

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
 Data File : BF086736.D
 Acq On : 6 May 2016 21:01
 Operator : UM/SJ
 Sample : H2802-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP

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-BF050416.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	4.041	169	171	174	rBV	78847	133109	2.29%	0.221%
2	4.247	187	189	196	rVB	39423	63347	1.09%	0.105%
3	4.750	231	233	244	rBV	275215	612680	10.52%	1.017%
4	4.899	244	246	250	rVV	102139	175006	3.00%	0.291%
5	5.013	254	256	261	rVB	44275	71615	1.23%	0.119%
6	5.241	274	276	279	rBV	39602	73909	1.27%	0.123%
7	5.310	280	282	292	rVV	1939655	2335232	40.09%	3.877%
8	5.493	295	298	303	rVV	283156	388338	6.67%	0.645%
9	5.573	303	305	308	rVV	56071	87334	1.50%	0.145%
10	5.676	312	314	316	rBV	121436	158994	2.73%	0.264%
11	5.722	316	318	326	rVB2	117630	280810	4.82%	0.466%
12	5.893	331	333	338	rBV	247324	326002	5.60%	0.541%
13	5.962	338	339	344	rBV3	64595	108731	1.87%	0.180%
14	6.122	351	353	354	rBV	64974	84702	1.45%	0.141%
15	6.144	354	355	360	rVB	565741	659223	11.32%	1.094%
16	6.236	360	363	366	rBV3	357139	765729	13.15%	1.271%
17	6.293	366	368	372	rBV3	125265	224989	3.86%	0.373%
18	6.373	372	375	378	rBV	1406965	1597400	27.42%	2.652%
19	6.442	378	381	382	rVV2	468929	692590	11.89%	1.150%
20	6.487	382	385	387	rVV	3867942	4718519	81.01%	7.833%
21	6.556	390	391	393	rBV2	63156	67812	1.16%	0.113%
22	6.590	393	394	399	rVB3	118047	178576	3.07%	0.296%
23	6.670	399	401	402	rBV	91258	92775	1.59%	0.154%
24	6.704	402	404	407	rVB	1200686	1132607	19.44%	1.880%
25	6.762	407	409	413	rBV2	245725	393921	6.76%	0.654%
26	6.864	415	418	420	rVV	4070621	4449089	76.38%	7.386%
27	6.956	422	426	429	rBV	206311	421957	7.24%	0.700%
28	7.013	429	431	432	rBV	225136	216726	3.72%	0.360%
29	7.059	432	435	437	rVB2	213539	332941	5.72%	0.553%
30	7.139	437	442	446	rBV4	364825	1170889	20.10%	1.944%
31	7.207	446	448	451	rVB3	140682	221693	3.81%	0.368%
32	7.276	451	454	457	rBV	2618549	4328966	74.32%	7.186%
33	7.367	460	462	464	rVB	152960	193638	3.32%	0.321%
34	7.413	464	466	469	rVB2	190199	234023	4.02%	0.388%

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Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

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Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.470	469	471	475	rVB5	47692	125149	2.15%	0.208%
36	7.562	475	479	481	rBV3	93123	220539	3.79%	0.366%
37	7.607	481	483	485	rBV3	65527	91162	1.57%	0.151%
38	7.665	486	488	491	rVB2	160756	194543	3.34%	0.323%
39	7.722	491	493	495	rBV	303683	346543	5.95%	0.575%
40	7.802	495	500	503	rBV2	482343	987806	16.96%	1.640%
41	7.927	508	511	514	rBV3	69203	181905	3.12%	0.302%
42	7.996	514	517	519	rVB	1311734	1499480	25.74%	2.489%
43	8.087	523	525	526	rVB	74322	98230	1.69%	0.163%
44	8.133	528	529	531	rBV2	75579	114379	1.96%	0.190%
45	8.179	531	533	535	rVB3	121175	149703	2.57%	0.249%
46	8.225	535	537	538	rVB2	84929	114327	1.96%	0.190%
47	8.282	539	542	544	rBV	166244	231315	3.97%	0.384%
48	8.316	544	545	548	rVB	122435	97786	1.68%	0.162%
49	8.396	548	552	555	rBV2	465004	975396	16.75%	1.619%
50	8.453	555	557	559	rVB3	93584	121212	2.08%	0.201%
51	8.499	559	561	562	rVB2	50625	68588	1.18%	0.114%
52	8.590	565	569	573	rVB4	127773	284804	4.89%	0.473%
53	8.659	573	575	576	rBV	55857	82313	1.41%	0.137%
54	8.705	576	579	581	rVB2	127547	232025	3.98%	0.385%
55	8.785	581	586	587	rBV3	127439	251954	4.33%	0.418%
56	8.888	591	595	597	rBV4	100995	245348	4.21%	0.407%
57	8.945	597	600	603	rBV2	296667	516948	8.87%	0.858%
58	9.002	603	605	607	rVV2	259325	427894	7.35%	0.710%
59	9.070	607	611	614	rVB	4475766	5824887	100.00%	9.670%
60	9.173	617	620	623	rBV5	83912	165071	2.83%	0.274%
61	9.230	623	625	627	rBV	1011429	1066855	18.32%	1.771%
62	9.322	631	633	634	rBV2	88601	149303	2.56%	0.248%
63	9.436	641	643	645	rVV	72523	82155	1.41%	0.136%
64	9.470	645	646	649	rVB2	188948	185153	3.18%	0.307%
65	9.573	654	655	658	rBV	123806	110174	1.89%	0.183%
66	9.619	658	659	660	rBV	120026	89425	1.54%	0.148%
67	9.688	663	665	667	rBV2	143175	228446	3.92%	0.379%
68	9.745	667	670	672	rVB	1829810	1709759	29.35%	2.838%
69	9.825	675	677	681	rVB5	72365	97045	1.67%	0.161%
70	9.905	681	684	687	rBV4	109848	278756	4.79%	0.463%
71	9.973	688	690	693	rBV2	143837	248797	4.27%	0.413%

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72	10.179	705	708	709	rVB	462001	548197	9.41%	0.910%
73	10.236	709	713	714	rVB3	46179	58930	1.01%	0.098%
74	10.533	735	739	742	rVB2	3222977	3941224	67.66%	6.543%
75	10.648	747	749	751	rBV2	102252	118648	2.04%	0.197%
76	10.751	756	758	760	rBV3	86593	112056	1.92%	0.186%
77	10.911	770	772	776	rBV	149290	203797	3.50%	0.338%
78	11.105	787	789	792	rVB2	69319	110618	1.90%	0.184%
79	11.219	797	799	802	rVV	1546471	1541512	26.46%	2.559%
80	11.265	802	803	808	rVB2	99038	147991	2.54%	0.246%
81	11.345	808	810	814	rBV3	39921	63063	1.08%	0.105%
82	11.768	845	847	853	rVB2	598990	603320	10.36%	1.002%
83	12.099	873	876	878	rBV	36643	68093	1.17%	0.113%
84	12.476	906	909	913	rVB5	49764	133900	2.30%	0.222%
85	12.545	913	915	921	rBV	502340	538984	9.25%	0.895%
86	12.808	935	938	940	rBV	4400239	4414581	75.79%	7.328%
87	12.842	940	941	946	rVB	417063	365676	6.28%	0.607%
88	13.699	1015	1016	1020	rVB	116810	125383	2.15%	0.208%
89	13.848	1026	1029	1032	rBV	1319382	1249872	21.46%	2.075%
90	14.922	1121	1123	1128	rBV2	38936	61310	1.05%	0.102%
91	15.231	1147	1150	1158	rBV	708965	943321	16.19%	1.566%

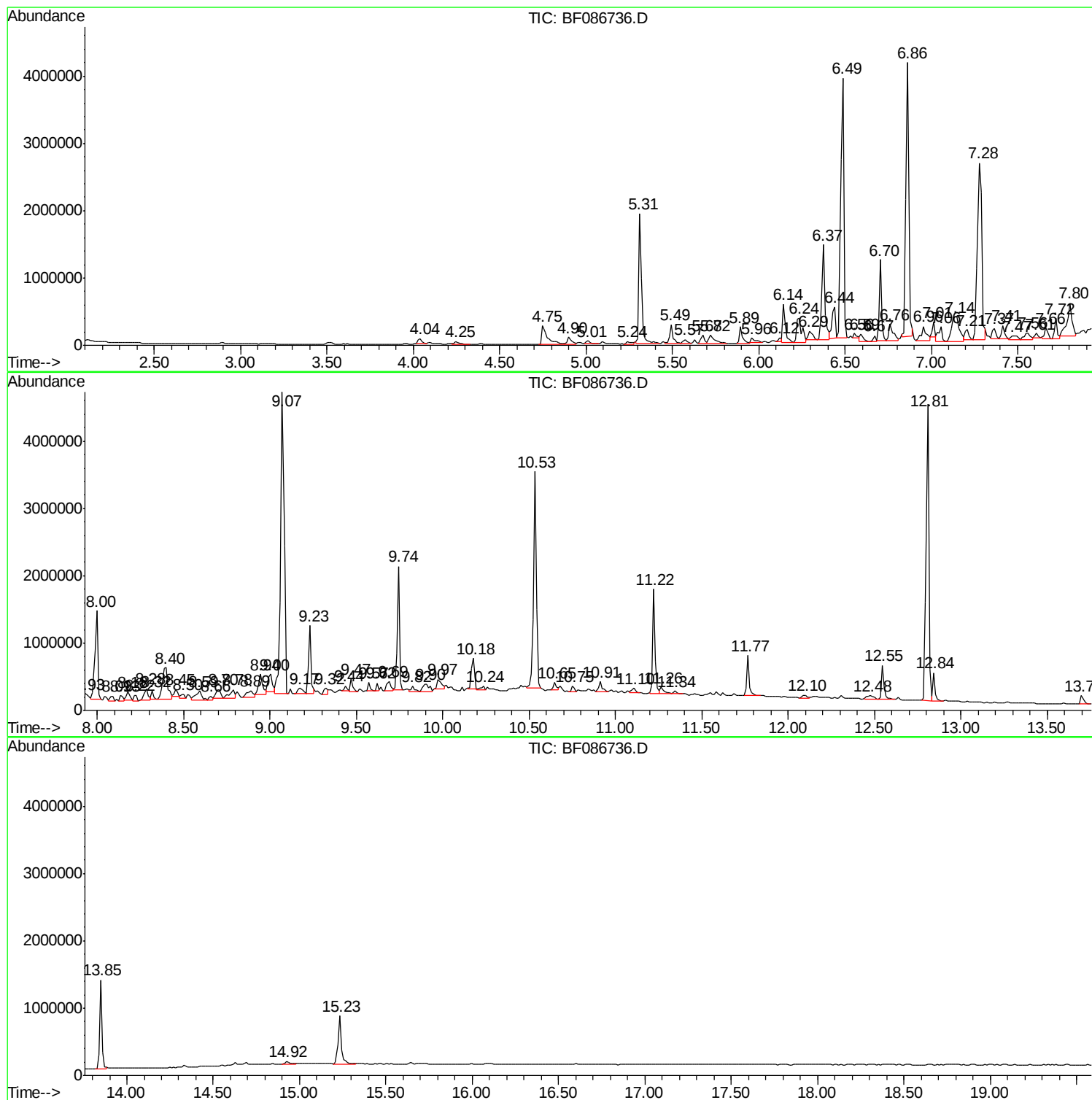
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Instrument :
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DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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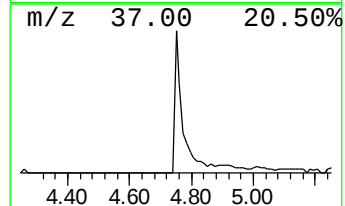
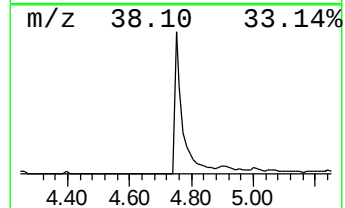
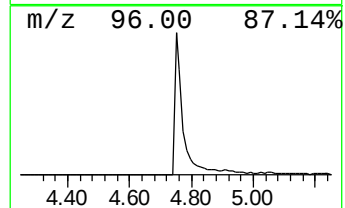
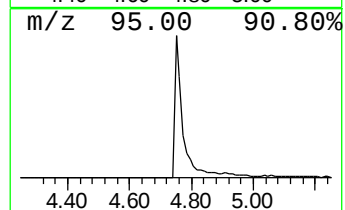
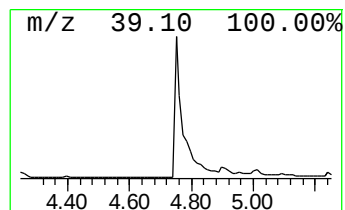
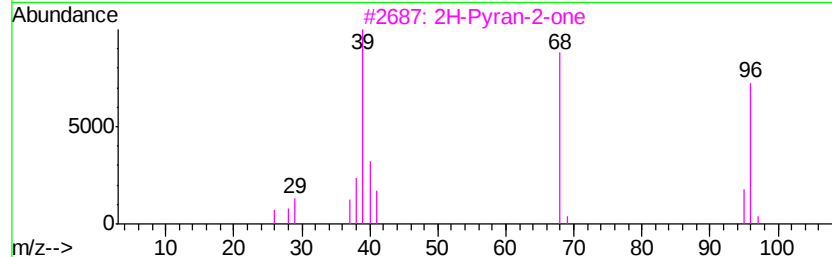
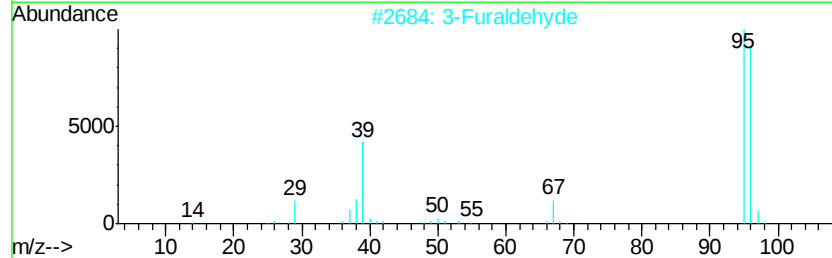
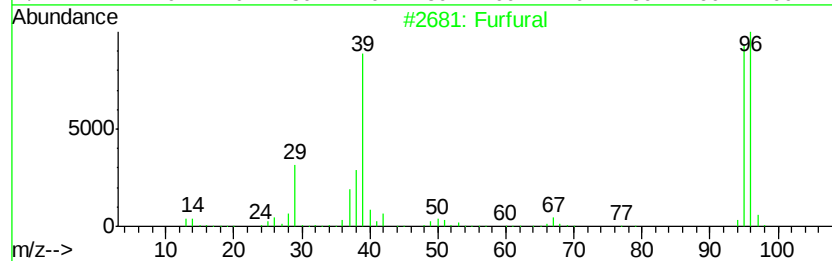
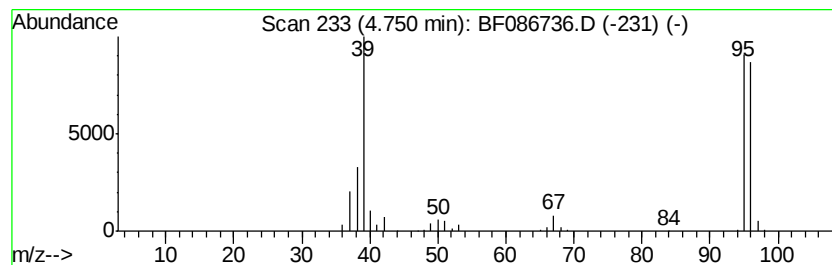
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Furfural Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	21.64 ng	612680	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furfural	96	C5H4O2	000098-01-1	97
2			3-Furaldehyde	96	C5H4O2	000498-60-2	91
3			2H-Pyran-2-one	96	C5H4O2	000504-31-4	50
4			1H-Imidazole, 1,4-dimethyl-	96	C5H8N2	006338-45-0	43
5			Cyclopropene	40	C3H4	002781-85-3	42



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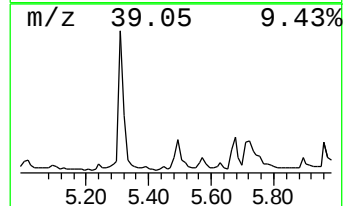
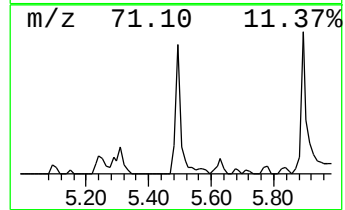
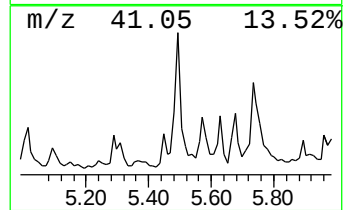
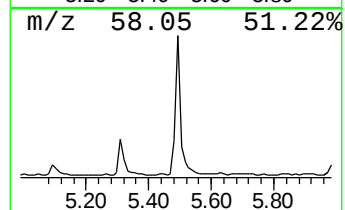
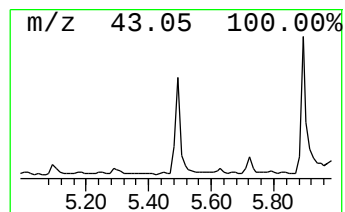
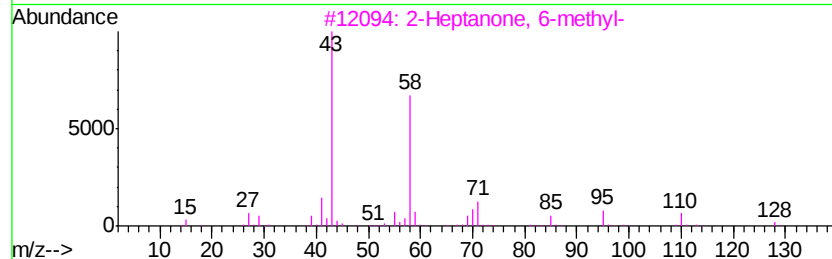
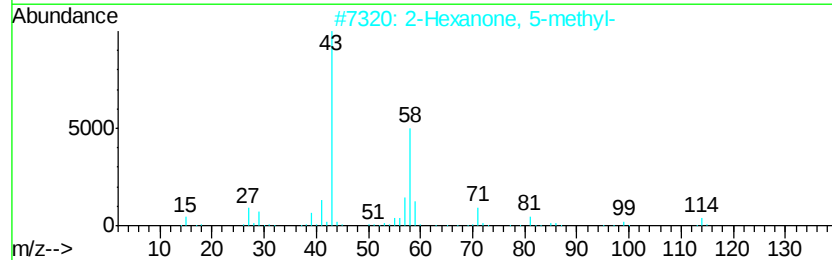
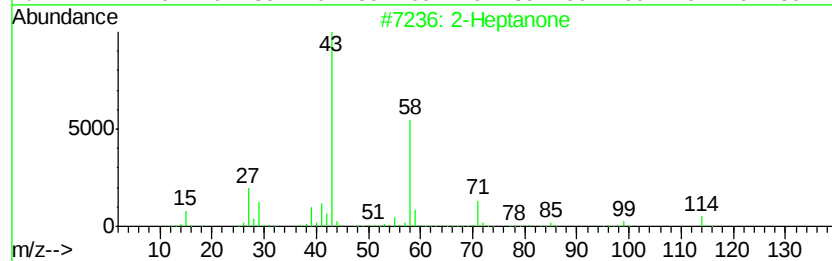
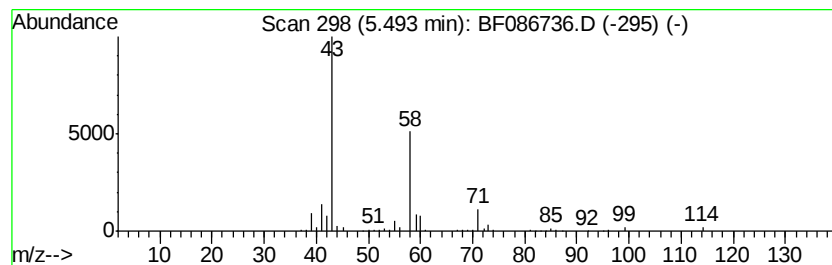
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Heptanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	13.71 ng	388338	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	72
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64
3			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	50
4			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	45
5			2-Nonanone	142	C9H18O	000821-55-6	45



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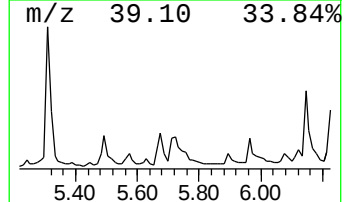
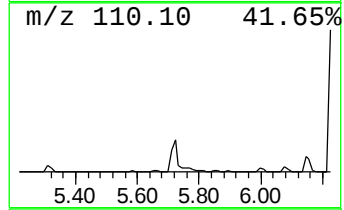
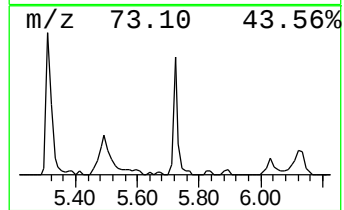
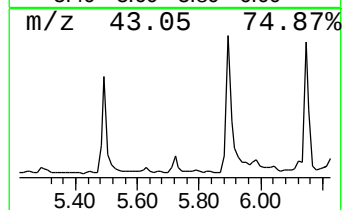
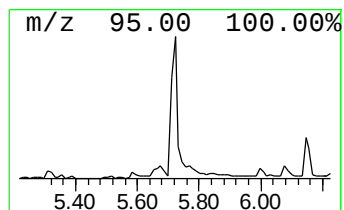
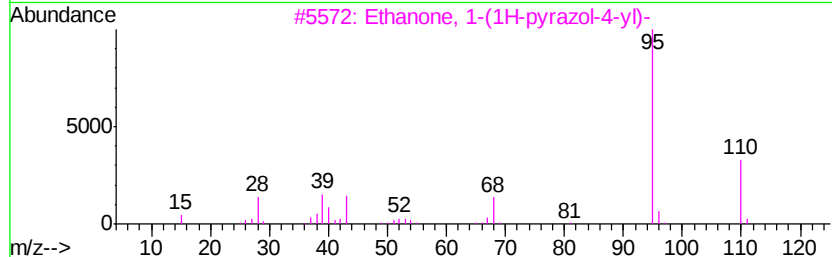
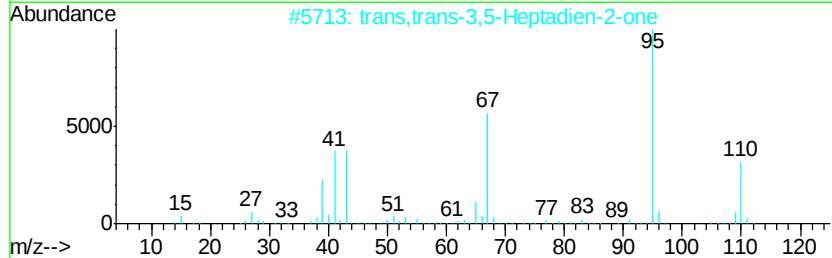
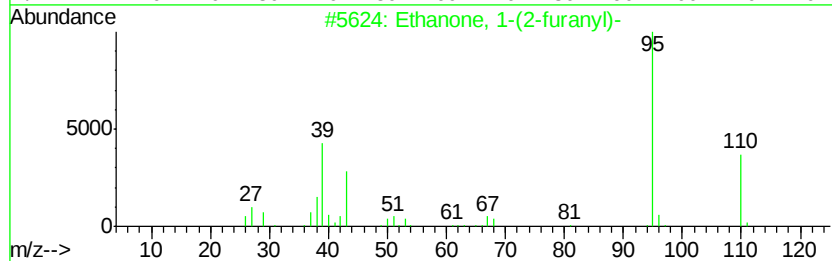
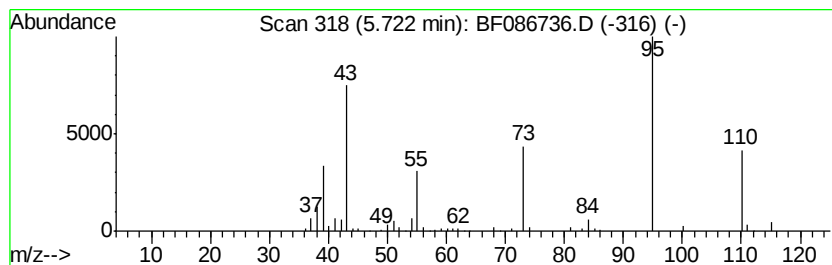
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanone, 1-(2-furanyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	9.92 ng	280810	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	64
2		trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	53
3		Ethanone, 1-(1H-pyrazol-4-yl)-	110	C5H6N2O	025016-16-4	53
4		Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	40
5		4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	40



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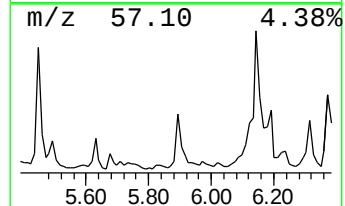
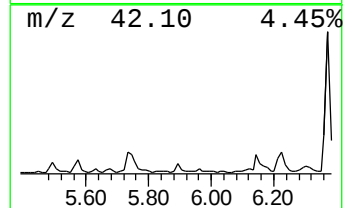
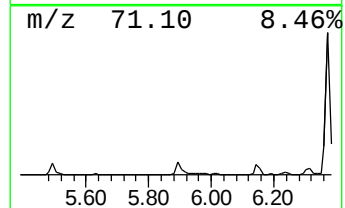
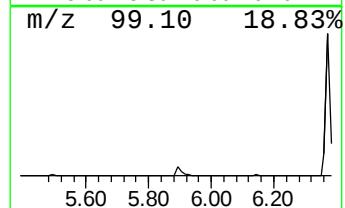
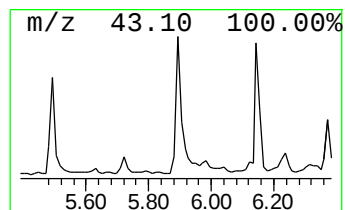
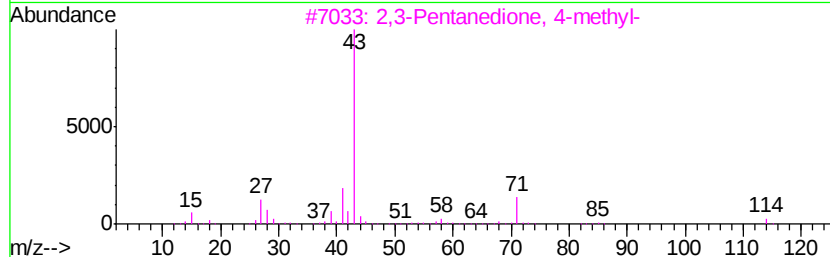
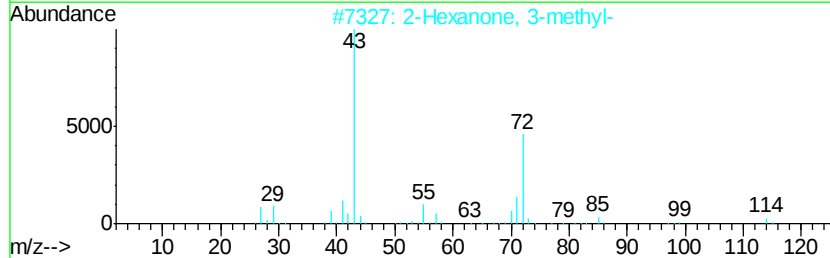
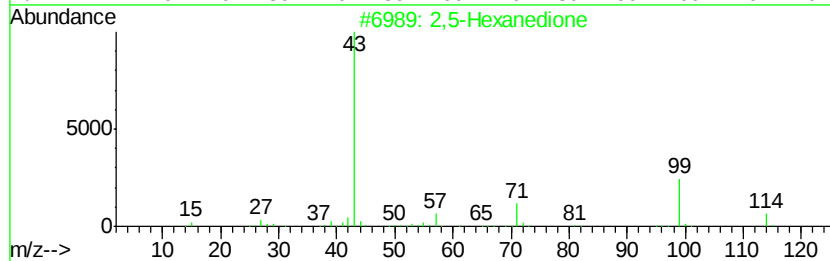
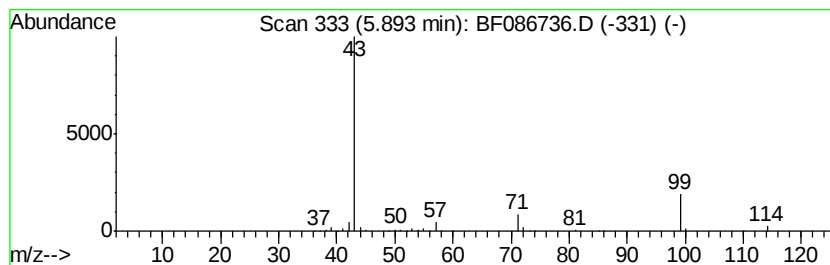
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2,5-Hexanedione Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	11.51 ng	326002	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Hexanedione	114	C6H10O2	000110-13-4	83
2		2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	25
3		2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	9
4		2,3-Hexanedione	114	C6H10O2	003848-24-6	9
5		2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
Operator : UM/SJ
Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

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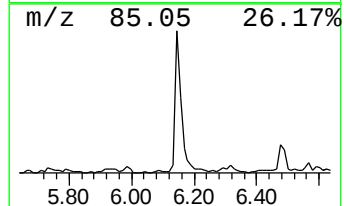
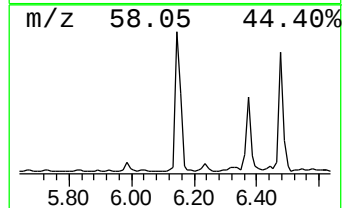
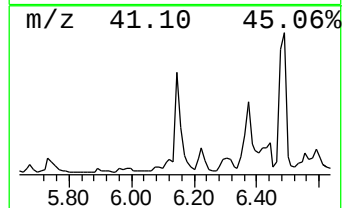
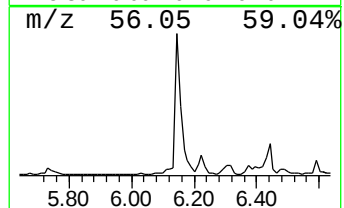
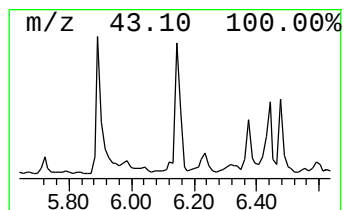
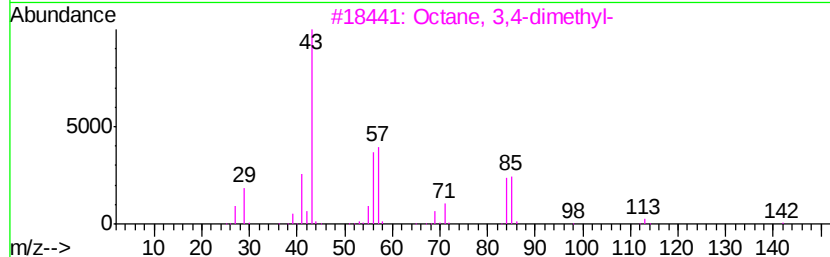
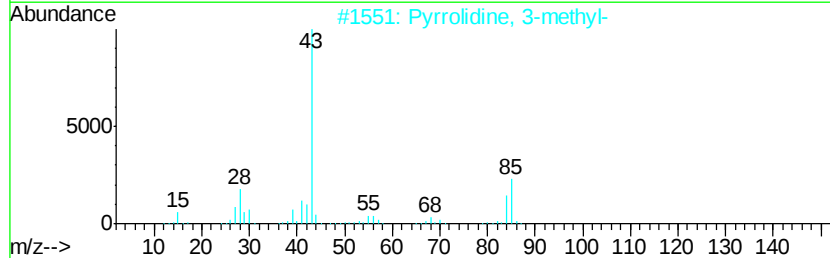
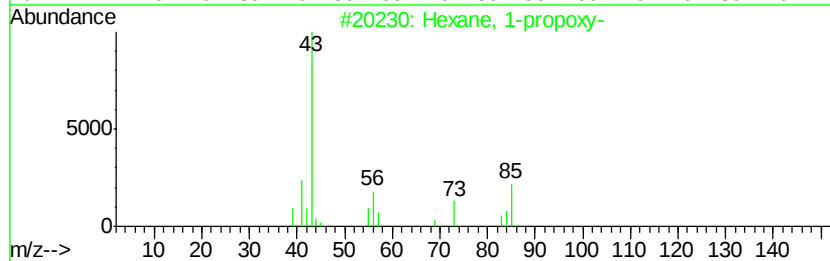
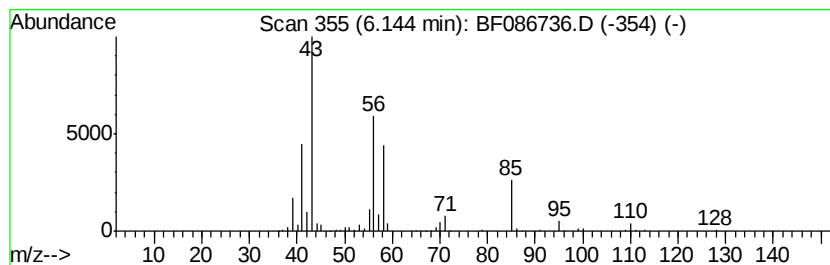
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.14 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	23.28 ng	659223	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 1-propoxy-	144	C9H20O	053685-78-2	27
2		Pyrrolidine, 3-methyl-	85	C5H11N	034375-89-8	22
3		Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	17
4		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	16
5		2(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
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Sample : H2802-07
Misc :
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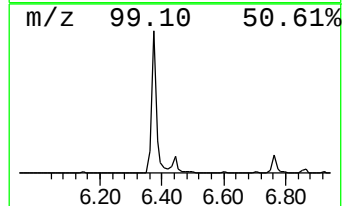
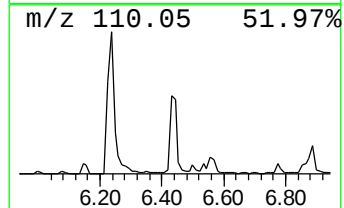
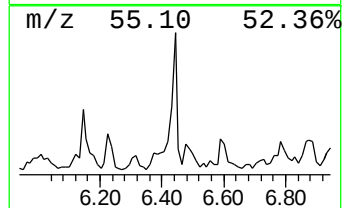
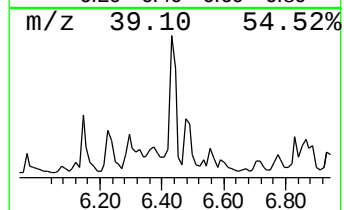
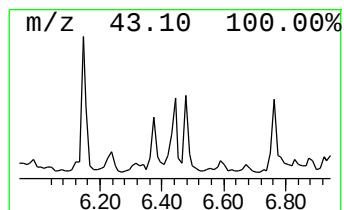
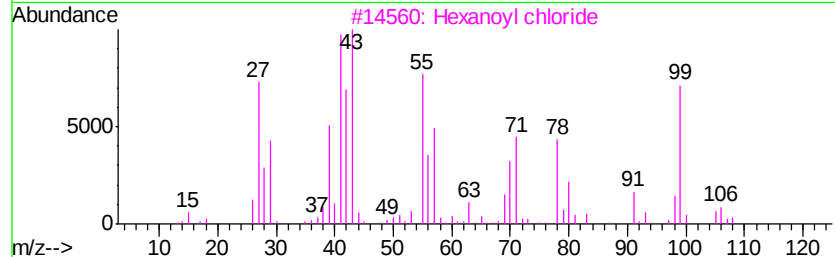
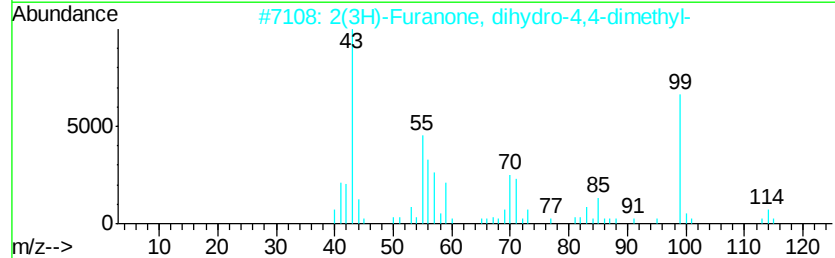
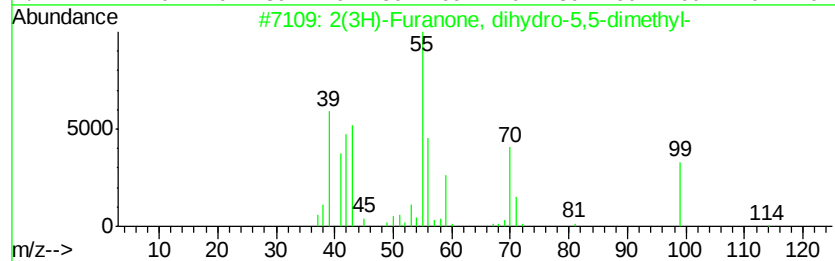
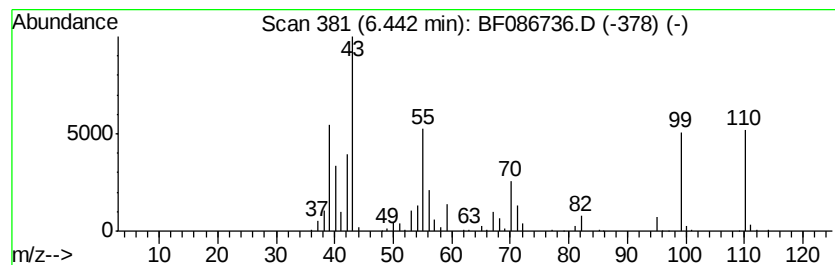
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2(3H)-Furanone, dihydro-5,5... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	24.46 ng	692590	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Furanone, dihydro-5,5-dime...	114	C6H10O2	003123-97-5	70
2		2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	38
3		Hexanoyl chloride	134	C6H11ClO	000142-61-0	37
4		Pentanedioic acid, monoamide, N-...	229	C10H19N3O3	1000263-87-8	37
5		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	35



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Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

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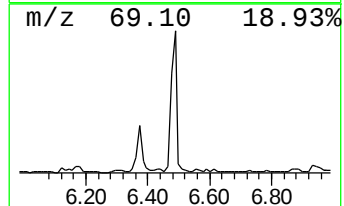
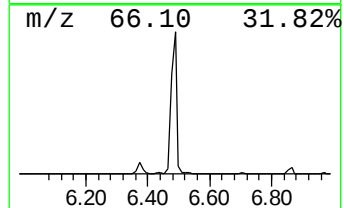
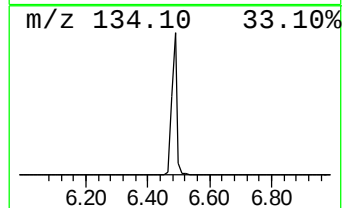
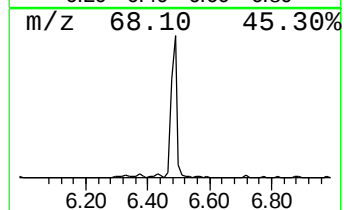
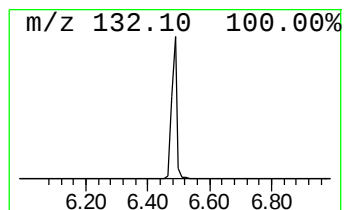
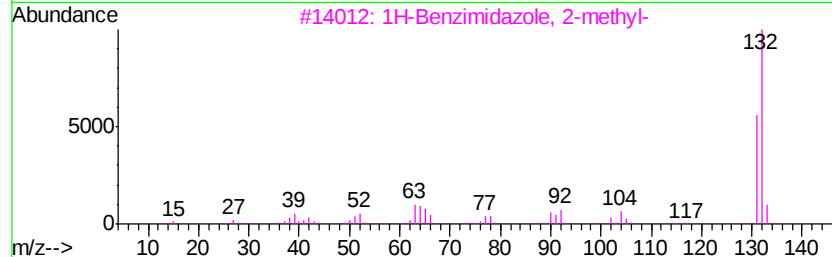
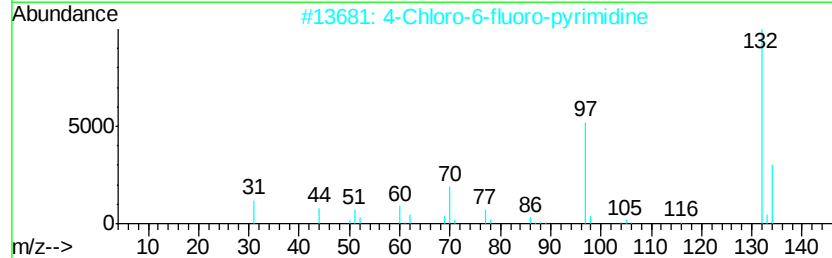
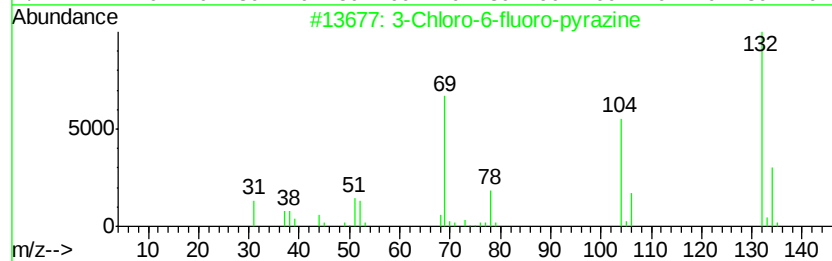
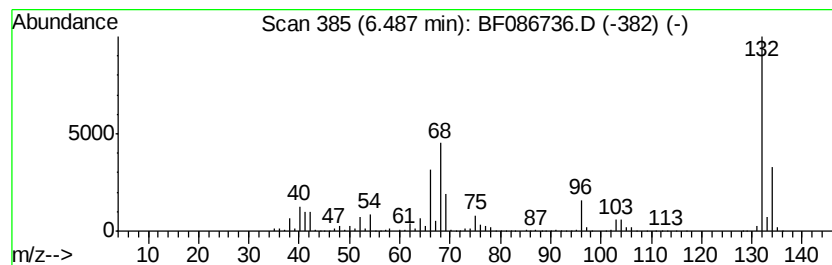
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	166.64 ng	4718520	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
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Sample : H2802-07
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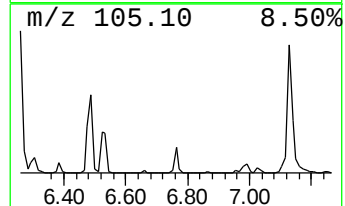
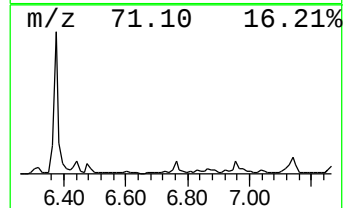
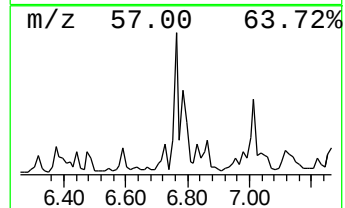
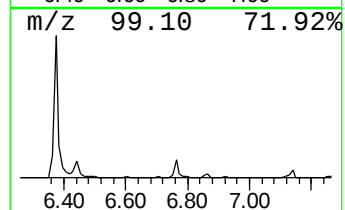
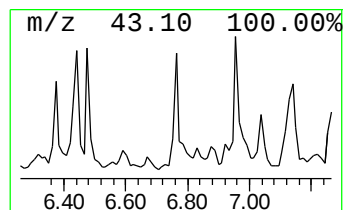
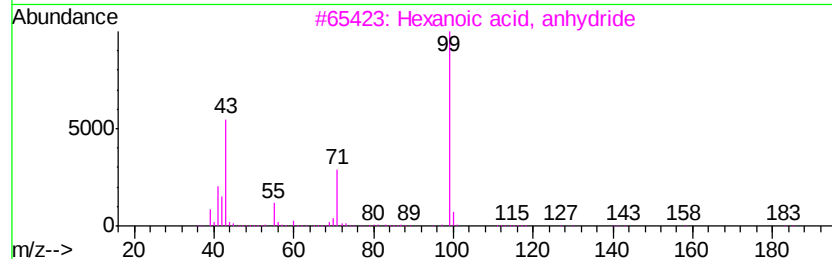
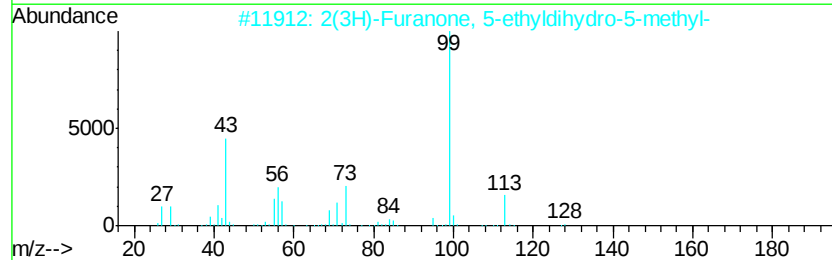
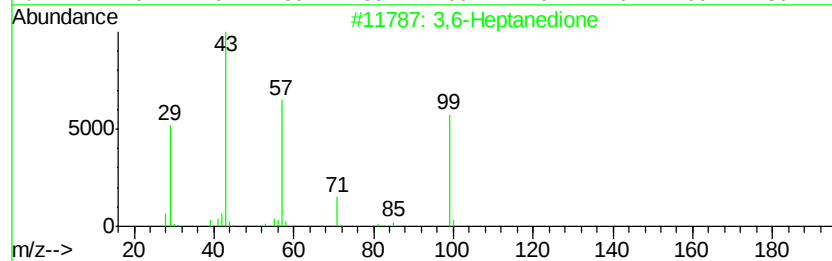
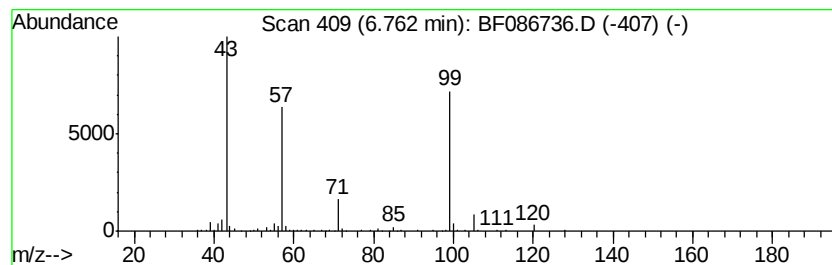
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 3,6-Heptanedione Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	13.91 ng	393921	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Heptanedione	128	C7H12O2	001703-51-1	78
2		2(3H)-Furanone, 5-ethylidihydro-5-methyl-	128	C7H12O2	002865-82-9	72
3		Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	50
4		4-Piperidinone	99	C5H9NO	041661-47-6	37
5		2,5-Pyrrolidinedione	99	C4H5NO2	000123-56-8	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
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Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

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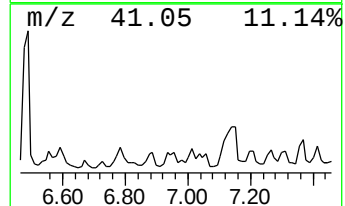
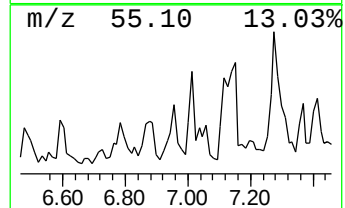
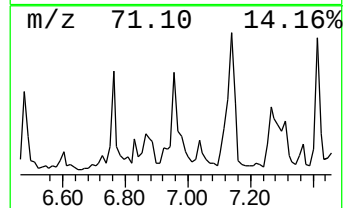
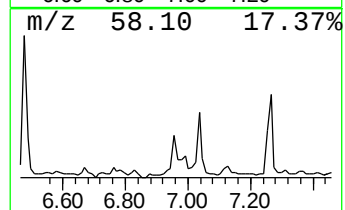
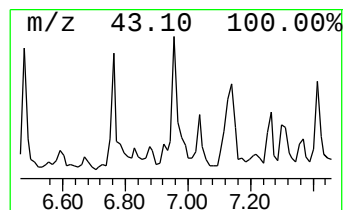
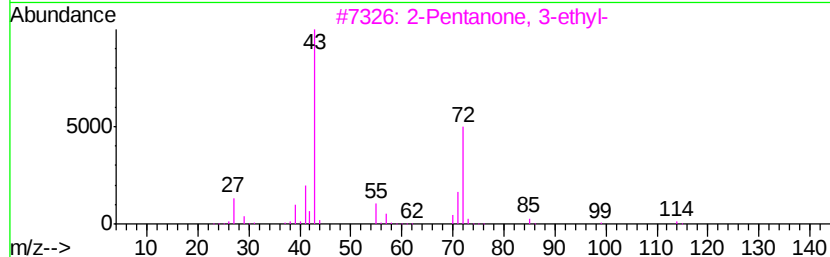
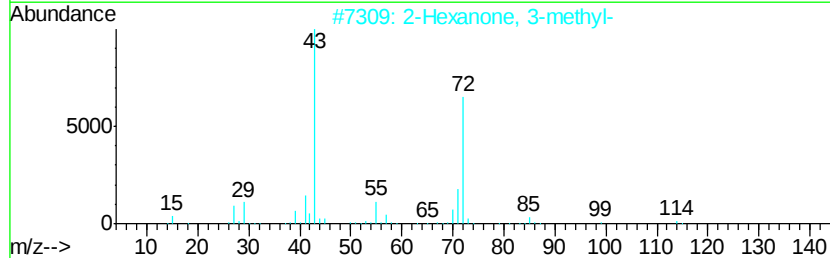
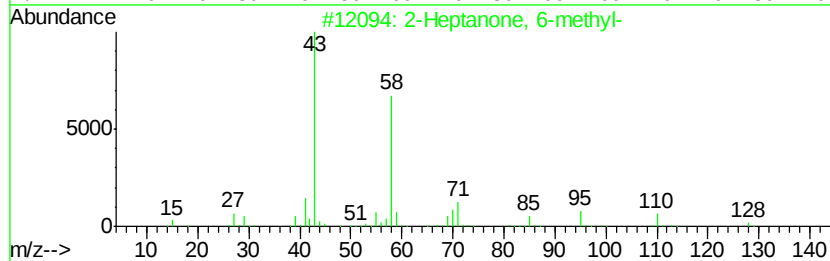
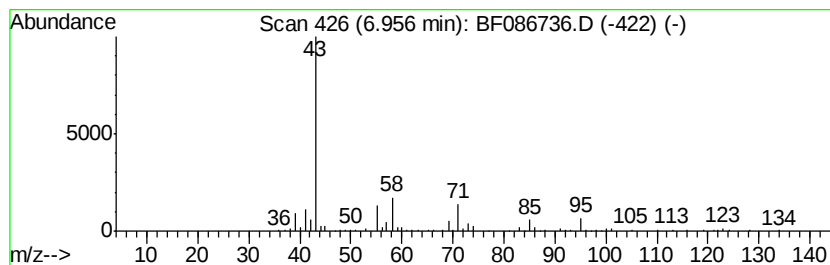
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown6.96 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	14.90 ng	421957	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-			128	C8H16O	000928-68-7	47
2	2-Hexanone, 3-methyl-			114	C7H14O	002550-21-2	38
3	2-Pentanone, 3-ethyl-			114	C7H14O	006137-03-7	37
4	2,9-Decanedione			170	C10H18O2	016538-91-3	36
5	Heptane, 2,3-dimethyl-			128	C9H20	003074-71-3	35



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Misc :
ALS Vial : 11 Sample Multiplier: 1

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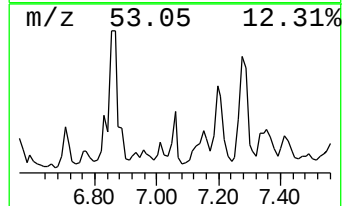
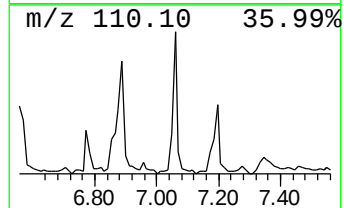
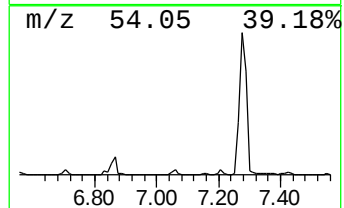
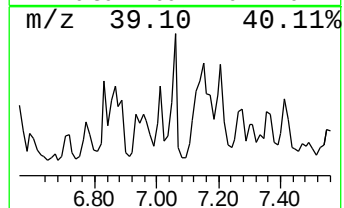
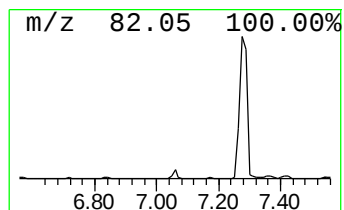
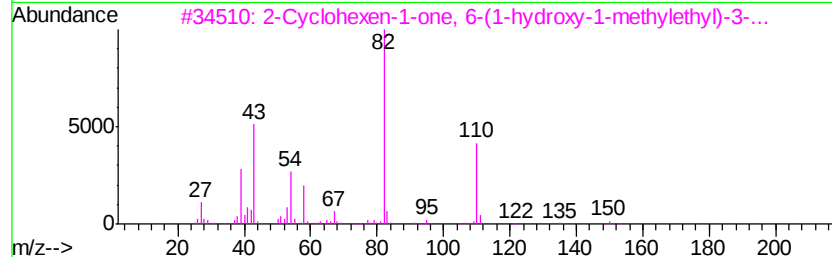
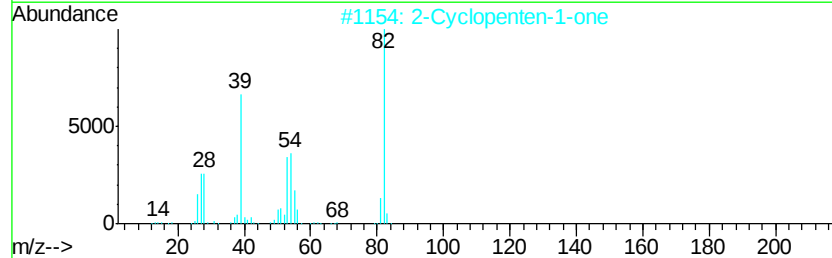
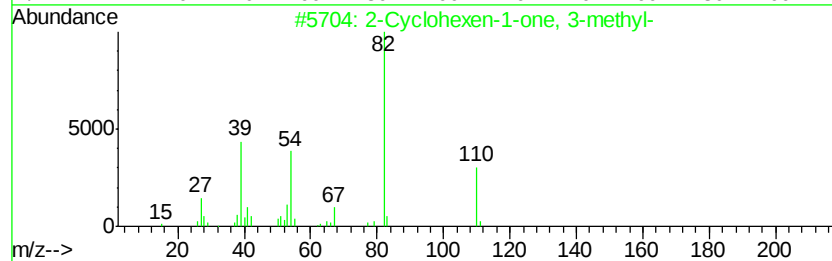
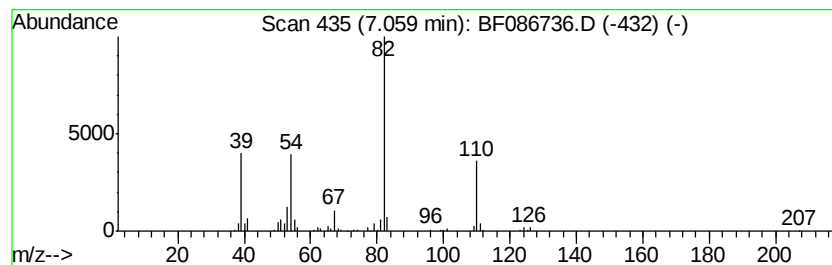
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	11.76 ng	332941	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2		2-Cyclopenten-1-one	82	C5H6O	000930-30-3	59
3		2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	50
4		1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	43
5		Azeleoneitrile	150	C9H14N2	001675-69-0	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
Operator : UM/SJ
Sample : H2802-07
Misc :
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Instrument :
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ClientSampled :
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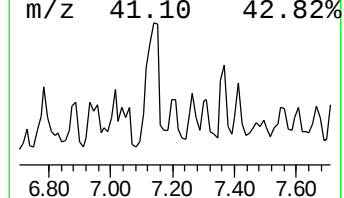
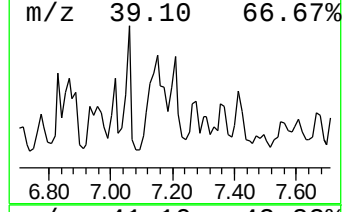
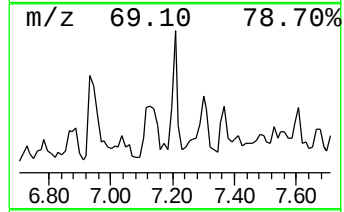
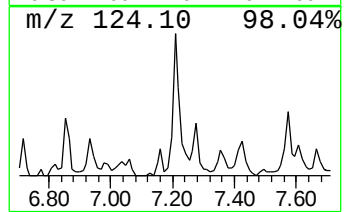
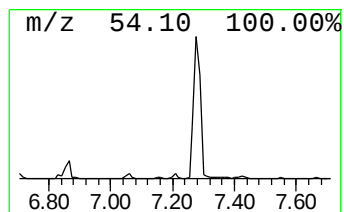
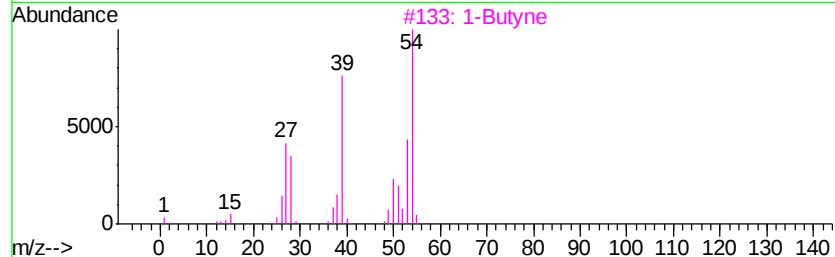
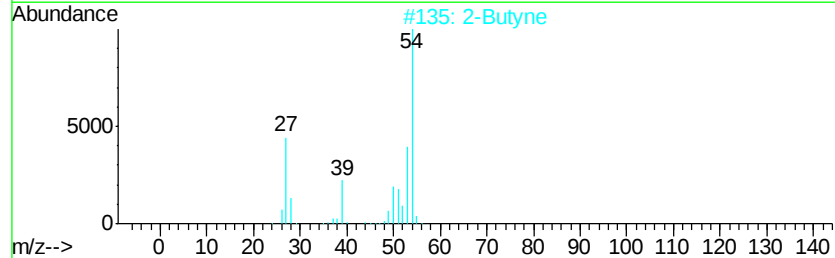
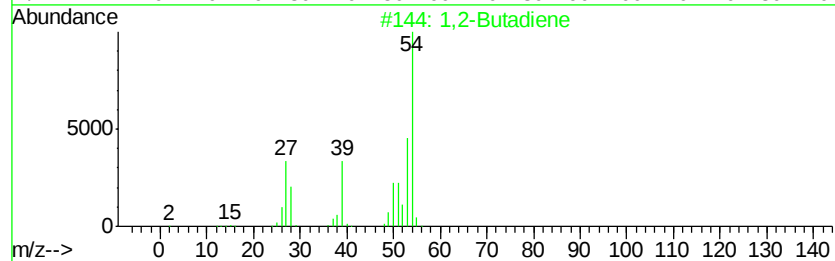
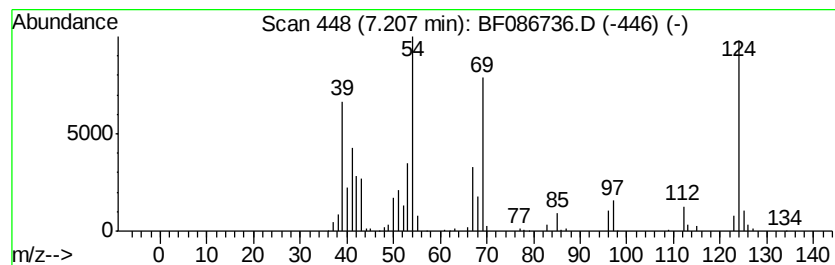
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown7.21 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	7.83 ng	221693	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Butadiene	54	C4H6	000590-19-2	49
2		2-Butyne	54	C4H6	000503-17-3	49
3		1-Butyne	54	C4H6	000107-00-6	47
4		2,5-Dihydrothiophene sulfone	118	C4H6O2S	000077-79-2	47
5		2-Oxazolidinone, 3-ethenyl-	113	C5H7N02	004271-26-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
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Sample : H2802-07
Misc :
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Instrument :
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ClientSampleId :
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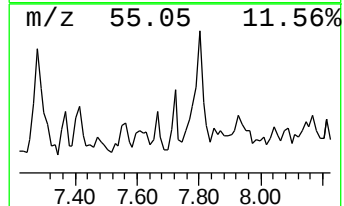
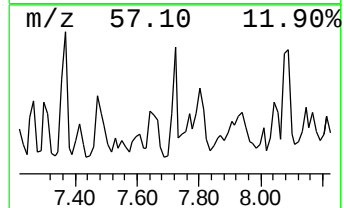
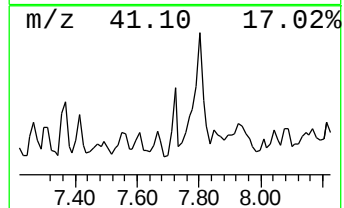
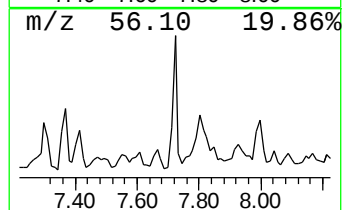
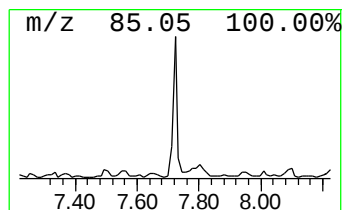
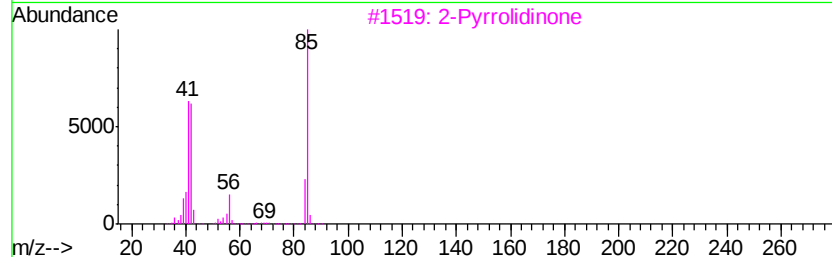
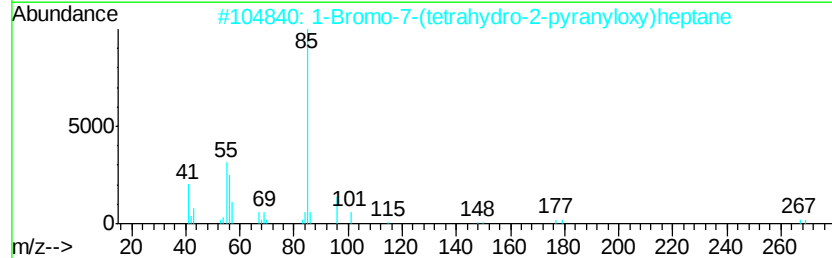
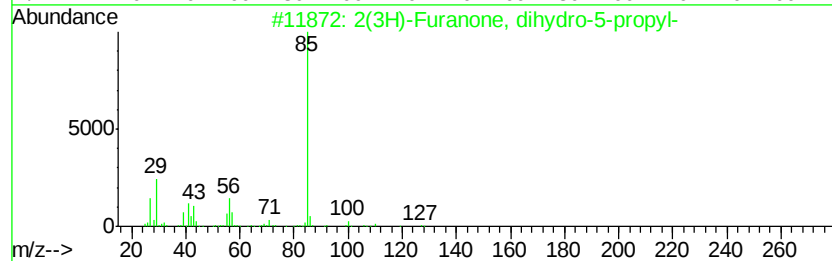
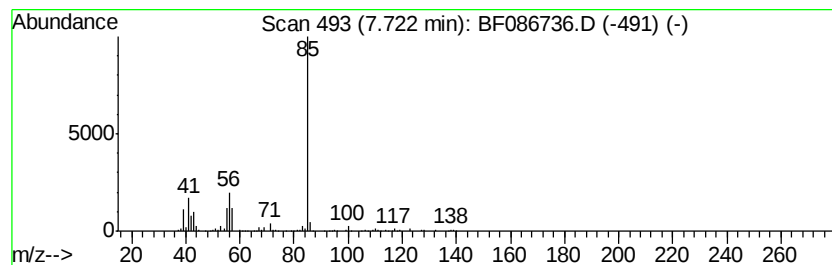
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Furanone, dihydro-5-p... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	9.24 ng	346543	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	83
2		1-Bromo-7-(tetrahydro-2-pyranylo...	278	C12H23BrO2	010160-25-5	72
3		2-Pyrrolidinone	85	C4H7NO	000616-45-5	64
4		2-(1-Methylpropoxy)-tetrahydropyran	158	C9H18O2	032767-69-4	64
5		Thiazole	85	C3H3NS	000288-47-1	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
Operator : UM/SJ
Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

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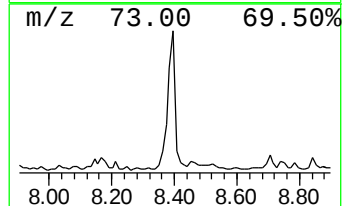
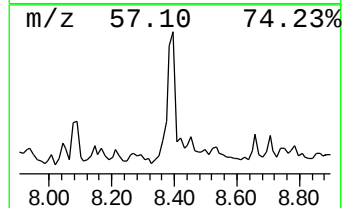
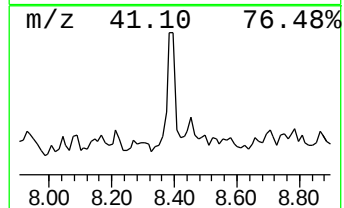
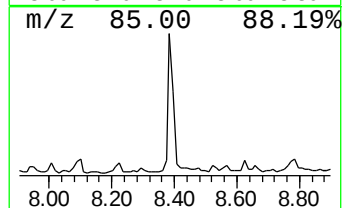
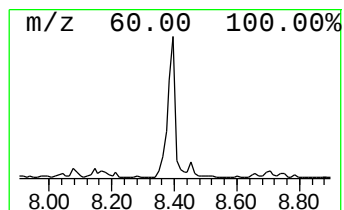
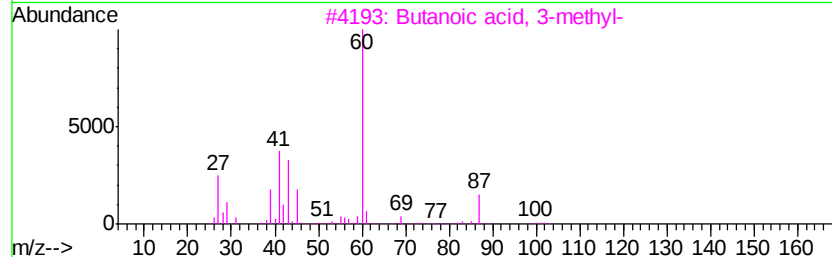
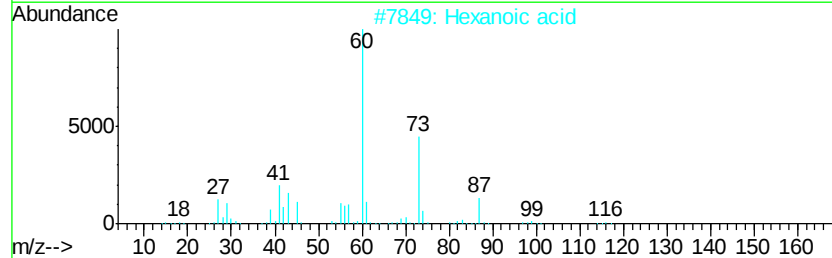
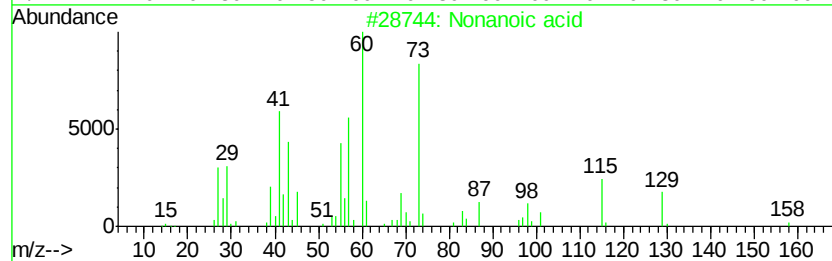
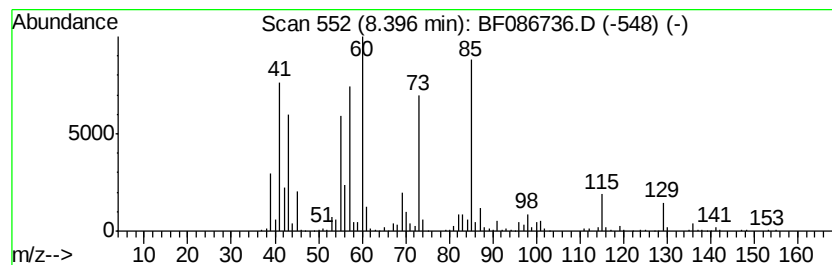
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown8.40 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	26.02 ng	975396	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	43
2		Hexanoic acid	116	C6H12O2	000142-62-1	35
3		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	35
4		Ether, hexyl isopropyl	144	C9H20O	018636-65-2	35
5		Oxirane, (2-methylbutyl)-	114	C7H14O	053229-42-8	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
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Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

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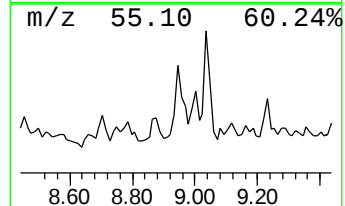
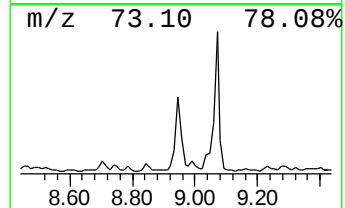
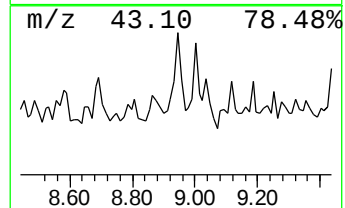
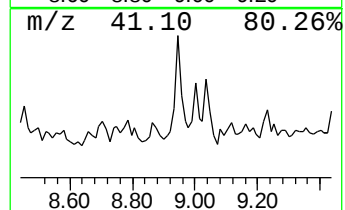
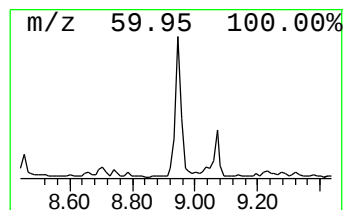
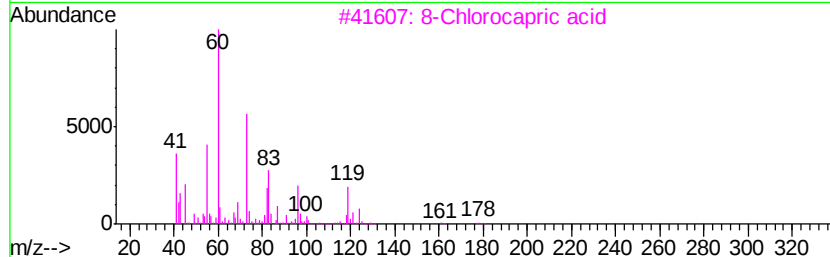
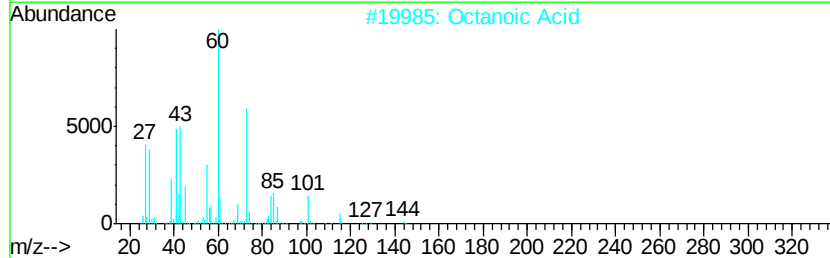
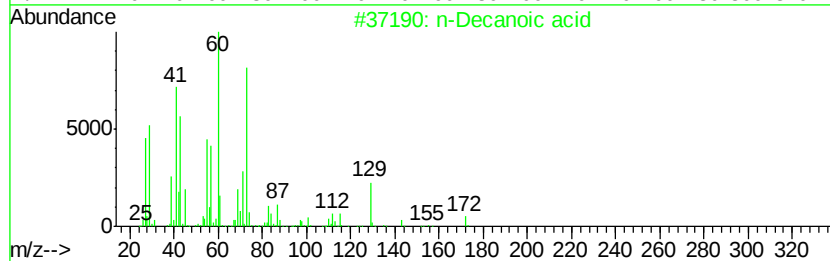
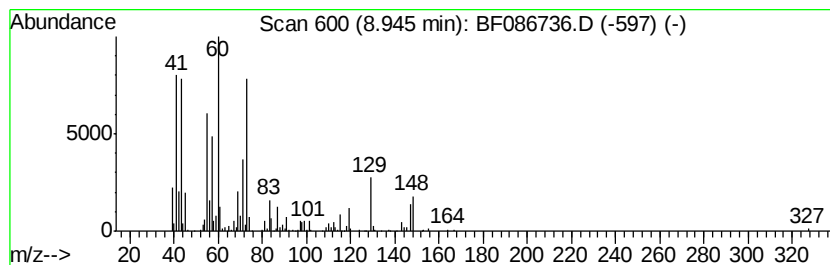
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 n-Decanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	12.09 ng	516948	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	64
2		Octanoic Acid	144	C8H16O2	000124-07-2	52
3		8-Chlorocapric acid	178	C8H15ClO2	001795-62-6	50
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	50
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
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Sample : H2802-07
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ClientSampleId :
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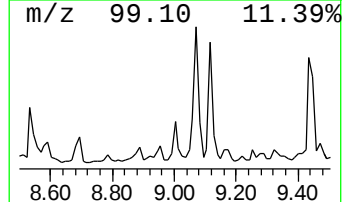
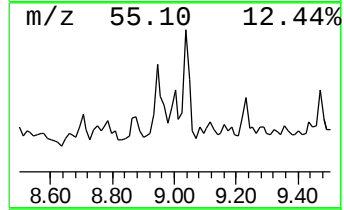
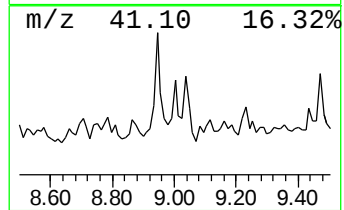
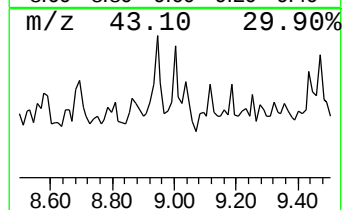
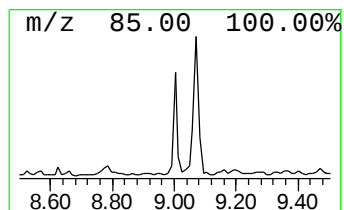
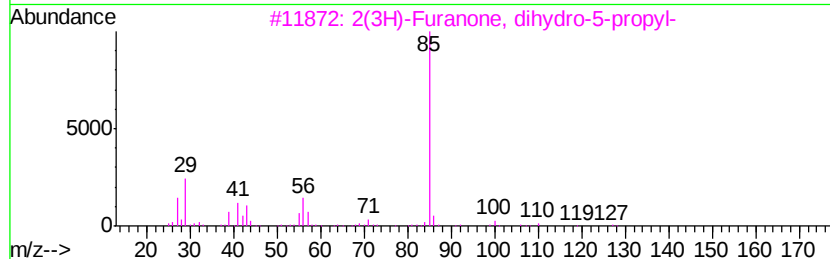
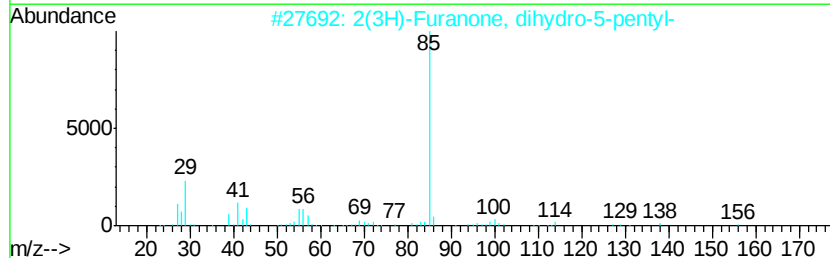
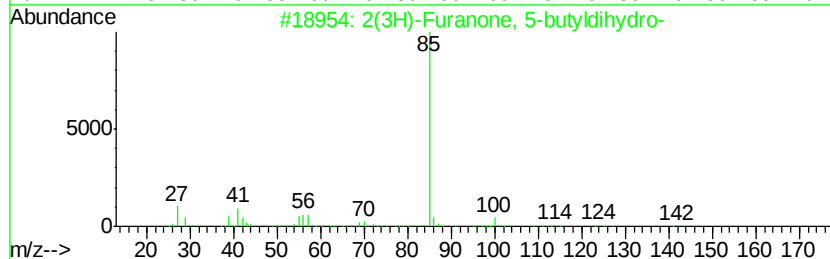
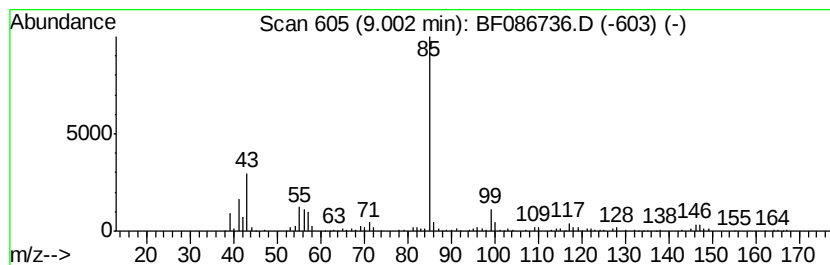
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 2(3H)-Furanone, 5-butyldihydro... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.00	10.01 ng	427894	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, 5-butyldihydro-	142	C8H14O2	000104-50-7	72
2		2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	64
3		2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	64
4		2(3H)-Furanone, 5-heptyldihydro-	184	C11H20O2	000104-67-6	56
5		2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	53



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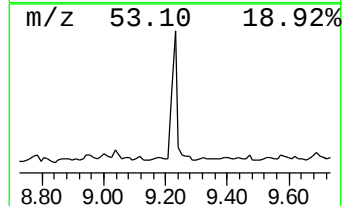
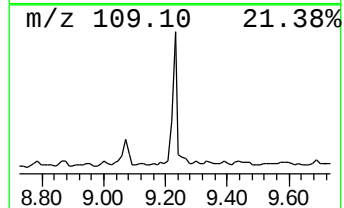
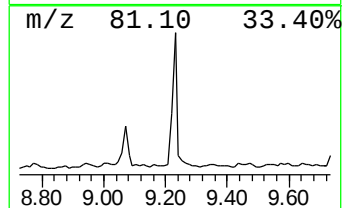
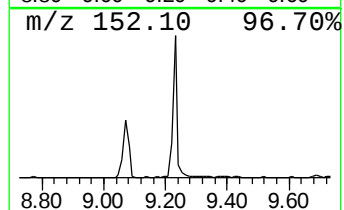
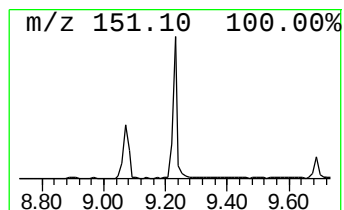
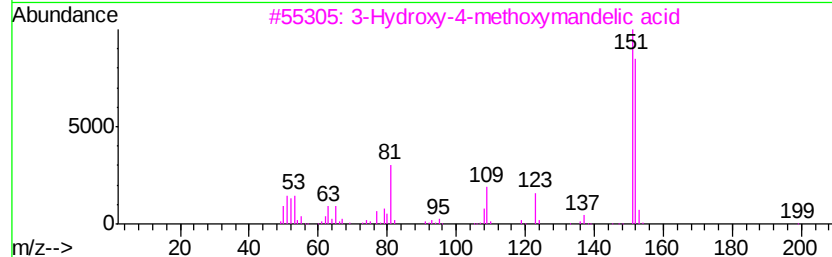
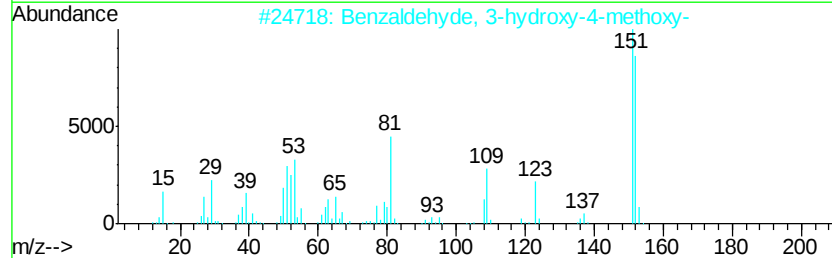
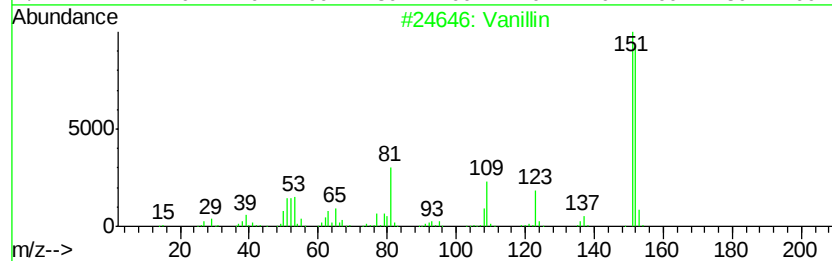
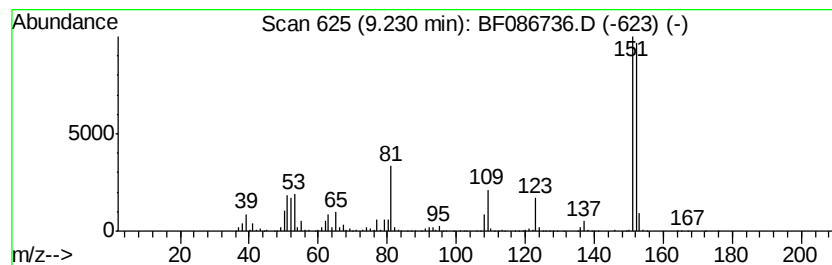
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Vanillin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	24.96 ng	1066860	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vanillin	152	C8H8O3	000121-33-5	97
2		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
3		3-Hydroxy-4-methoxymandelic acid	198	C9H10O5	003695-24-7	91
4		4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	87
5		Vanillin lactoside	476	C20H28O13	1000129-94-7	72



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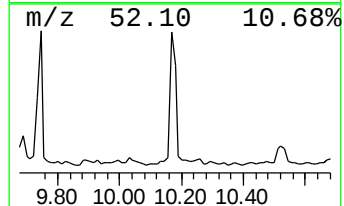
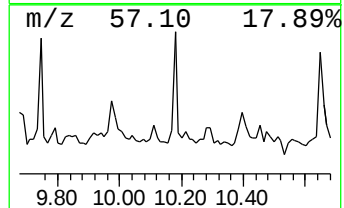
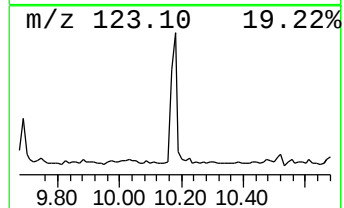
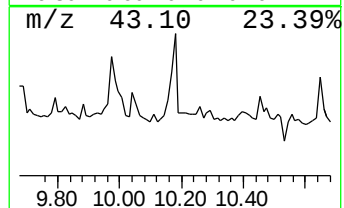
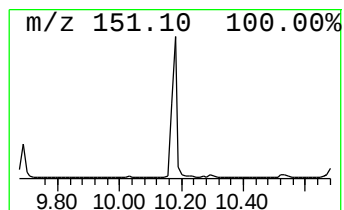
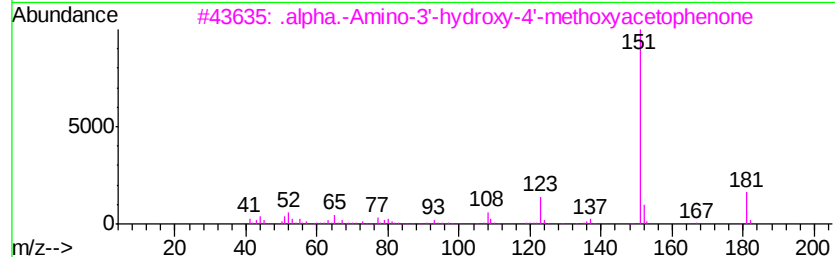
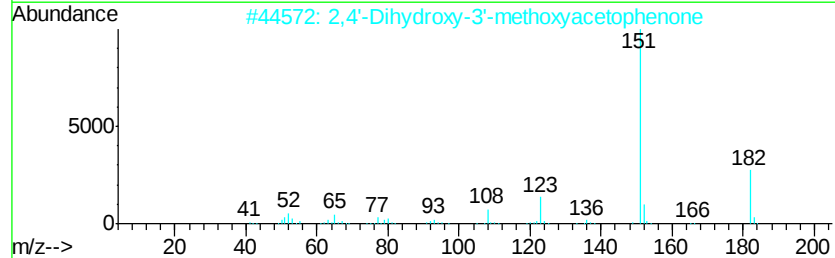
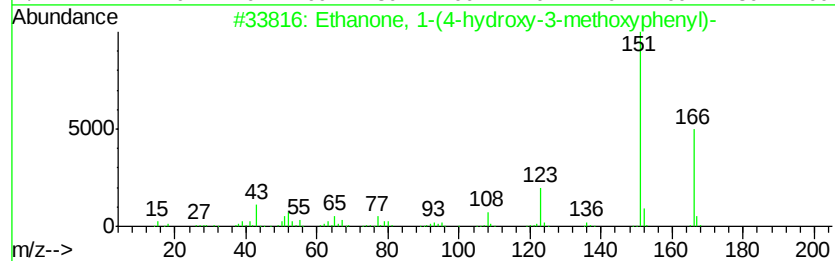
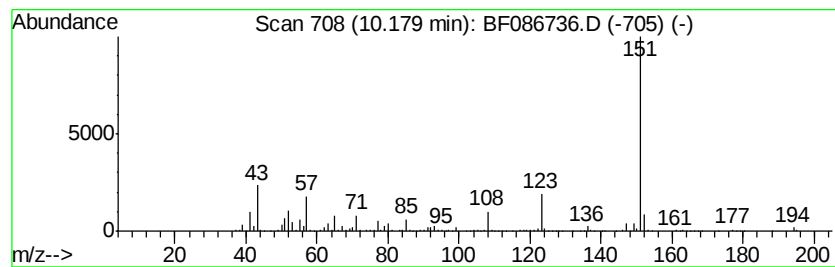
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Ethanone, 1-(4-hydroxy-3-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	12.83 ng	548197	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(4-hydroxy-3-methoxy...	166	C9H10O3	000498-02-2	64
2		2,4'-Dihydroxy-3'-methoxyacetoph...	182	C9H10O4	018256-48-9	59
3		.alpha.-Amino-3'-hydroxy-4'-meth...	181	C9H11NO3	090765-44-9	45
4		Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	42
5		Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
Operator : UM/SJ
Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP

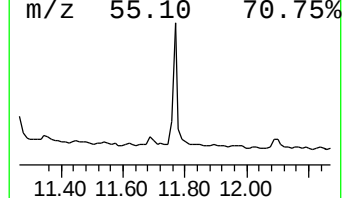
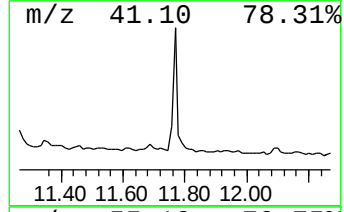
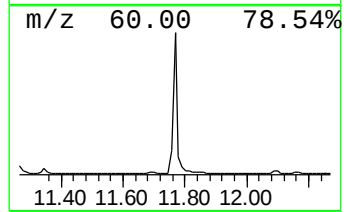
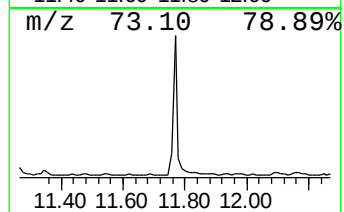
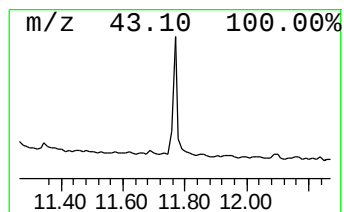
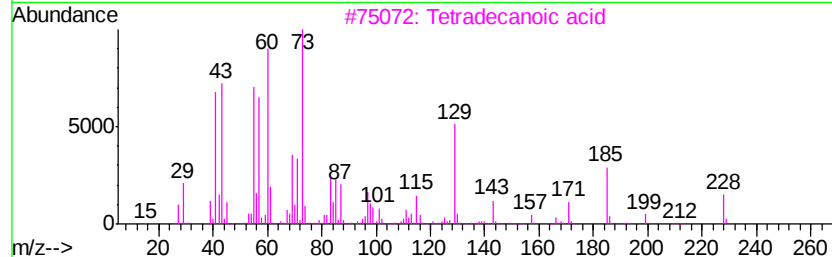
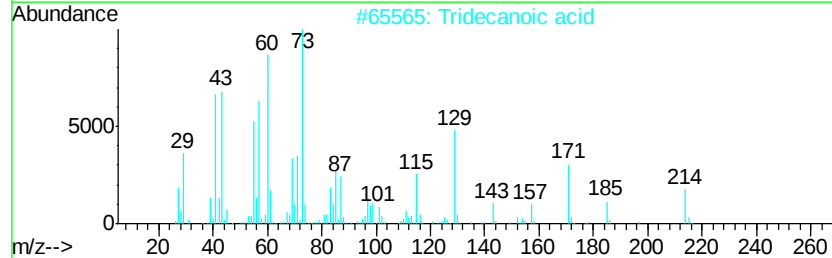
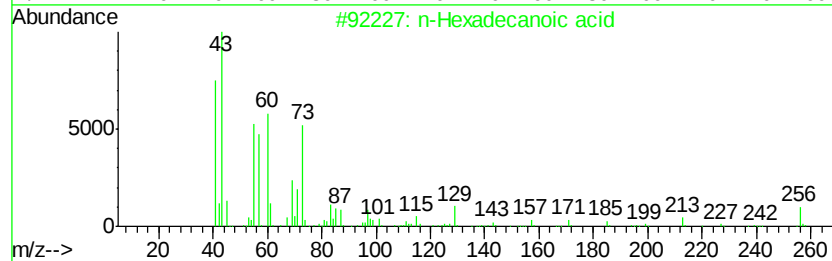
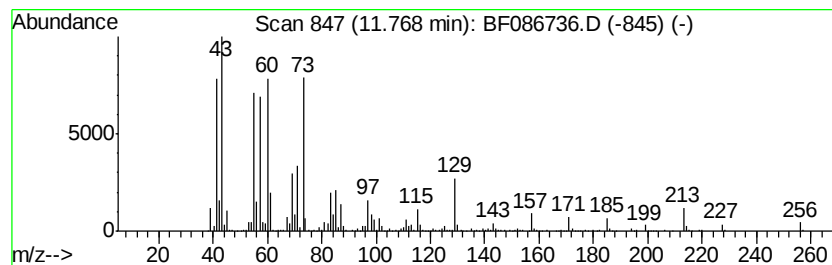
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	15.66 ng	603320	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086736.D
Acq On : 6 May 2016 21:01
Operator : UM/SJ
Sample : H2802-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

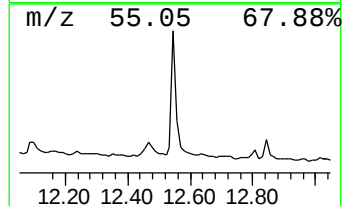
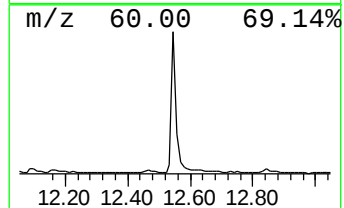
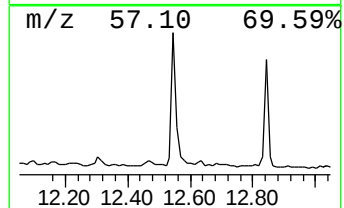
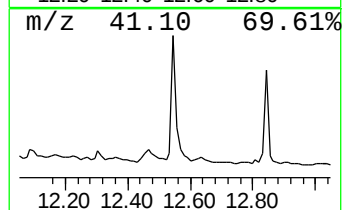
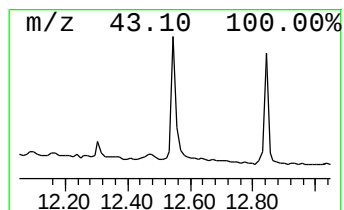
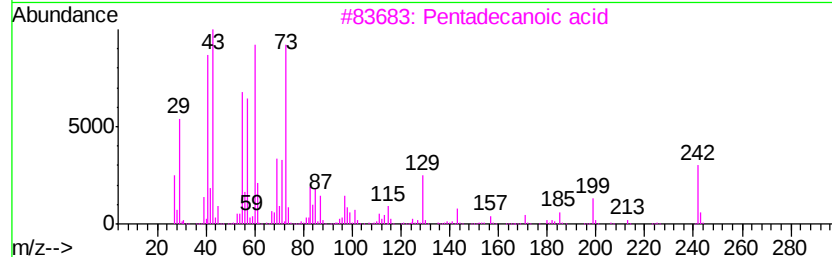
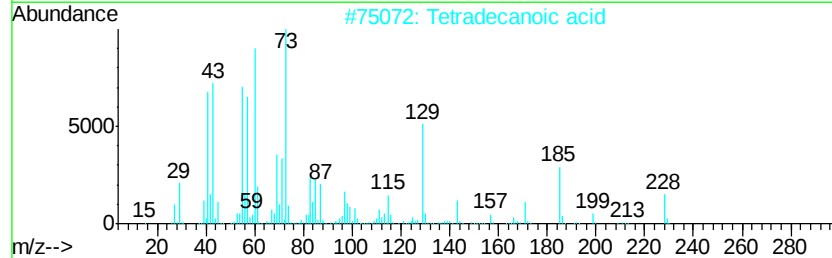
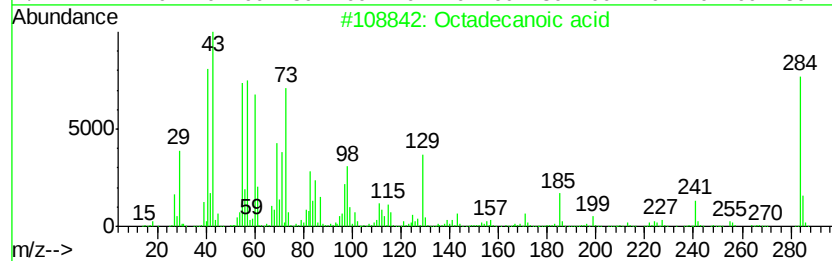
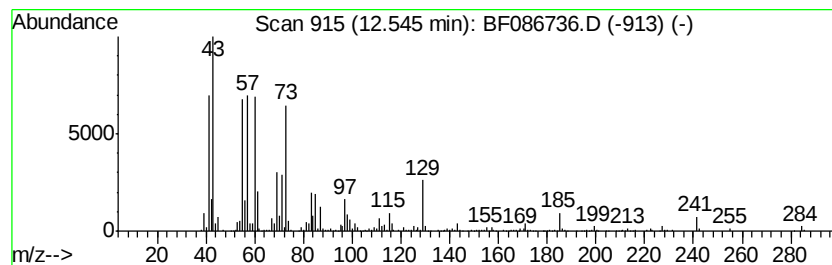
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	17.25 ng	538984	Chrysene-d12	13.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octadecanoic acid	284 C18H36O2	000057-11-4 94
2		Tetradecanoic acid	228 C14H28O2	000544-63-8 94
3		Pentadecanoic acid	242 C15H30O2	001002-84-2 86
4		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 64
5		n-Decanoic acid	172 C10H20O2	000334-48-5 52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
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 Acq On : 6 May 2016 21:01
 Operator : UM/SJ
 Sample : H2802-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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
Furfural	4.75	21.6	ng	612680	1	6.70	1132610	40.0
2-Heptanone	5.49	13.7	ng	388338	1	6.70	1132610	40.0
Ethanone, 1-(2-fu...	5.72	9.9	ng	280810	1	6.70	1132610	40.0
2,5-Hexanedione	5.89	11.5	ng	326002	1	6.70	1132610	40.0
unknown6.14	6.14	23.3	ng	659223	1	6.70	1132610	40.0
2(3H)-Furanone, d...	6.44	24.5	ng	692590	1	6.70	1132610	40.0
unknown6.49	6.49	166.6	ng	4718520	1	6.70	1132610	40.0
3,6-Heptanedione	6.76	13.9	ng	393921	1	6.70	1132610	40.0
unknown6.96	6.96	14.9	ng	421957	1	6.70	1132610	40.0
2-Cyclohexen-1-on...	7.06	11.8	ng	332941	1	6.70	1132610	40.0
unknown7.21	7.21	7.8	ng	221693	1	6.70	1132610	40.0
2(3H)-Furanone, d...	7.72	9.2	ng	346543	2	8.00	1499480	40.0
unknown8.40	8.40	26.0	ng	975396	2	8.00	1499480	40.0
n-Decanoic acid	8.94	12.1	ng	516948	3	9.74	1709760	40.0
2(3H)-Furanone, 5...	9.00	10.0	ng	427894	3	9.74	1709760	40.0
Vanillin	9.23	25.0	ng	1066860	3	9.74	1709760	40.0
Ethanone, 1-(4-hy...	10.18	12.8	ng	548197	3	9.74	1709760	40.0
n-Hexadecanoic acid	11.77	15.7	ng	603320	4	11.22	1541510	40.0
Octadecanoic acid	12.55	17.3	ng	538984	5	13.85	1249870	40.0