

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
 Data File : BF081659.D
 Acq On : 16 Sep 2015 21:04
 Operator : UM/IZ
 Sample : G3654-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP203(27-29)

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-BF090115.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	1.440	8	9	15	rBV	273692	707624	17.78%	3.062%
2	1.531	15	17	59	rVB	1153318	3980264	100.00%	17.222%
3	4.480	270	275	293	rBV	339447	1031097	25.91%	4.461%
4	5.349	347	351	373	rBV	954900	1802327	45.28%	7.798%
5	7.612	544	549	553	rBV	912448	1836018	46.13%	7.944%
6	7.703	553	557	560	rVB	1085239	1829072	45.95%	7.914%
7	8.183	596	599	608	rVB	210578	331177	8.32%	1.433%
8	8.515	624	628	631	rBV	780730	1327837	33.36%	5.745%
9	9.486	708	713	716	rBV	620909	1166802	29.31%	5.048%
10	11.086	849	853	854	rBV	240373	428031	10.75%	1.852%
11	11.132	854	857	861	rVB	334137	555946	13.97%	2.405%
12	12.778	998	1001	1007	rBB	75291	132031	3.32%	0.571%
13	12.995	1016	1020	1025	rBB	57667	99532	2.50%	0.431%
14	13.727	1079	1084	1087	rBV	960518	1919039	48.21%	8.303%
15	14.778	1173	1176	1181	rVB	178732	289903	7.28%	1.254%
16	15.212	1210	1214	1218	rBV	272955	456316	11.46%	1.974%
17	16.515	1326	1328	1333	rVB	22152	42170	1.06%	0.182%
18	17.121	1376	1381	1384	rBV	713727	1301871	32.71%	5.633%
19	18.721	1516	1521	1523	rBV	255713	481635	12.10%	2.084%
20	18.767	1523	1525	1528	rVV	95500	148504	3.73%	0.643%
21	19.681	1602	1605	1616	rBV2	40423	95924	2.41%	0.415%
22	20.470	1671	1674	1686	rVB	67918	137329	3.45%	0.594%
23	21.739	1781	1785	1790	rBV	56316	81927	2.06%	0.354%
24	21.876	1794	1797	1805	rBV2	25238	45941	1.15%	0.199%
25	22.082	1812	1815	1818	rBV	1297466	1867493	46.92%	8.080%
26	23.328	1921	1924	1925	rBV	146199	227985	5.73%	0.986%
27	23.350	1925	1926	1928	rVV	401225	419700	10.54%	1.816%
28	24.791	2050	2052	2055	rBV	303261	310931	7.81%	1.345%
29	25.225	2089	2090	2097	rVB2	27052	57738	1.45%	0.250%

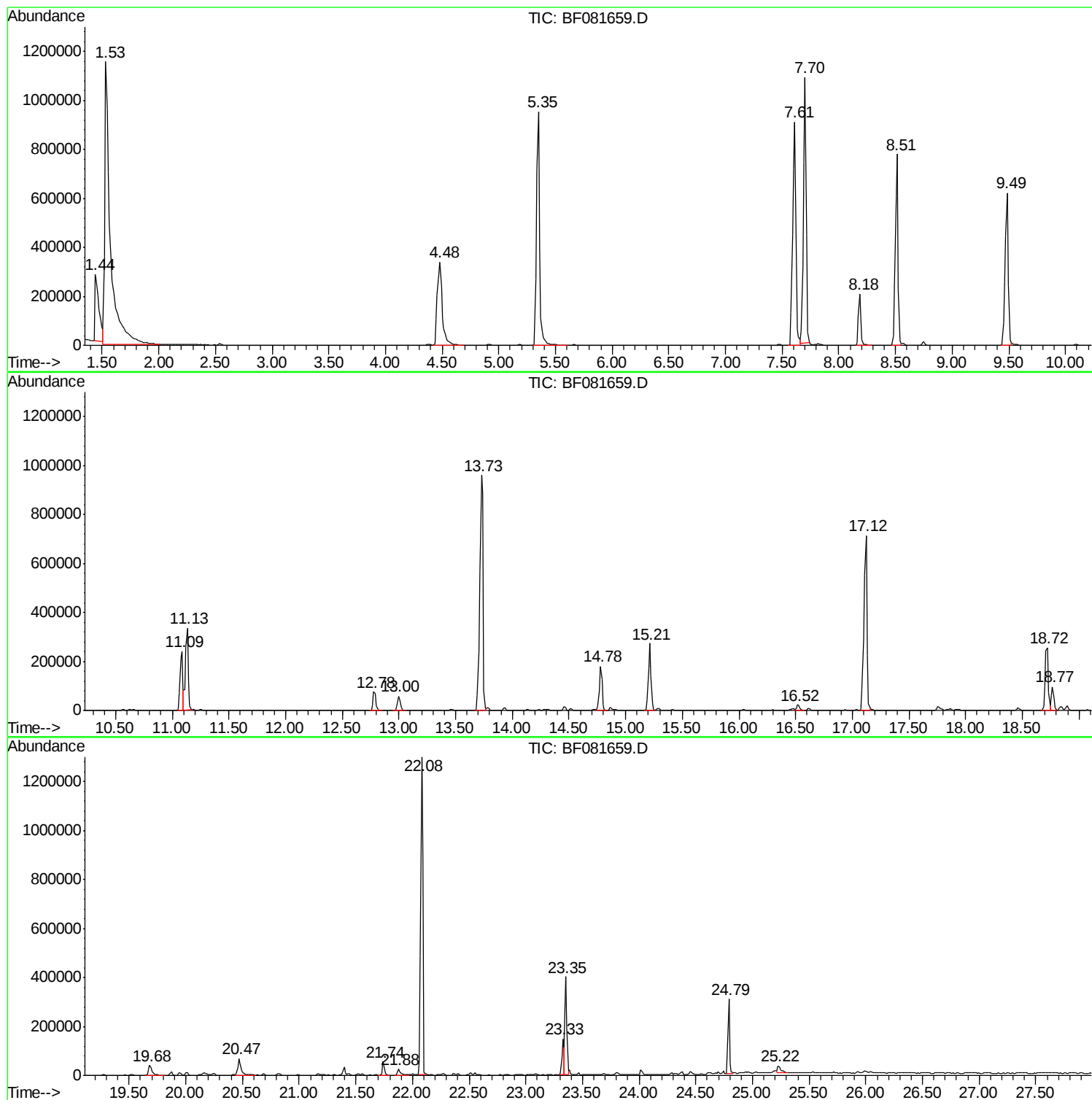
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MGP203(27-29)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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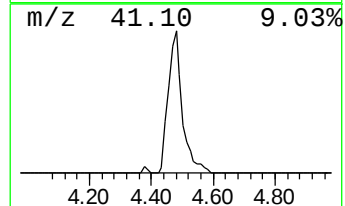
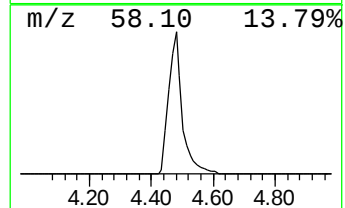
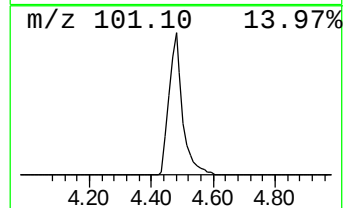
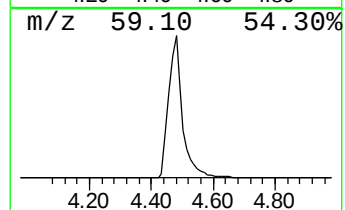
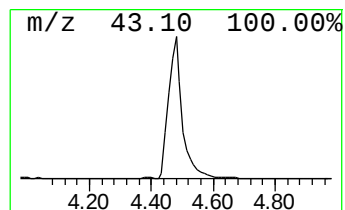
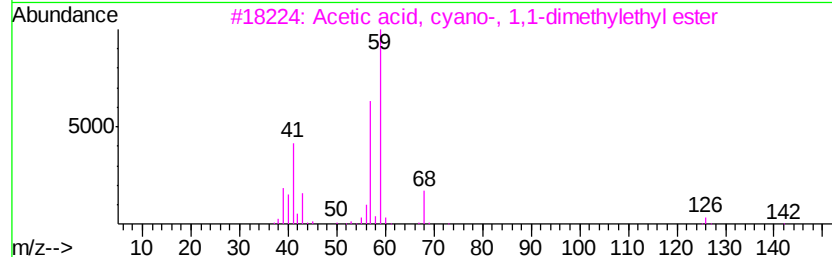
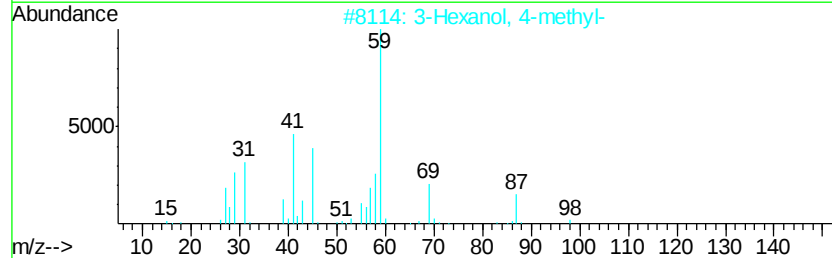
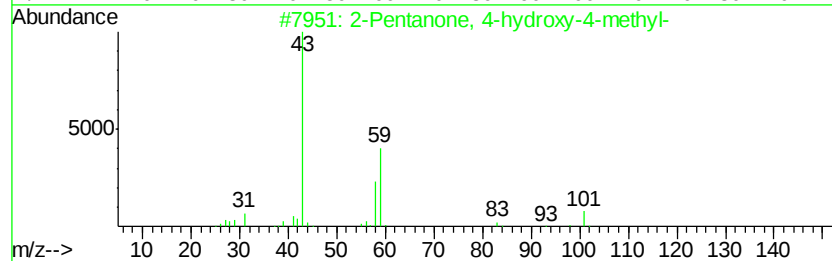
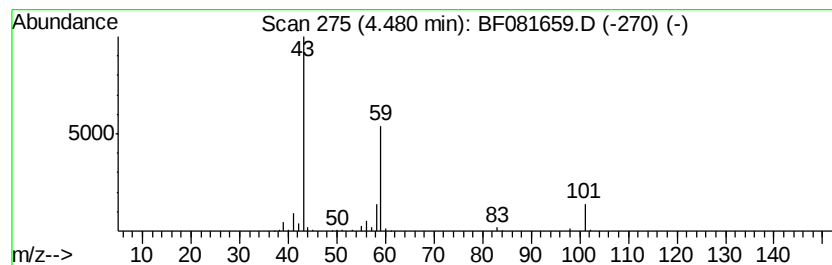
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	62.27 ng	1031100	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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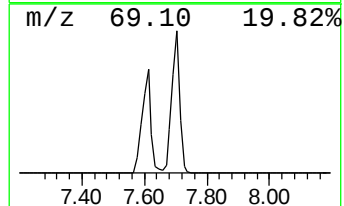
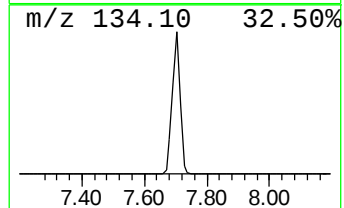
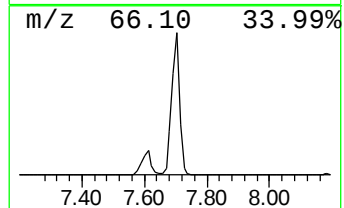
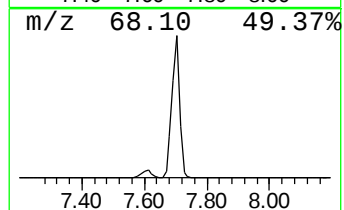
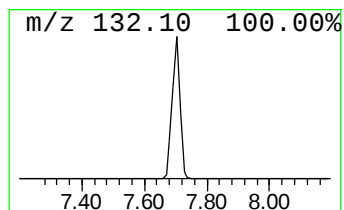
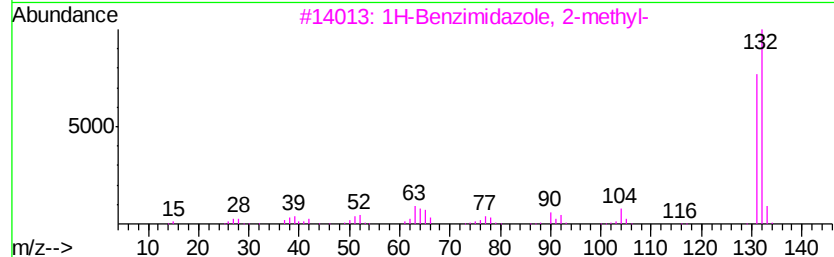
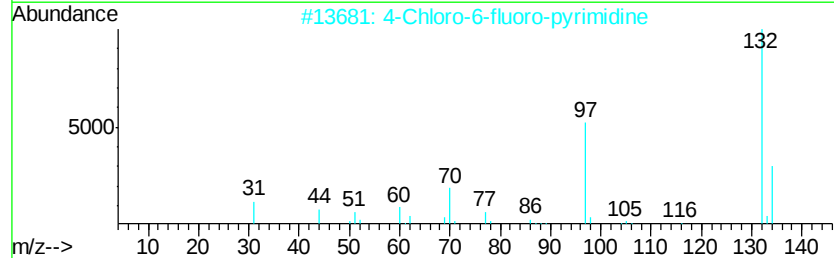
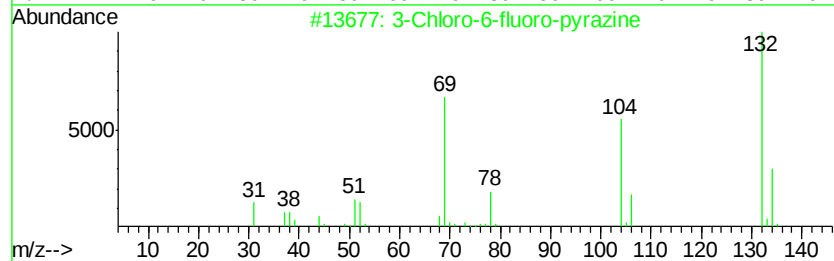
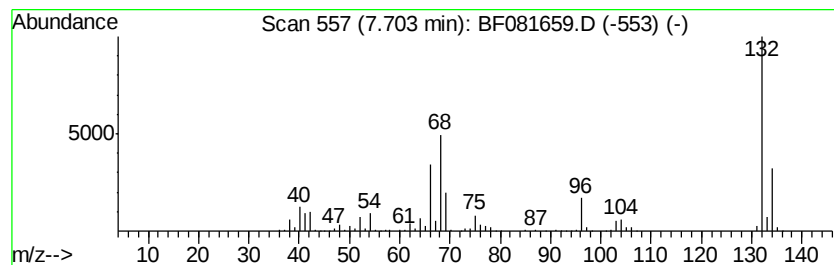
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Peak Number 4 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	110.46 ng	1829070	1,4-Dichlorobenzene-d4	8.18

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	25
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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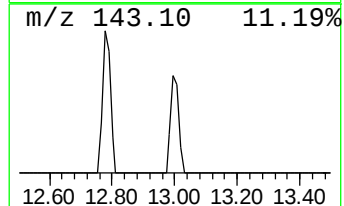
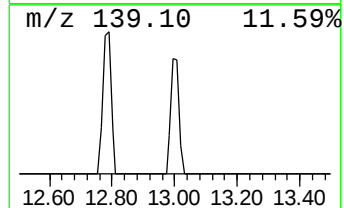
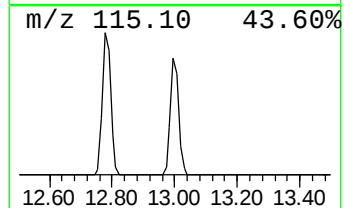
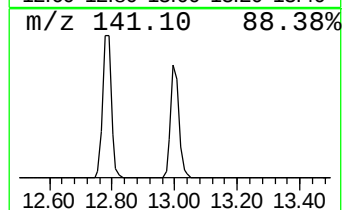
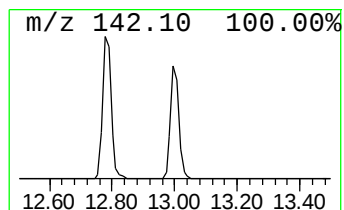
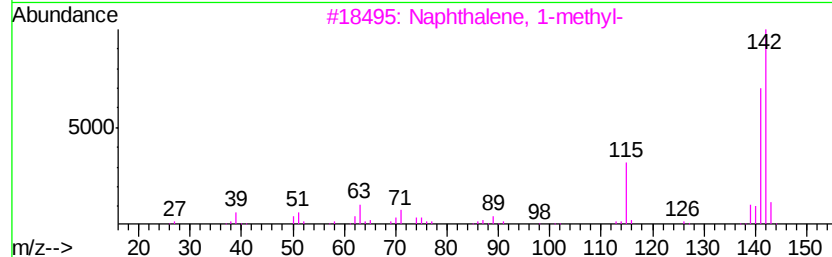
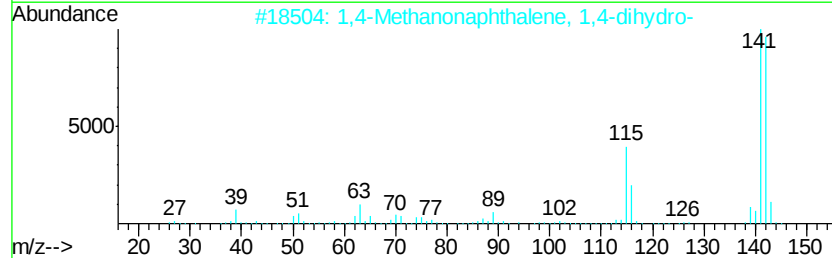
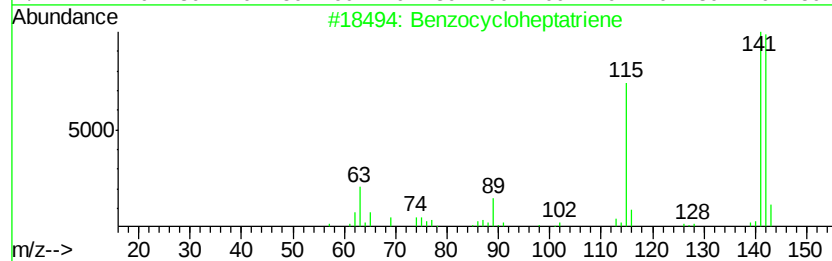
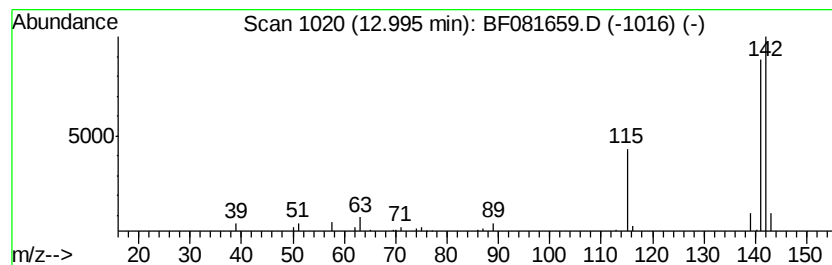
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Peak Number 6 Benzocycloheptatriene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	4.65 ng	99532	Naphthalene-d8	11.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzocycloheptatriene	142	C11H10	000264-09-5	91
2		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
3		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
4		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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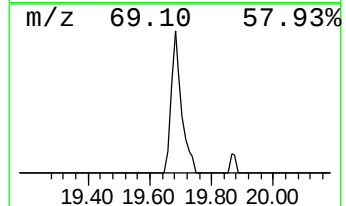
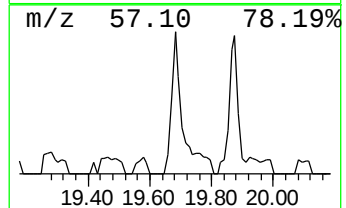
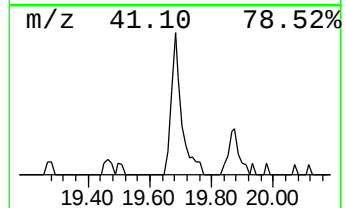
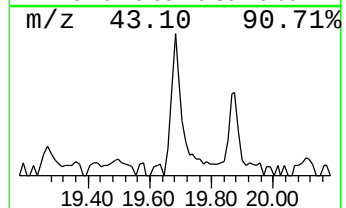
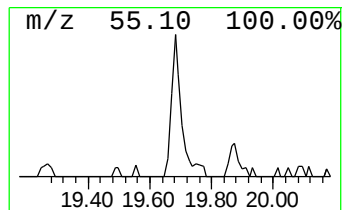
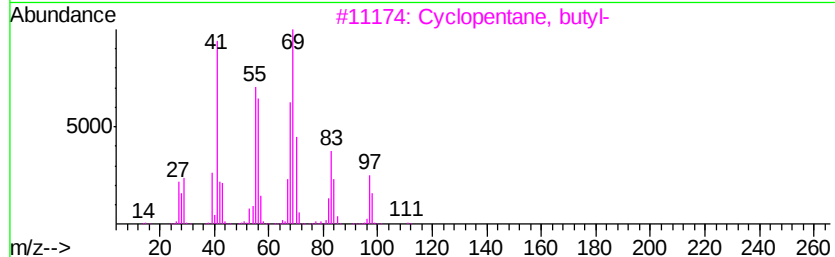
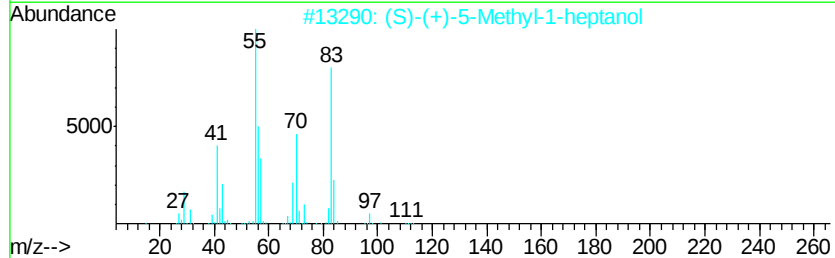
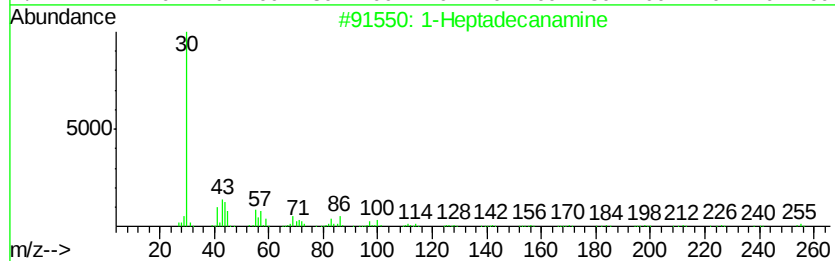
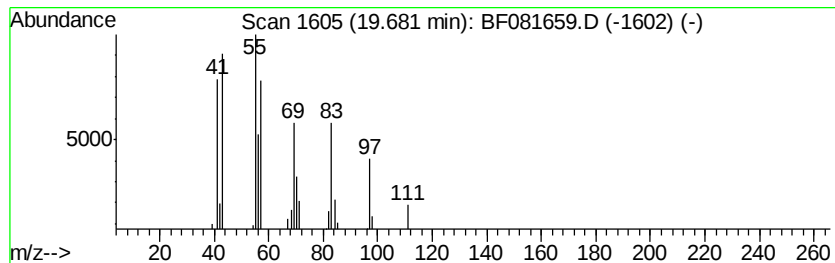
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Peak Number 7 1-Heptadecanamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	3.98 ng	95924	Phenanthrene-d10	18.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptadecanamine	255	C17H37N	004200-95-7	53
2		(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	38
3		Cyclopentane, butyl-	126	C9H18	002040-95-1	38
4		Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	35
5		Isooctanol	130	C8H18O	026952-21-6	35



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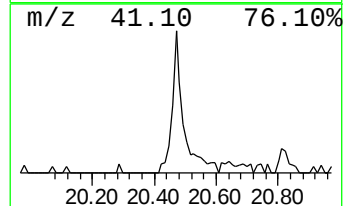
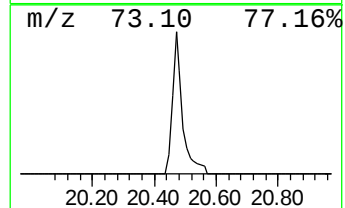
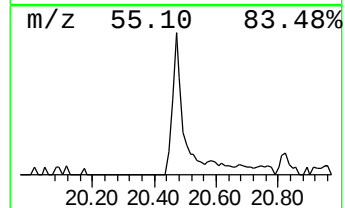
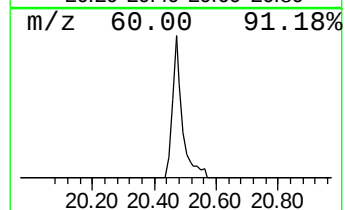
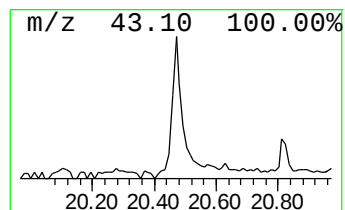
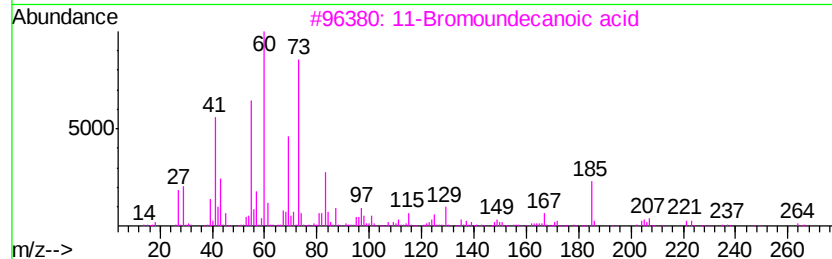
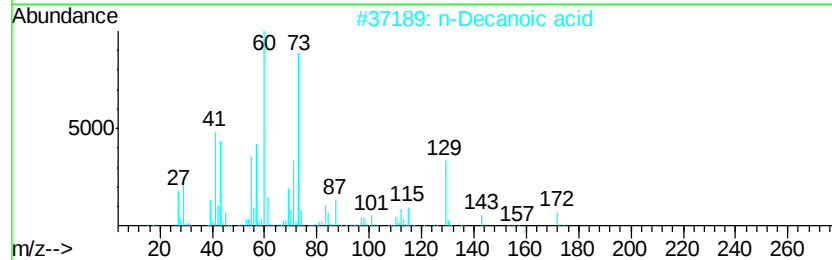
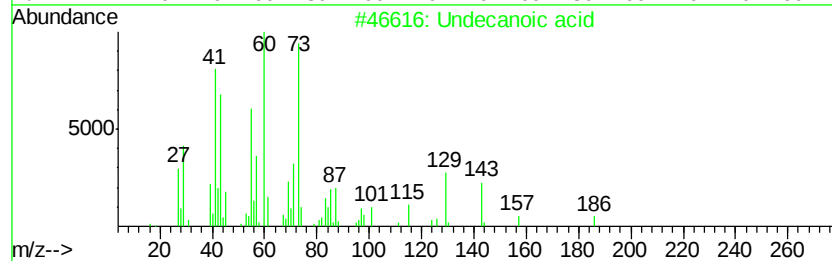
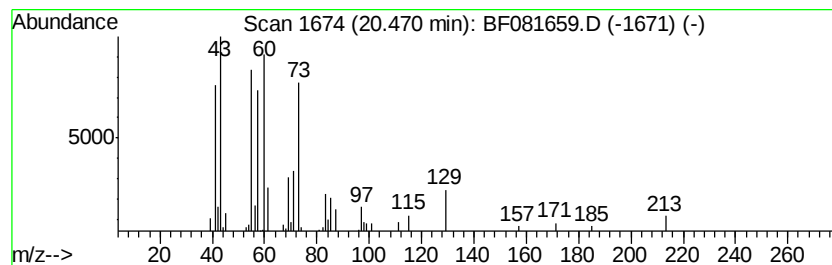
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TIC Integration Parameters: LSCINT.P

Peak Number 8 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.47	5.70 ng	137329	Phenanthrene-d10	18.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Heptanoic acid	130	C7H14O2	000111-14-8	43



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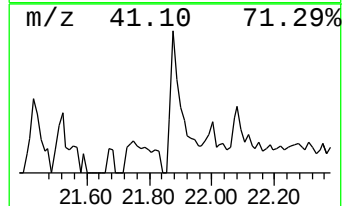
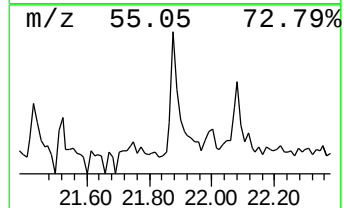
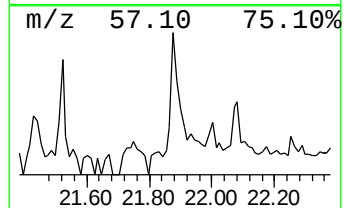
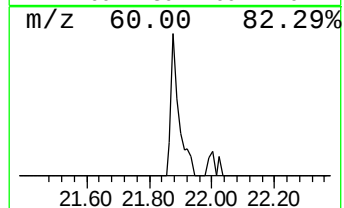
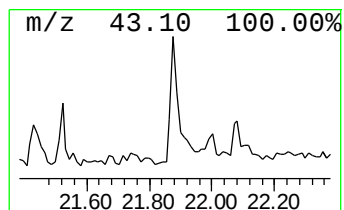
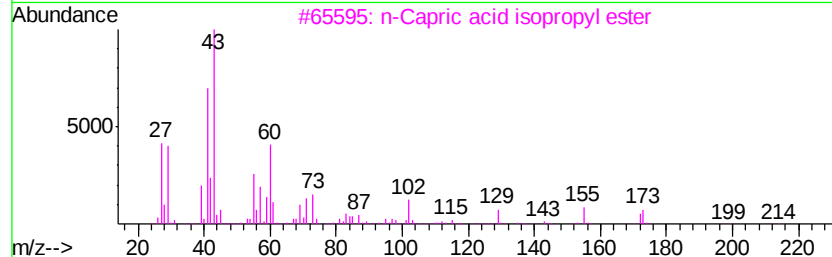
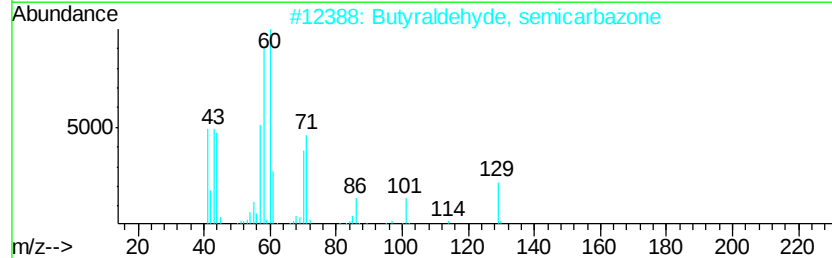
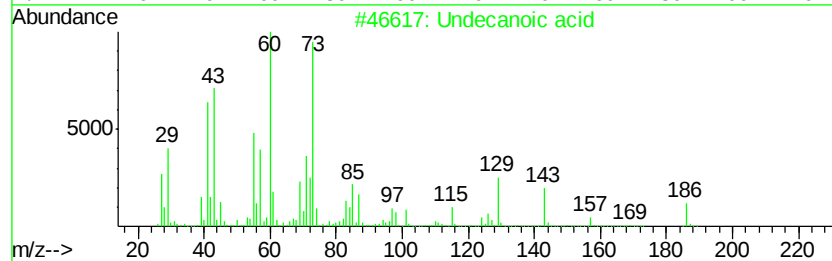
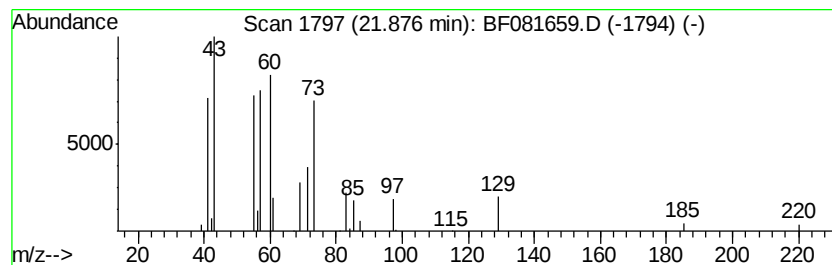
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Butyraldehyde, semicarbazone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	2.19 ng	45941	Chrysene-d12	23.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Undecanoic acid	186	C11H22O2	000112-37-8	59
2		Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	58
3		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081659.D
Acq On : 16 Sep 2015 21:04
Operator : UM/IZ
Sample : G3654-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP203(27-29)

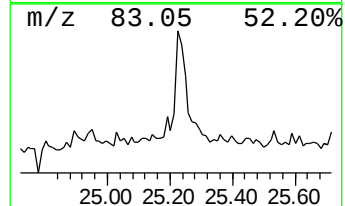
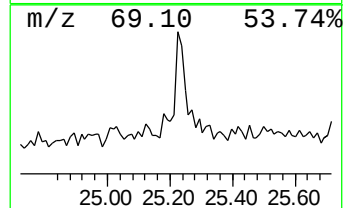
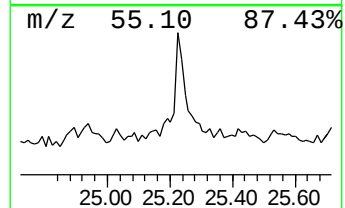
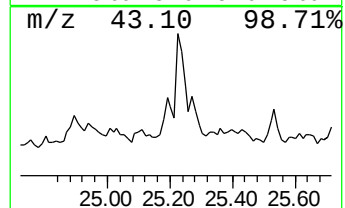
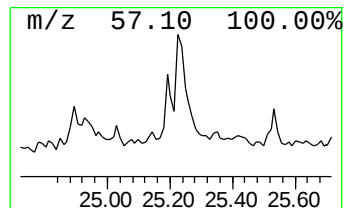
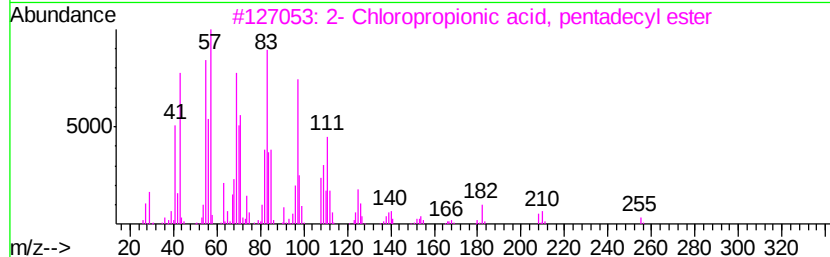
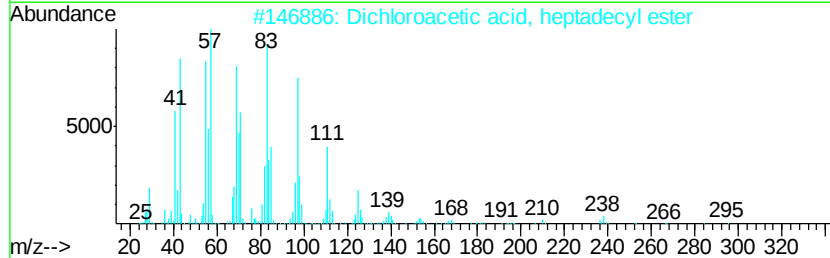
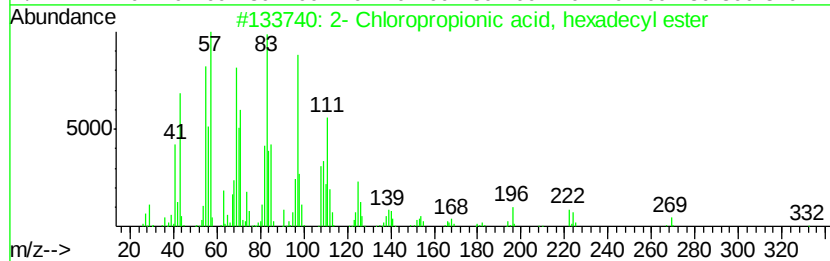
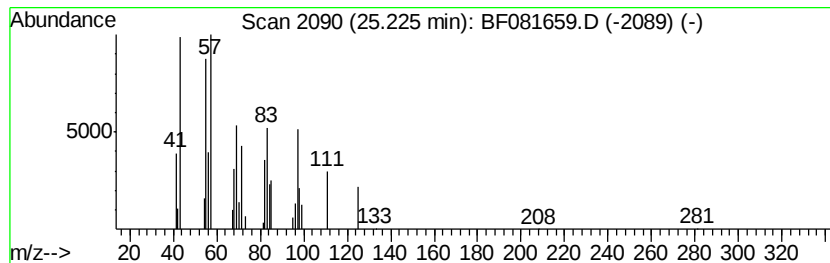
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2- Chloropropionic acid, he... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.22	3.71 ng	57738	Perylene-d12	24.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	86
3			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	86
4			1-Docosene	308	C22H44	001599-67-3	86
5			Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081659.D
Acq On : 16 Sep 2015 21:04
Operator : UM/IZ
Sample : G3654-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP203(27-29)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.48	62.3	ng	1031100	1	8.18	331177	20.0
unknown7.70	7.70	110.5	ng	1829070	1	8.18	331177	20.0
Benzocycloheptatr...	13.00	4.7	ng	99532	2	11.09	428031	20.0
1-Heptadecanamine	19.68	4.0	ng	95924	4	18.72	481635	20.0
Undecanoic acid	20.47	5.7	ng	137329	4	18.72	481635	20.0
Butyraldehyde, se...	21.88	2.2	ng	45941	5	23.35	419700	20.0
2- Chloropropioni...	25.22	3.7	ng	57738	6	24.79	310931	20.0