
unknown11.06	11.06	22.8	ng	1921280	4	11.18	1685920	20.0
n-Hexadecanoic acid	11.74	13.1	ng	1103720	4	11.18	1685920	20.0
Octadecanoic acid	12.52	9.7	ng	714928	5	13.81	1477710	20.0