

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
 Data File : BF091515.D
 Acq On : 8 Dec 2016 21:07
 Operator : UM/SJ
 Sample : H5886-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 URSMW-07

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-BF112916.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	3.624	113	117	124	rVB	36531	65931	1.80%	0.186%
2	4.996	234	237	243	rBV	372758	481502	13.15%	1.359%
3	5.418	271	274	276	rBV	2486704	2414364	65.92%	6.815%
4	6.447	362	364	367	rVB	1435411	1498114	40.90%	4.229%
5	6.584	374	376	379	rBV	2989866	3081317	84.13%	8.698%
6	6.813	394	396	399	rBV	963476	1047738	28.61%	2.958%
7	6.893	400	403	405	rVV	692917	830642	22.68%	2.345%
8	6.973	407	410	412	rVB	2513389	2335336	63.76%	6.592%
9	7.224	430	432	434	rBV	23947	42336	1.16%	0.120%
10	7.339	438	442	443	rBV3	24253	37888	1.03%	0.107%
11	7.384	443	446	448	rBV	2227133	2251215	61.46%	6.355%
12	7.544	456	460	463	rVB3	21427	46563	1.27%	0.131%
13	7.773	476	480	483	rBV3	21213	43907	1.20%	0.124%
14	7.910	490	492	495	rBV3	27461	46138	1.26%	0.130%
15	8.013	498	501	506	rBV5	46958	94086	2.57%	0.266%
16	8.104	506	509	511	rBV	1779905	1563396	42.68%	4.413%
17	8.196	515	517	518	rBV	39993	40730	1.11%	0.115%
18	8.264	520	523	524	rBV3	27804	52678	1.44%	0.149%
19	8.299	524	526	529	rVB4	26502	60605	1.65%	0.171%
20	8.367	531	532	536	rVB2	30361	47727	1.30%	0.135%
21	8.436	536	538	540	rBV2	65866	86660	2.37%	0.245%
22	8.493	540	543	546	rBV4	45312	117908	3.22%	0.333%
23	8.550	546	548	549	rBV2	43264	64238	1.75%	0.181%
24	8.585	549	551	554	rVB2	102994	126966	3.47%	0.358%
25	8.642	554	556	557	rBV	57883	81768	2.23%	0.231%
26	8.665	557	558	562	rVB2	32491	76487	2.09%	0.216%
27	8.745	562	565	567	rBV4	53336	110985	3.03%	0.313%
28	8.790	567	569	571	rBV2	58182	106149	2.90%	0.300%
29	8.836	571	573	574	rBV	30427	39627	1.08%	0.112%
30	8.859	574	575	576	rBV	47931	56681	1.55%	0.160%
31	8.939	580	582	583	rBV2	38084	44389	1.21%	0.125%
32	8.973	583	585	587	rBV	120862	155144	4.24%	0.438%
33	9.019	587	589	590	rBV2	34553	43843	1.20%	0.124%
34	9.065	590	593	595	rBV4	60454	119918	3.27%	0.339%

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35	9.110	595	597	600	rBV3	85389	214470	5.86%	0.605%
36	9.179	600	603	605	rBV	3337813	3662672	100.00%	10.339%
37	9.247	607	609	610	rBV2	37019	53529	1.46%	0.151%
38	9.305	611	614	616	rVB4	65408	105944	2.89%	0.299%
39	9.362	617	619	621	rBV3	120139	154185	4.21%	0.435%
40	9.442	624	626	629	rBV3	151703	300084	8.19%	0.847%
41	9.510	629	632	634	rBV2	129509	214561	5.86%	0.606%
42	9.579	634	638	641	rVB5	103089	325819	8.90%	0.920%
43	9.705	645	649	650	rBV4	93174	269353	7.35%	0.760%
44	9.807	654	658	660	rBV5	88004	296687	8.10%	0.837%
45	9.853	660	662	664	rVV	1661445	1451511	39.63%	4.097%
46	10.139	685	687	688	rBV2	60433	73982	2.02%	0.209%
47	10.173	688	690	691	rBV2	62090	62322	1.70%	0.176%
48	10.436	711	713	714	rBV	134068	203726	5.56%	0.575%
49	10.642	728	731	733	rVB	2352918	2501589	68.30%	7.061%
50	10.688	733	735	736	rBV	97951	100455	2.74%	0.284%
51	10.768	740	742	745	rBV3	115628	186912	5.10%	0.528%
52	11.339	790	792	794	rBV	1767343	1604304	43.80%	4.529%
53	11.888	838	840	844	rVB	355792	350006	9.56%	0.988%
54	12.665	906	908	910	rBV2	200566	234883	6.41%	0.663%
55	12.928	928	931	933	rBV	3482398	3507582	95.77%	9.901%
56	13.968	1019	1022	1024	rBV	1206060	1069279	29.19%	3.018%
57	14.814	1095	1096	1101	rVB	52454	83679	2.28%	0.236%
58	15.385	1143	1146	1149	rBV	784514	966378	26.38%	2.728%
59	16.288	1222	1225	1234	rVB5	24504	80729	2.20%	0.228%
60	16.962	1280	1284	1289	rVB4	15099	38652	1.06%	0.109%

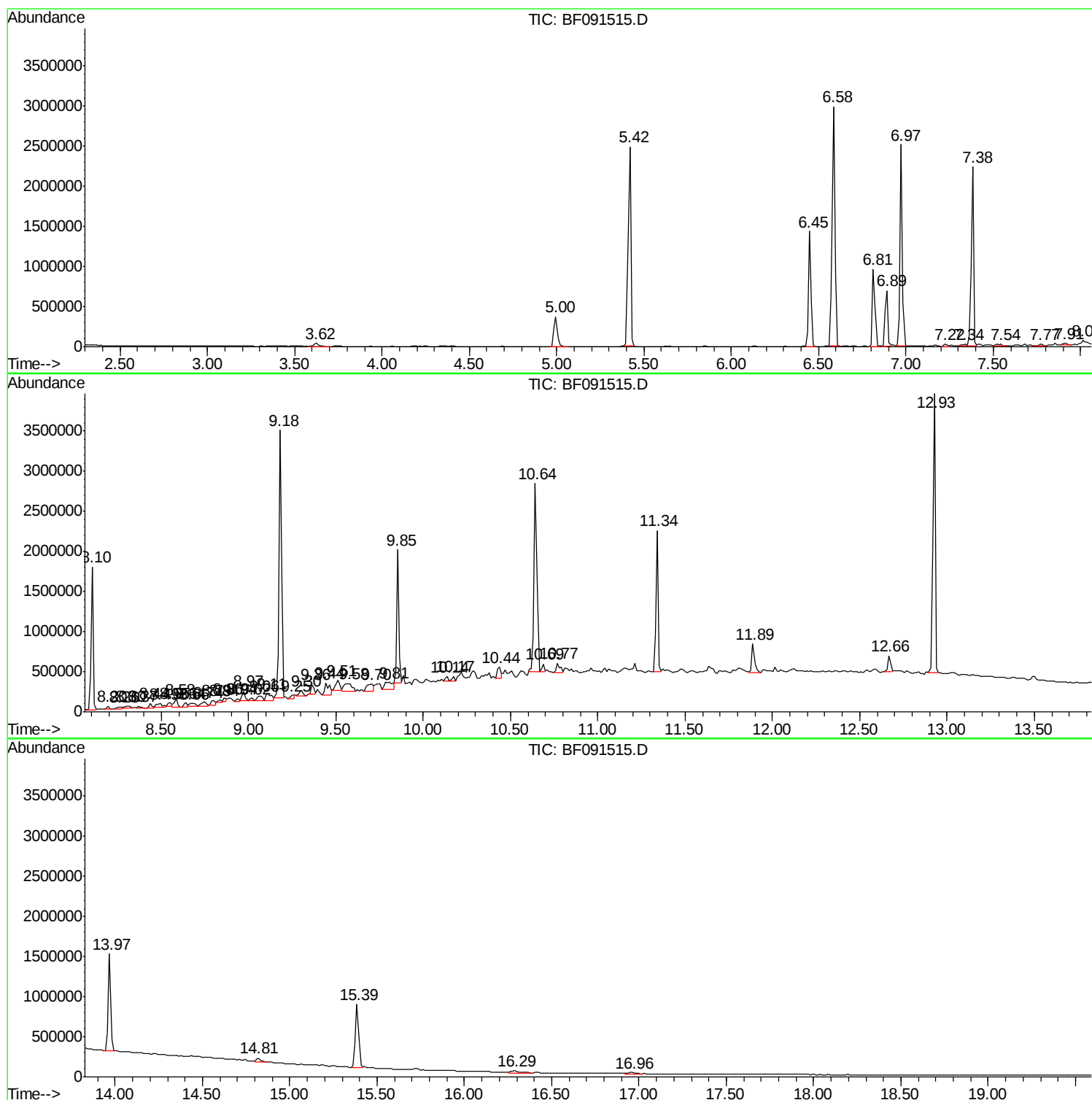
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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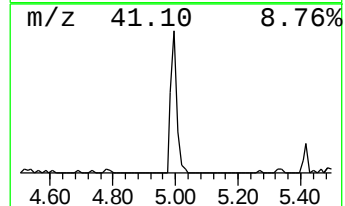
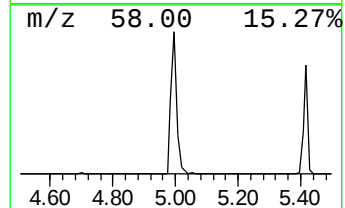
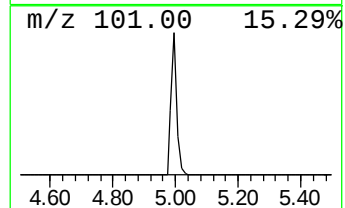
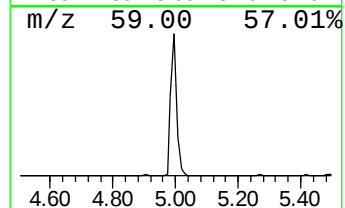
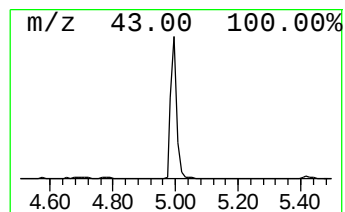
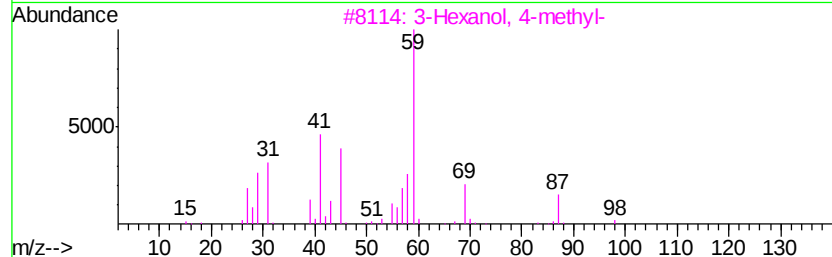
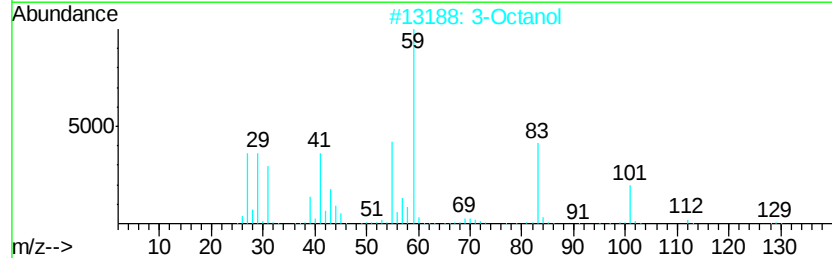
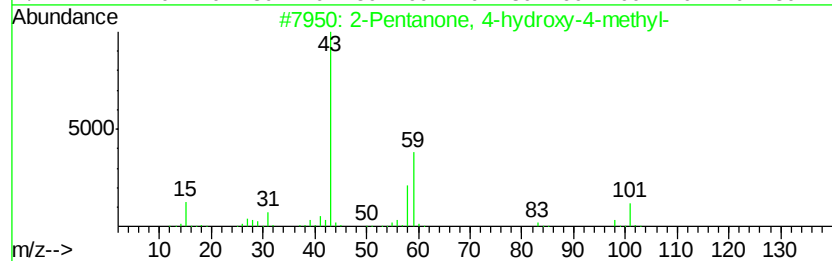
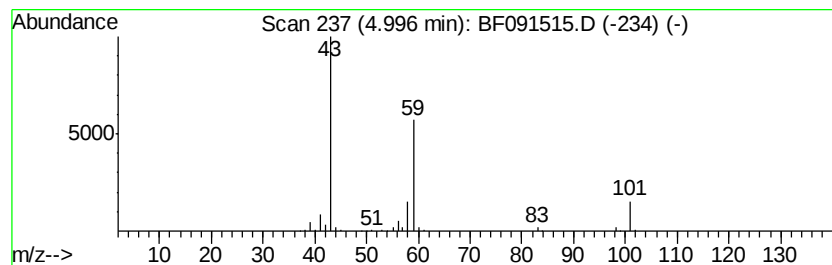
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	9.19 ng	481502	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	3-Octanol	130	C8H18O	000589-98-0	33	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9	



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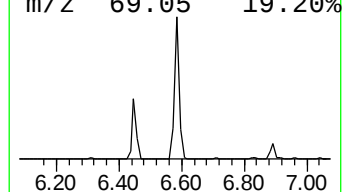
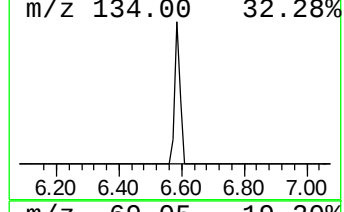
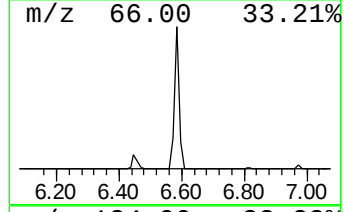
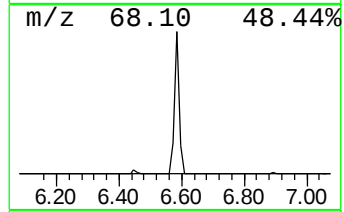
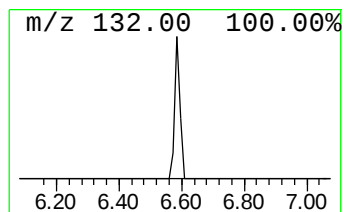
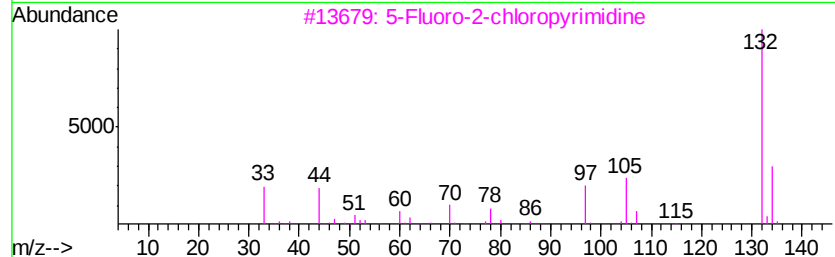
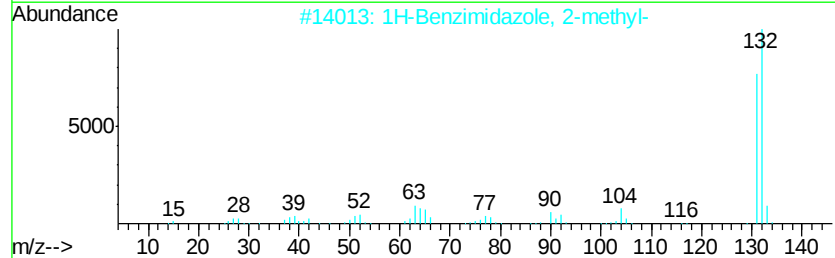
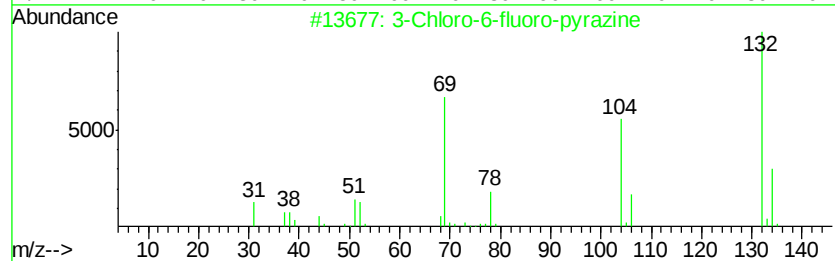
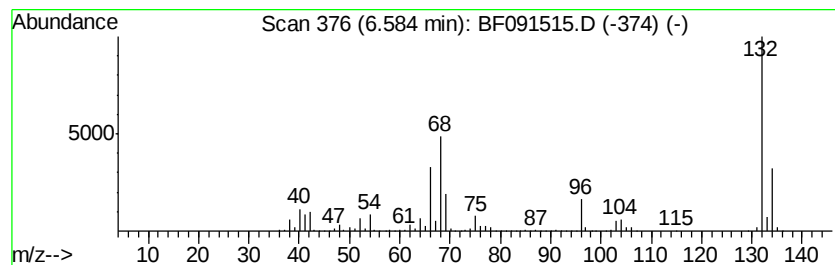
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	58.82 ng	3081320	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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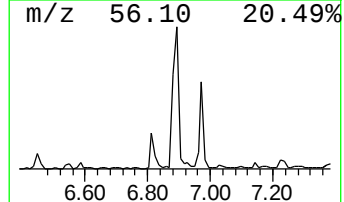
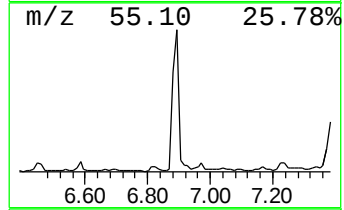
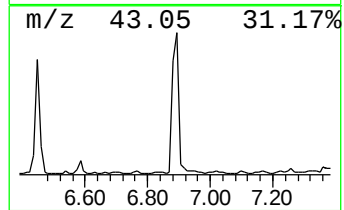
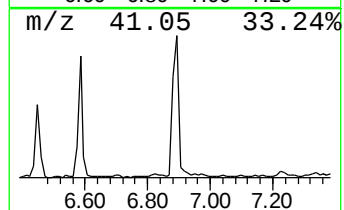
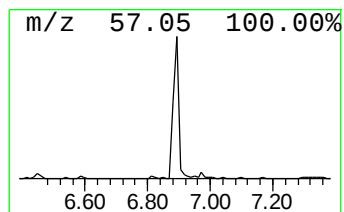
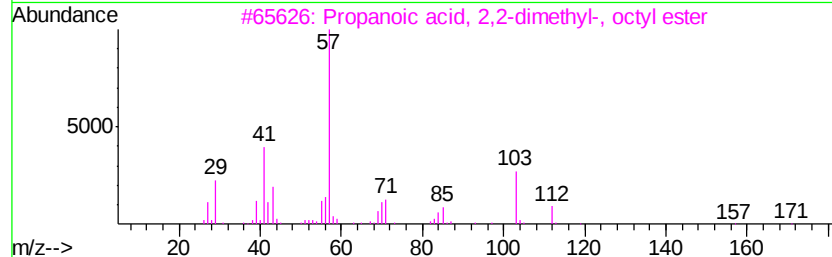
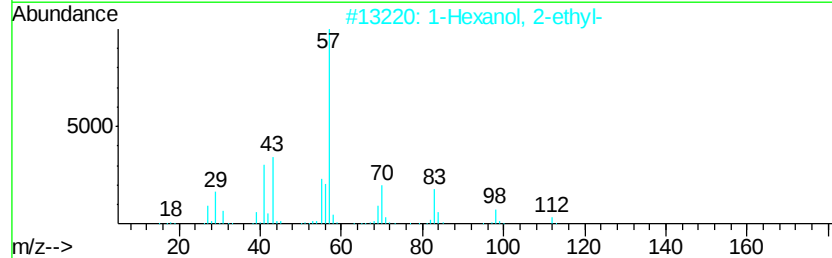
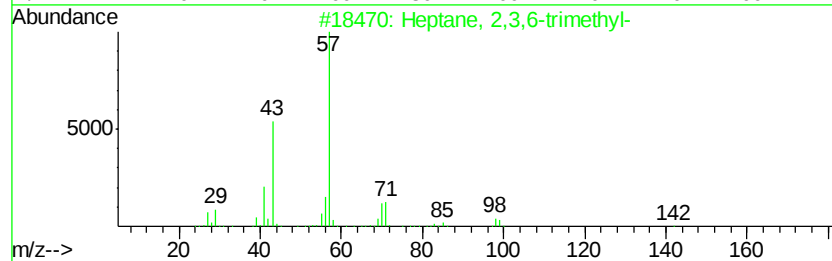
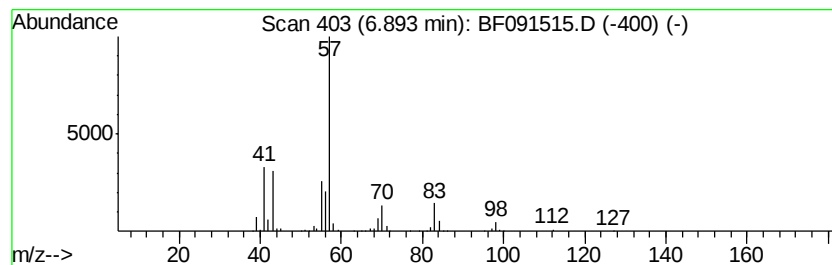
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 Heptane, 2,3,6-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	15.86 ng	830642	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3		Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	64
4		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
5		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50



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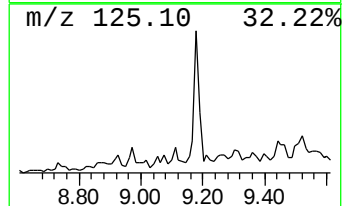
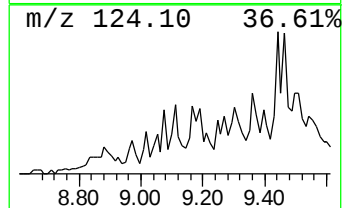
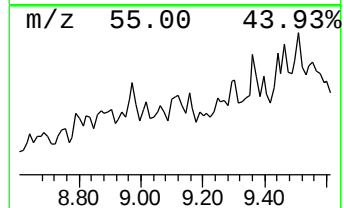
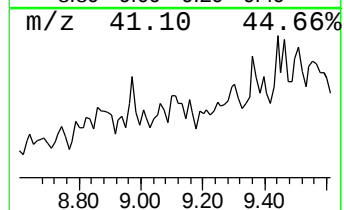
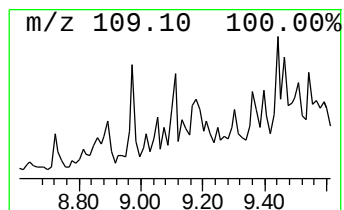
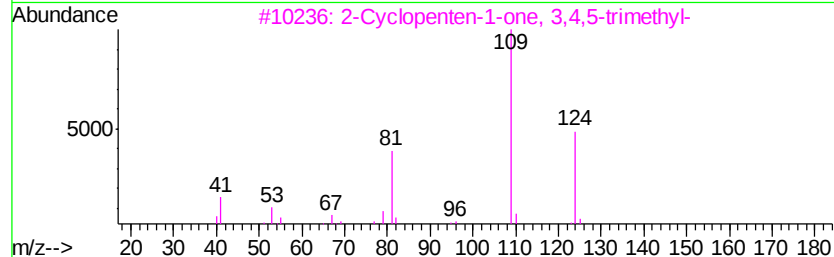
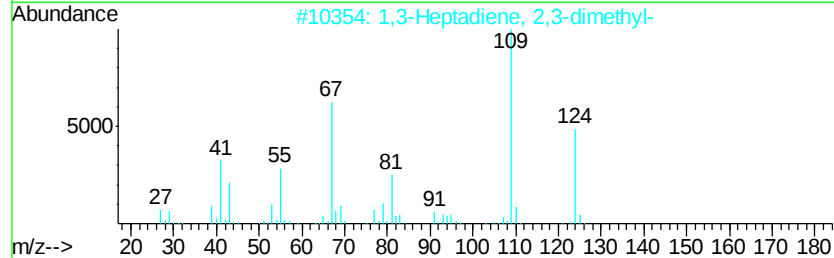
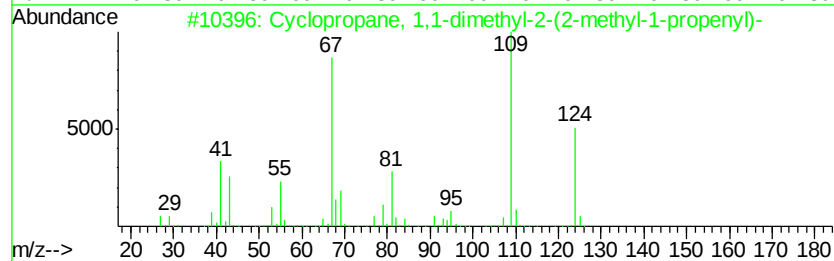
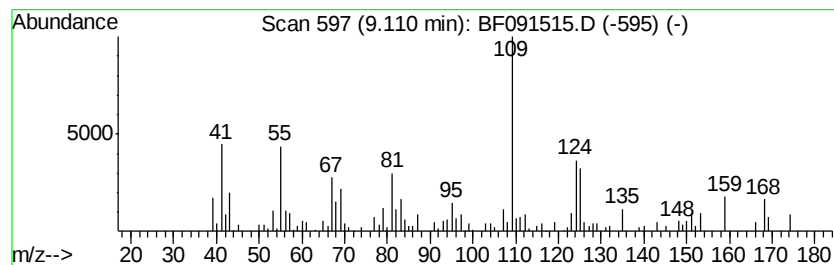
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Cyclopropane, 1,1-dimethyl-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.11	2.96 ng	214470	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	033422-32-1	50
2		1,3-Heptadiene, 2,3-dimethyl-	124	C9H16	074779-65-0	46
3		2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	43
4		2,4-Heptadiene, 2,6-dimethyl-	124	C9H16	004634-87-1	43
5		2-Cyclopenten-1-one, 3,5,5-trime...	124	C8H12O	024156-95-4	43



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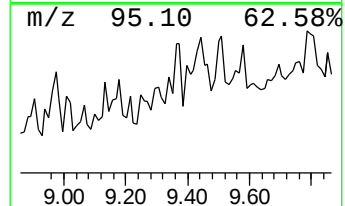
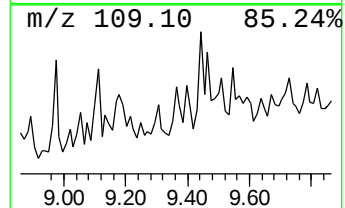
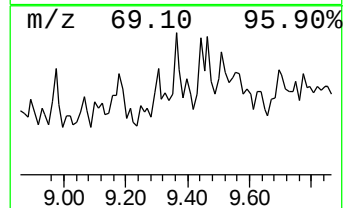
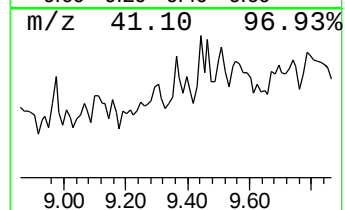
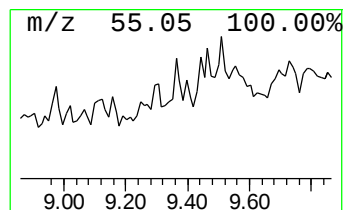
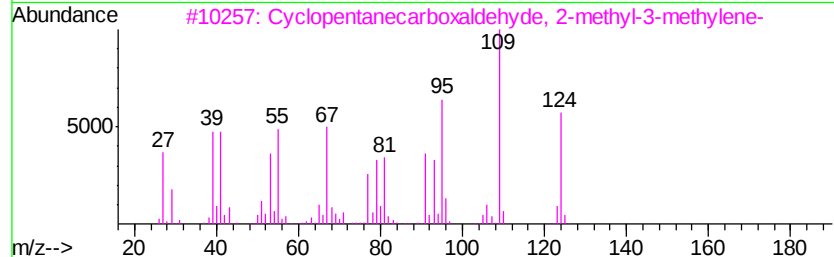
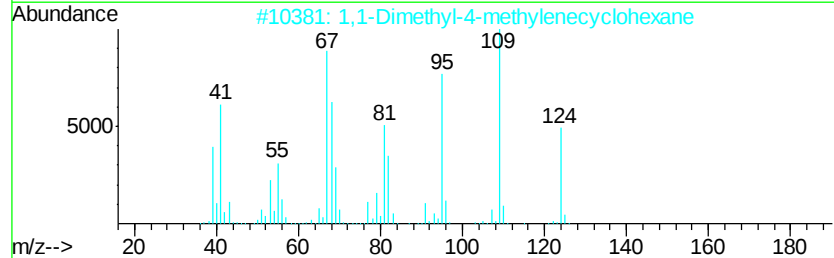
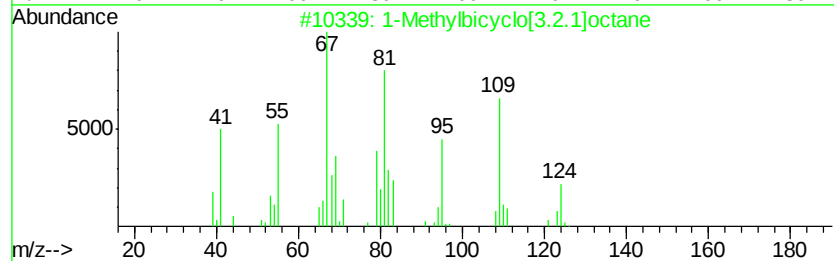
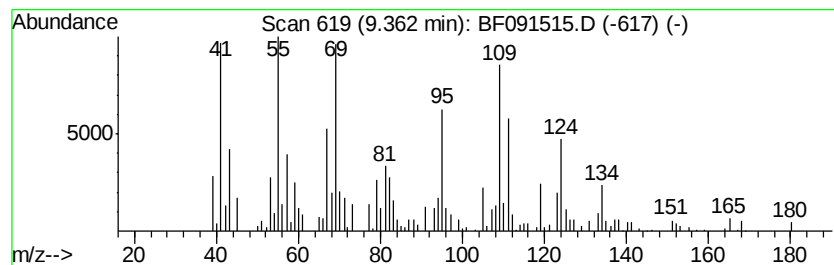
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Methylbicyclo[3.2.1]octane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	2.12 ng	154185	Acenaphthene-d10	9.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methylbicyclo[3.2.1]octane	124	C9H16	119972-41-7	50
2			1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	50
3			Cyclopentanecarboxaldehyde, 2-me...	124	C8H12O	1000154-24-0	43
4			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	30
5			9-Oxabicyclo[6.1.0]nonane, 1-met...	140	C9H16O	052954-47-9	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
Data File : BF091515.D
Acq On : 8 Dec 2016 21:07
Operator : UM/SJ
Sample : H5886-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

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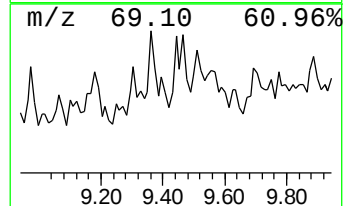
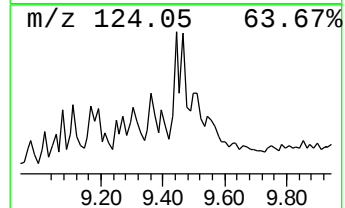
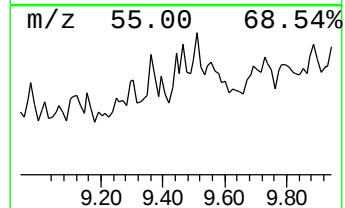
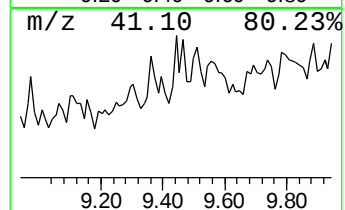
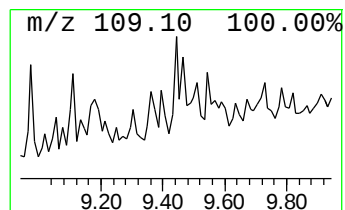
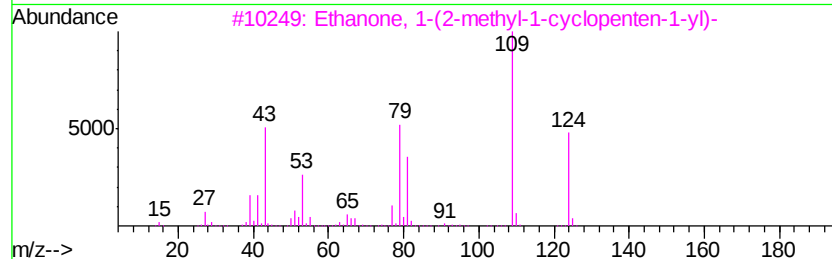
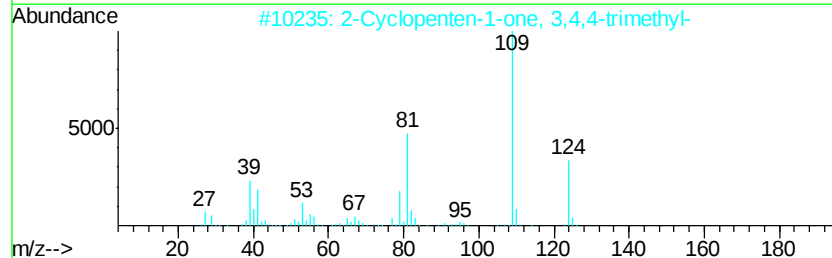
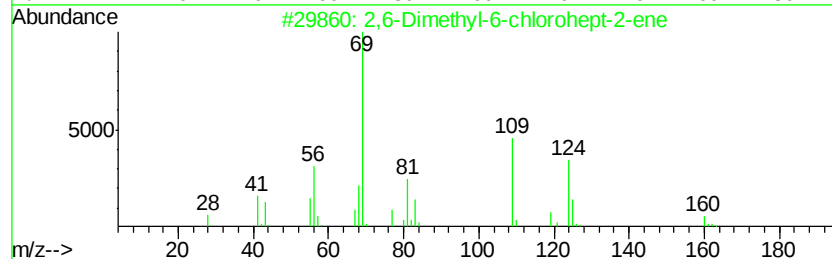
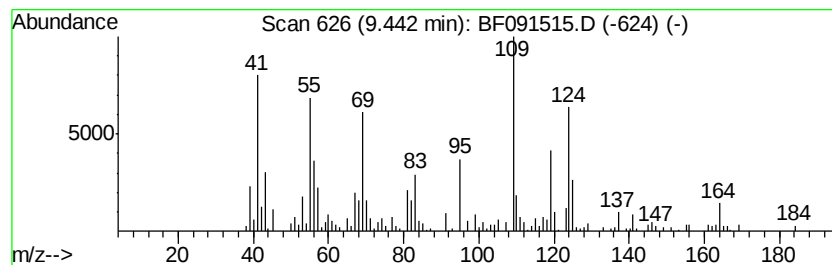
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.44 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	4.13 ng	300084	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6-Dimethyl-6-chlorohept-2-ene	160	C9H17Cl	006076-48-8	47
2		2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	43
3		Ethanone, 1-(2-methyl-1-cyclopen...	124	C8H12O	003168-90-9	38
4		Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	033422-32-1	38
5		p-Fluoroethylbenzene	124	C8H9F	000459-47-2	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
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Acq On : 8 Dec 2016 21:07
Operator : UM/SJ
Sample : H5886-03
Misc :
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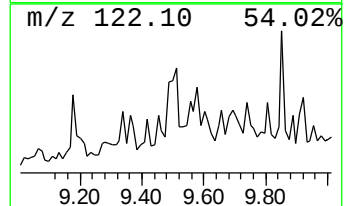
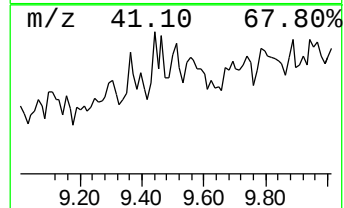
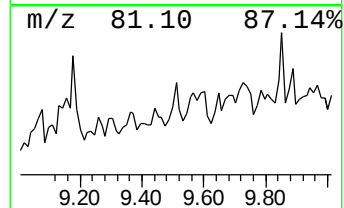
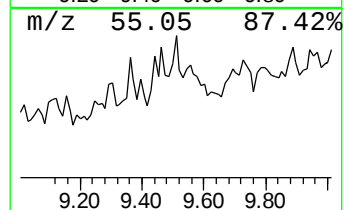
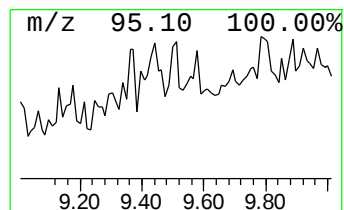
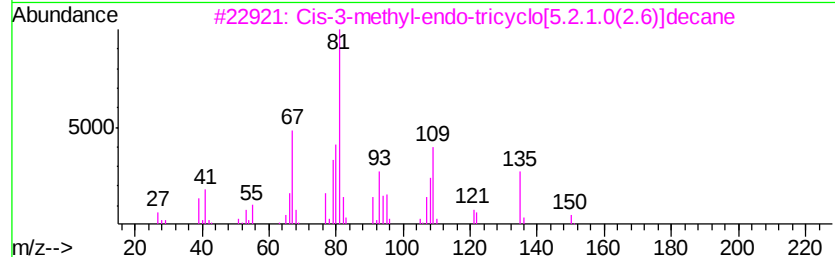
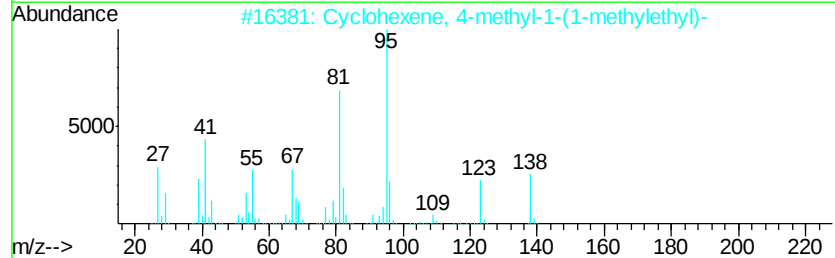
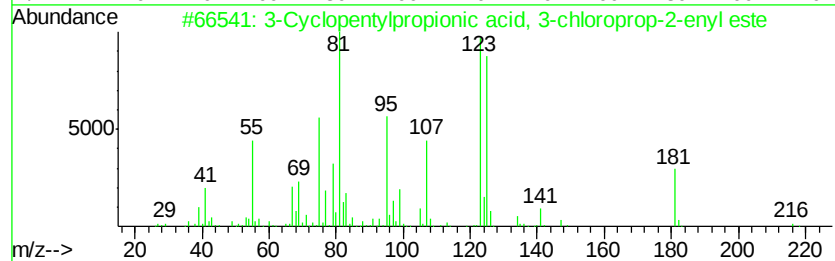
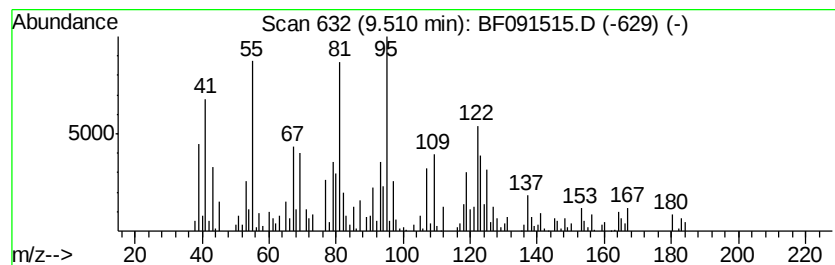
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.51 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	2.96 ng	214561	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Cyclopentylpropionic acid, 3-c...	216	C11H17ClO2	1000292-47-2	35
2		Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	35
3		Cis-3-methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	30
4		Bicyclo[3.3.1]nonan-3-ol, exo-	140	C9H16O	010036-08-5	22
5		Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
Data File : BF091515.D
Acq On : 8 Dec 2016 21:07
Operator : UM/SJ
Sample : H5886-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

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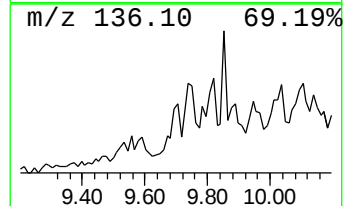
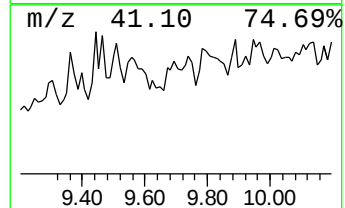
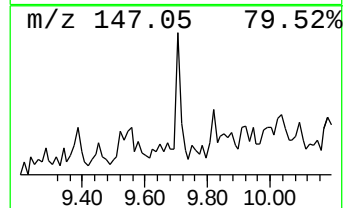
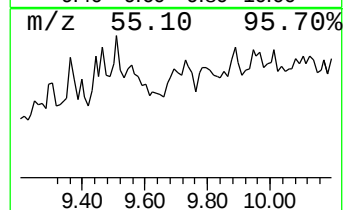
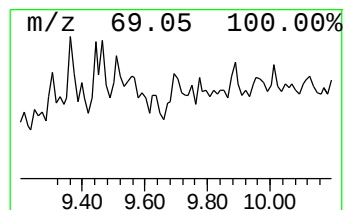
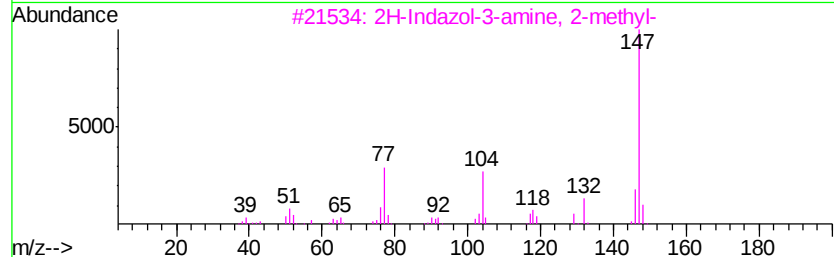
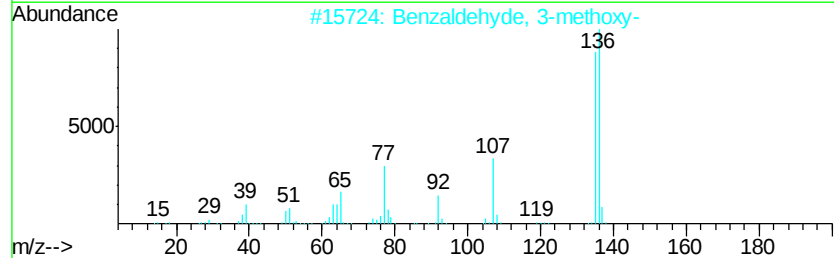
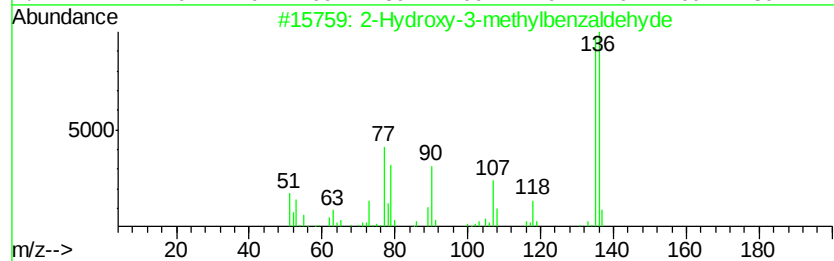
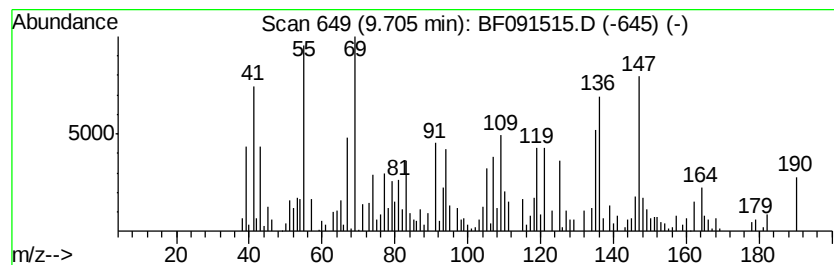
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.70 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	3.71 ng	269353	Acenaphthene-d10	9.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroxy-3-methylbenzaldehyde	136	C8H8O2	000824-42-0	25
2			Benzaldehyde, 3-methoxy-	136	C8H8O2	000591-31-1	25
3			2H-Indazol-3-amine, 2-methyl-	147	C8H9N3	097990-19-7	25
4			2-Ethyl-5-n-butylphenol	178	C12H18O	072386-21-1	14
5			Benzene, 1-(1,1-dimethylethyl)-3...	162	C12H18	000098-19-1	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
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Operator : UM/SJ
Sample : H5886-03
Misc :
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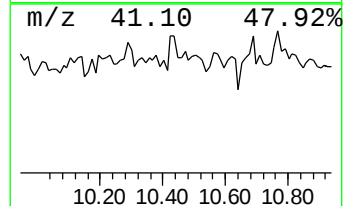
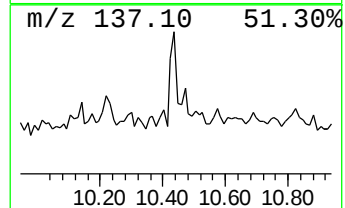
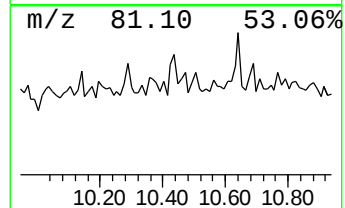
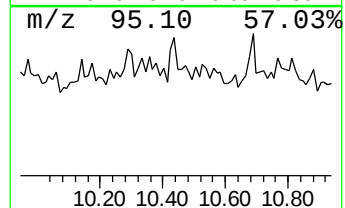
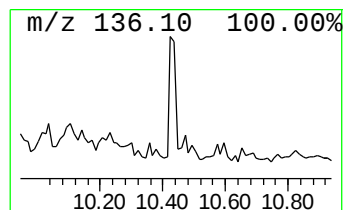
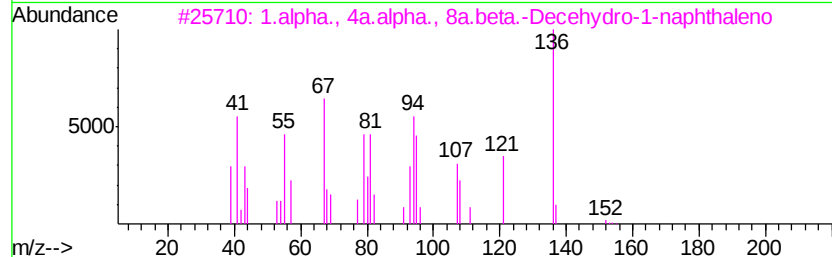
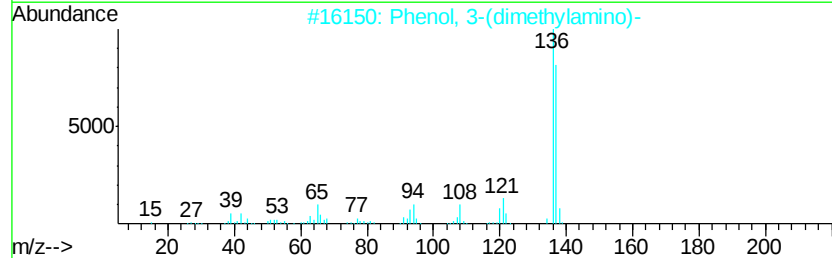
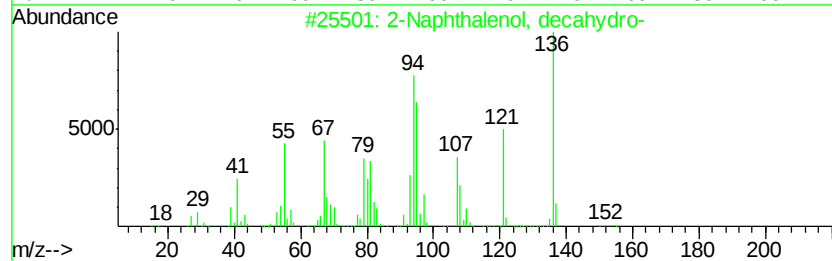
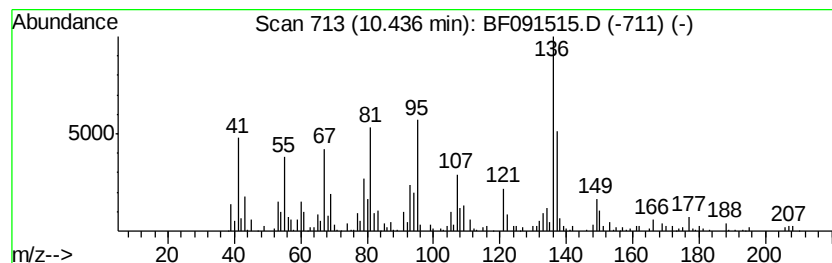
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Naphthalenol, decahydro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.81 ng	203726	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Naphthalenol, decahydro-	154 C10H18O	000825-51-4	58
2	Phenol, 3-(dimethylamino)-	137 C8H11NO	000099-07-0	55
3	1.alpha., 4a.alpha., 8a.beta.-De...	154 C10H18O	002529-03-5	47
4	2.alpha., 4a.beta., 8a.beta.-Dec...	154 C10H18O	001424-37-9	47
5	1,2,3,4,4a,5,6,8a-Octahydro-naph...	136 C10H16	031244-58-3	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
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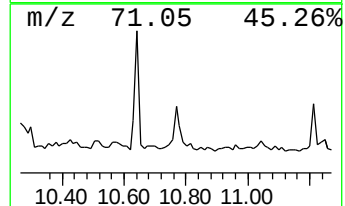
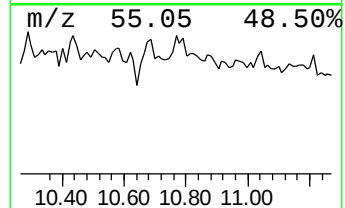
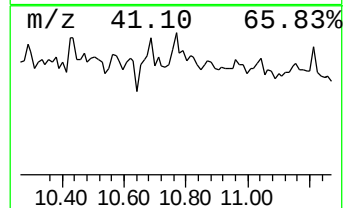
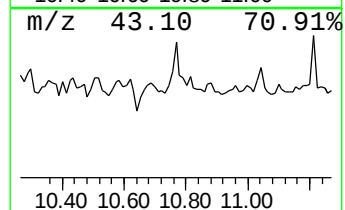
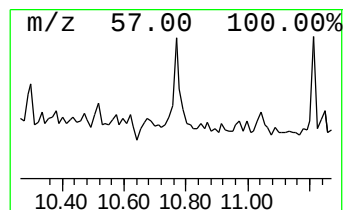
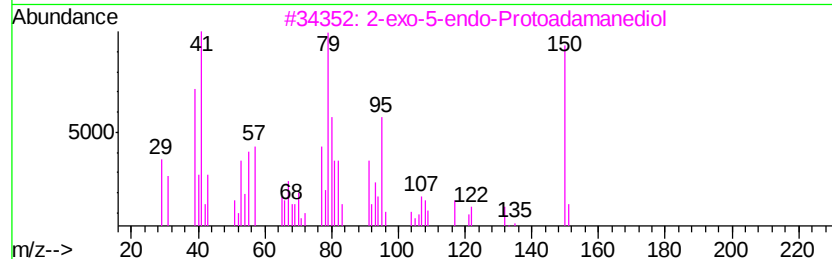
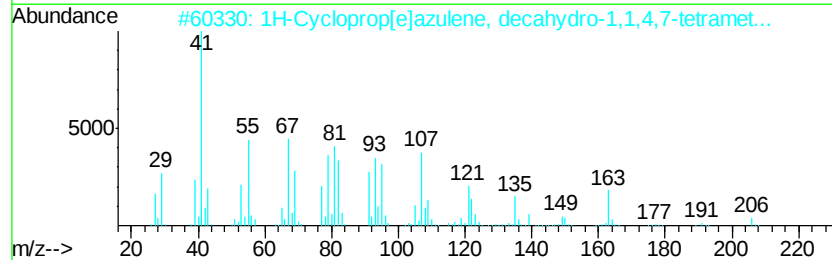
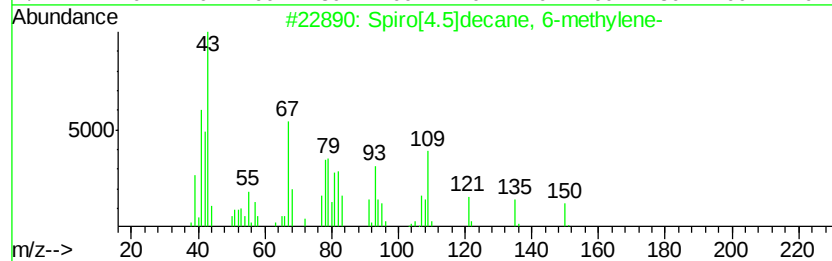
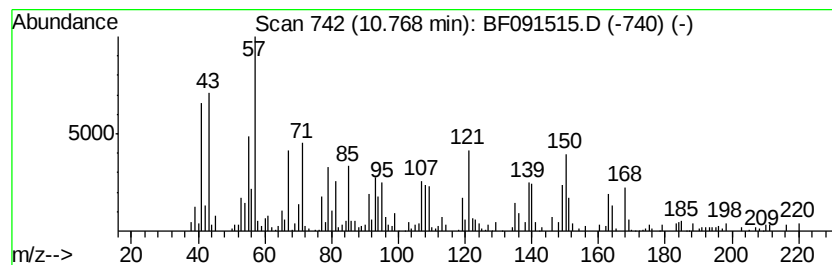
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.77 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.33 ng	186912	Phenanthrene-d10	11.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Spiro[4.5]decane, 6-methylene-	150 C11H18	019144-01-5 27
2		1H-Cycloprop[e]azulene, decahydr...	206 C15H26	028580-43-0 22
3		2-exo-5-endo-Protoadamanediol	168 C10H16O2	1000143-28-8 12
4		2,5-exo,exo-protoadamanediol	168 C10H16O2	1000143-28-7 12
5		7,11-Epoxy megastigma-5(6)-en-9-one	208 C13H20O2	064243-62-5 12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
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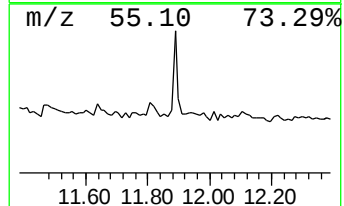
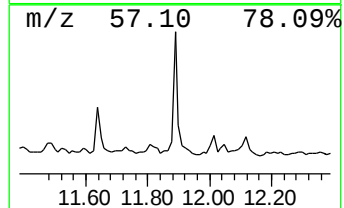
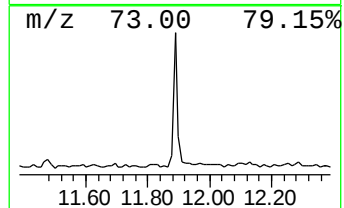
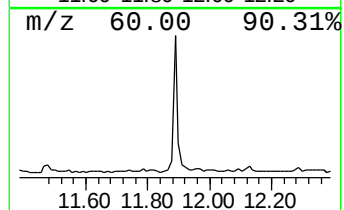
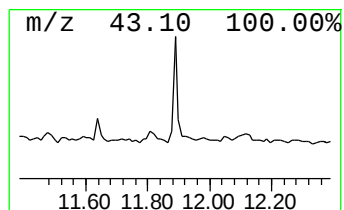
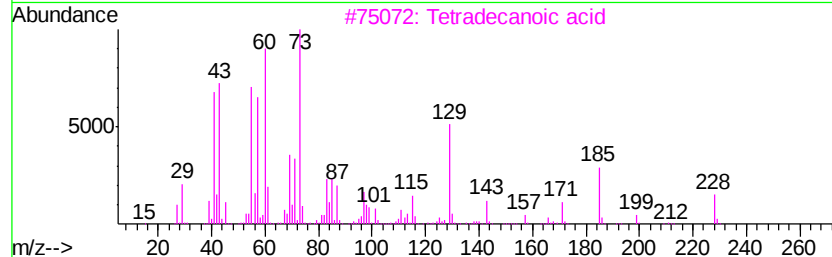
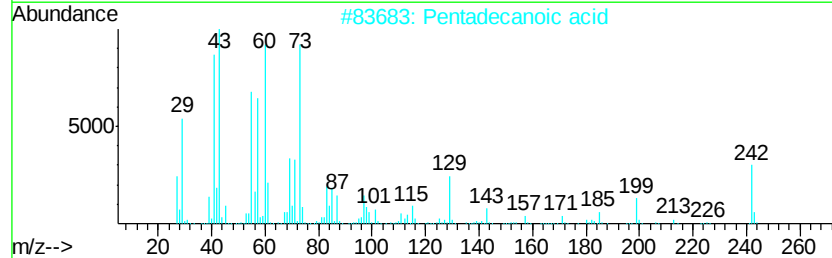
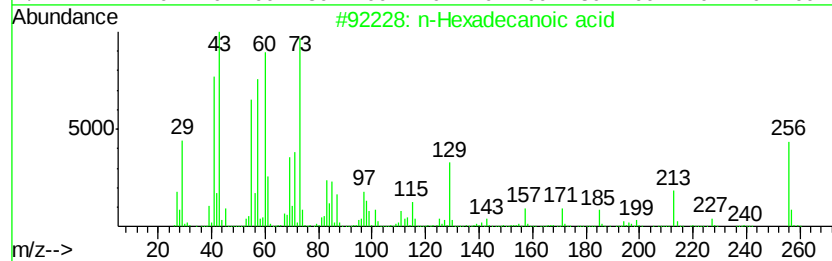
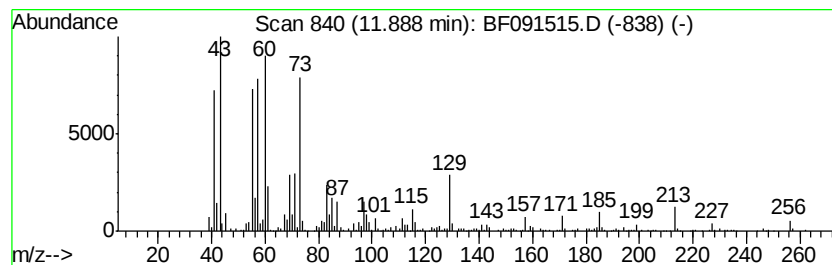
Instrument :
BNA_F
ClientSampleId :
URSMW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.89	4.36 ng	350006	Phenanthrene-d10		11.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
Data File : BF091515.D
Acq On : 8 Dec 2016 21:07
Operator : UM/SJ
Sample : H5886-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
URSMW-07

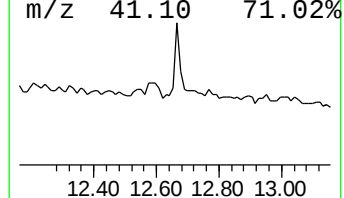
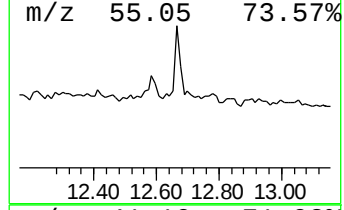
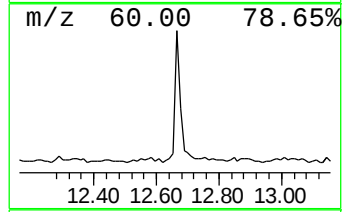
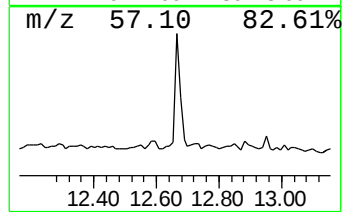
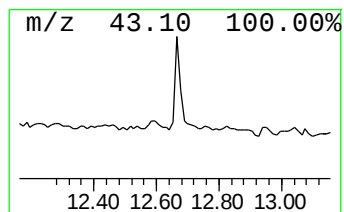
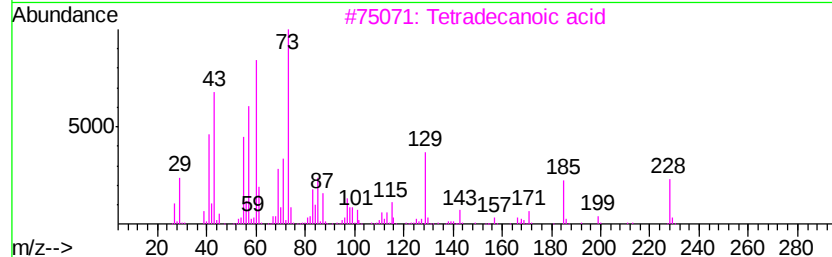
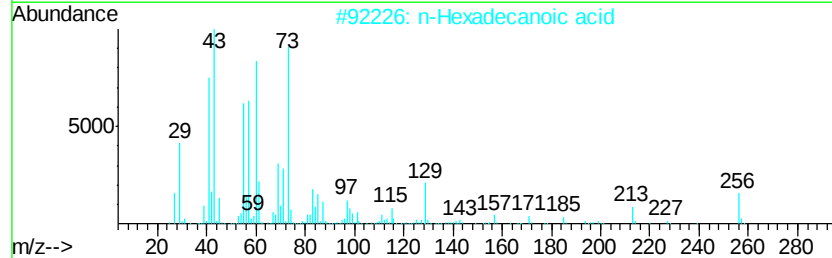
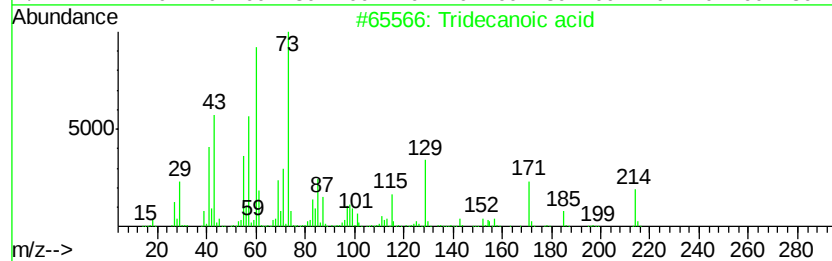
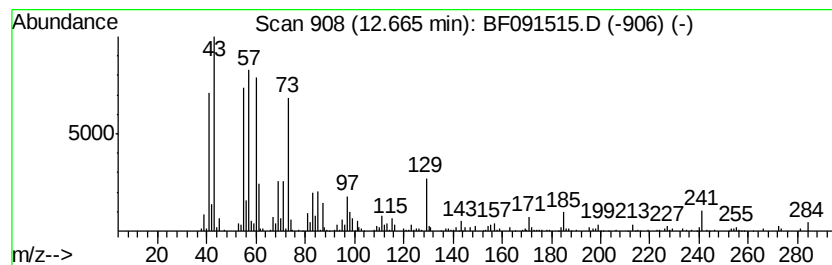
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	4.39 ng	234883	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	83
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
Data File : BF091515.D
Acq On : 8 Dec 2016 21:07
Operator : UM/SJ
Sample : H5886-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
URSMW-07

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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...	5.00	9.2 ng		481502	1	6.81	1047740	20.0
unknown6.58	6.58	58.8 ng		3081320	1	6.81	1047740	20.0
Heptane, 2,3,6-tr...	6.89	15.9 ng		830642	1	6.81	1047740	20.0
Cyclopropane, 1,1...	9.11	3.0 ng		214470	3	9.85	1451510	20.0
1-Methylbicyclo[3...	9.36	2.1 ng		154185	3	9.85	1451510	20.0
unknown9.44	9.44	4.1 ng		300084	3	9.85	1451510	20.0
unknown9.51	9.51	3.0 ng		214561	3	9.85	1451510	20.0
unknown9.70	9.70	3.7 ng		269353	3	9.85	1451510	20.0
2-Naphthalenol, d...	10.44	2.8 ng		203726	3	9.85	1451510	20.0
unknown10.77	10.77	2.3 ng		186912	4	11.34	1604300	20.0
n-Hexadecanoic acid	11.89	4.4 ng		350006	4	11.34	1604300	20.0
Tridecanoic acid	12.66	4.4 ng		234883	5	13.97	1069280	20.0