

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
 Data File : BF080755.D
 Acq On : 1 Aug 2015 2:03
 Operator : TP/UM
 Sample : G3127-07
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-3RD-7(0-2)

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-BF073015.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	3.207	97	98	113	rBV	14516	67251	2.77%	0.273%
2	4.384	199	201	205	rBV	67977	91456	3.77%	0.371%
3	5.036	255	258	261	rBV	1594377	1868436	77.03%	7.580%
4	5.447	291	294	296	rBV	2376595	2178123	89.80%	8.836%
5	5.859	328	330	333	rVB	86552	74854	3.09%	0.304%
6	6.476	381	384	386	rBV	2353208	2422905	99.89%	9.829%
7	6.613	394	396	399	rBV	2161787	2048244	84.45%	8.309%
8	6.853	415	417	419	rVB	943424	846833	34.91%	3.435%
9	7.002	428	430	433	rVB	1193770	1390422	57.32%	5.640%
10	7.413	463	466	468	rBV	1298166	1410415	58.15%	5.722%
11	8.133	526	529	531	rVB	1227045	1057403	43.59%	4.289%
12	9.208	620	623	625	rBV	2314693	1951052	80.44%	7.915%
13	9.608	655	658	660	rBV	223125	275727	11.37%	1.119%
14	9.882	680	682	685	rBV	1095845	1043046	43.00%	4.231%
15	10.671	748	751	753	rBV	1327502	1452825	59.90%	5.894%
16	10.773	758	760	761	rBV	82897	73062	3.01%	0.296%
17	10.796	761	762	766	rVB	24024	25052	1.03%	0.102%
18	11.242	797	801	802	rBV	39209	34340	1.42%	0.139%
19	11.368	809	812	814	rVB	881837	1027471	42.36%	4.168%
20	11.665	836	838	840	rBV	50266	54328	2.24%	0.220%
21	11.768	840	847	849	rVV5	32985	150047	6.19%	0.609%
22	11.894	856	858	870	rVB	127555	197902	8.16%	0.803%
23	12.076	871	874	876	rVV	26446	28413	1.17%	0.115%
24	12.156	878	881	883	rBV	1020535	1015892	41.88%	4.121%
25	12.682	925	927	933	rBV	28784	47666	1.97%	0.193%
26	12.774	933	935	938	rVB	36935	35627	1.47%	0.145%
27	12.945	948	950	953	rBV	2484383	2425535	100.00%	9.839%
28	13.985	1039	1041	1044	rBV	619408	697048	28.74%	2.828%
29	14.065	1044	1048	1050	rVV3	11088	43188	1.78%	0.175%
30	14.168	1056	1057	1064	rVB	26775	31913	1.32%	0.129%
31	15.402	1162	1165	1168	rBV	441963	584663	24.10%	2.372%

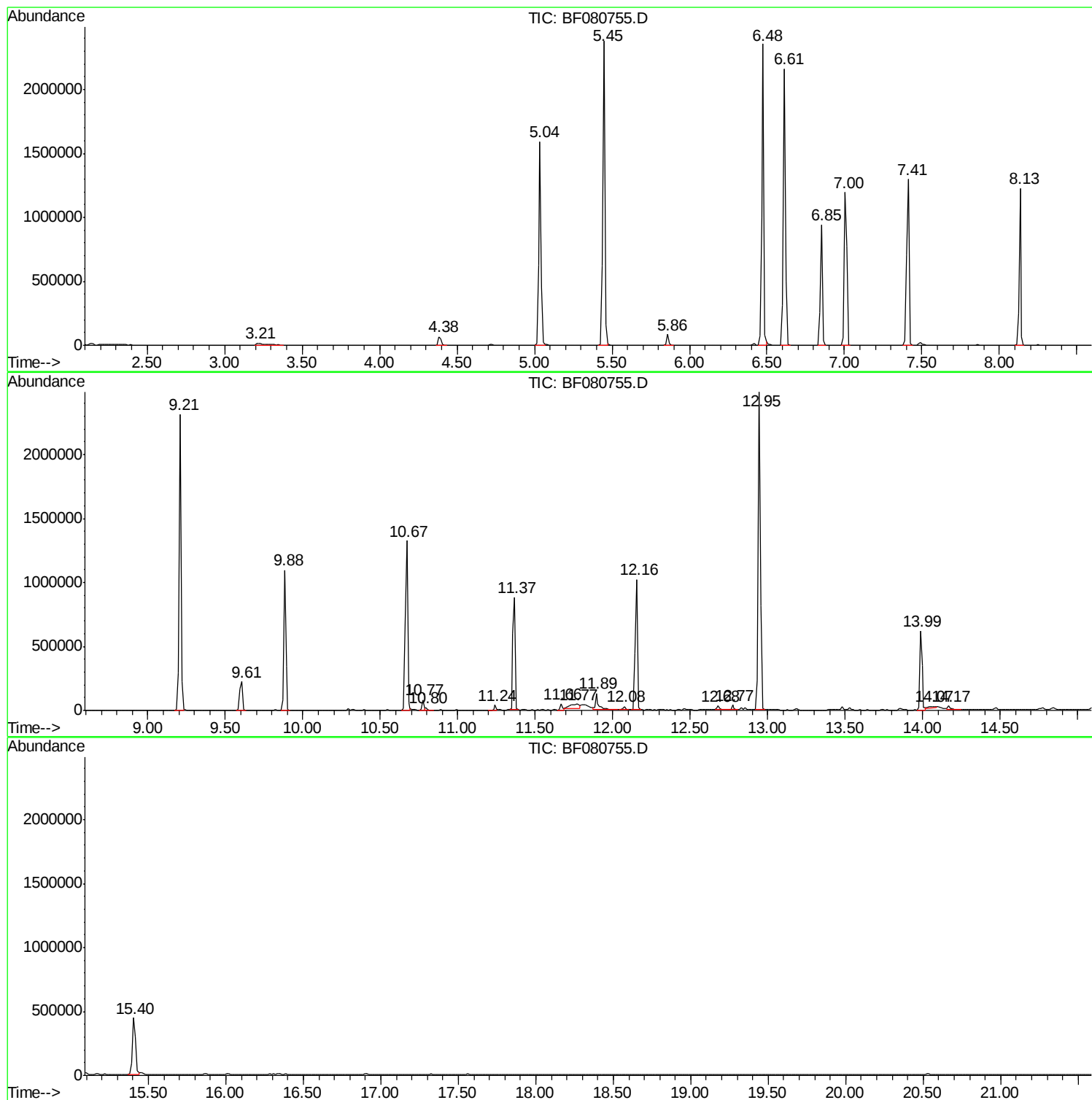
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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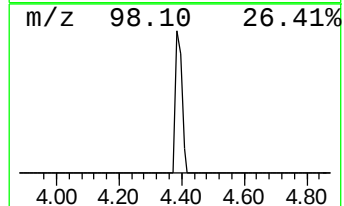
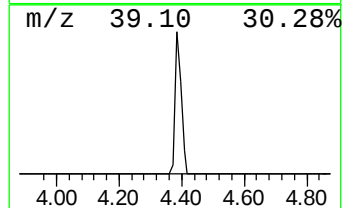
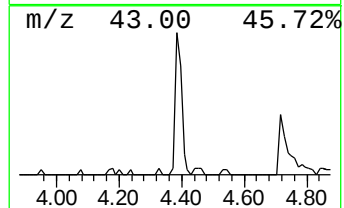
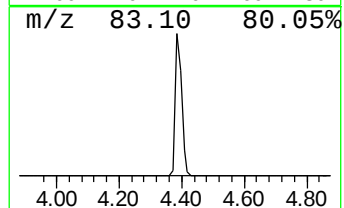
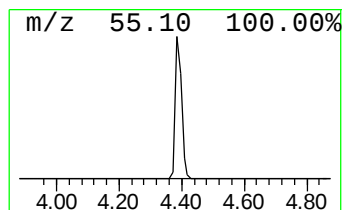
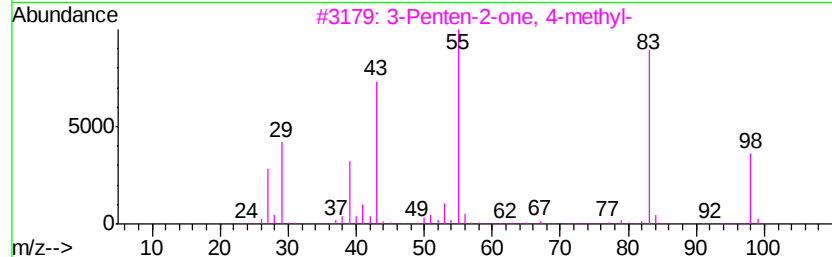
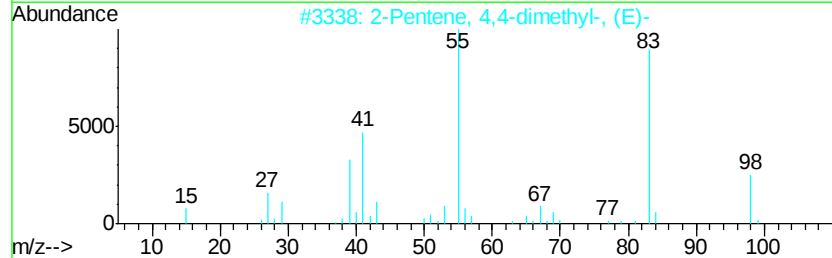
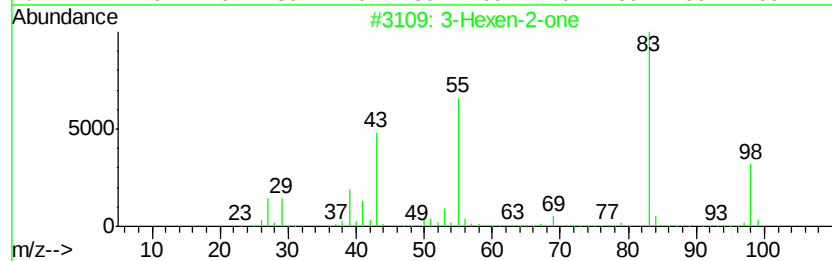
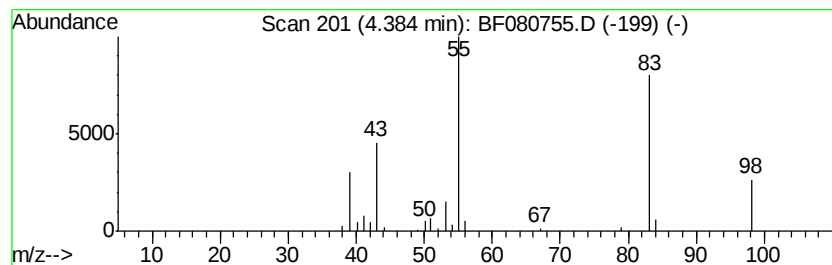
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	2.16 ng	91456	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	86
2		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
3		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	80
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72



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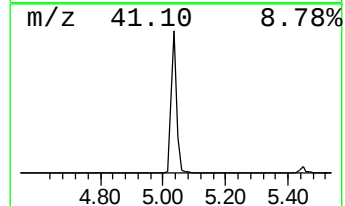
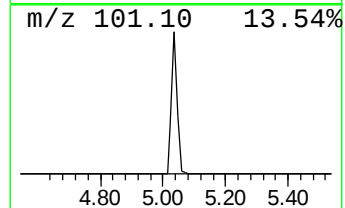
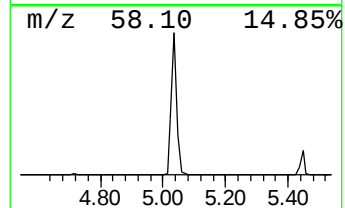
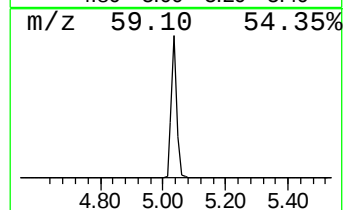
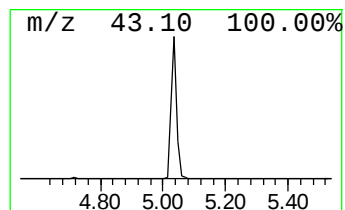
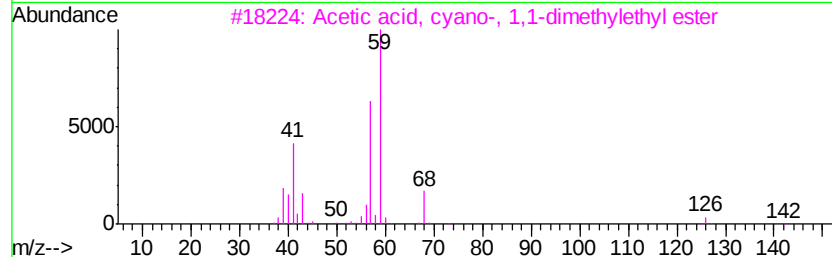
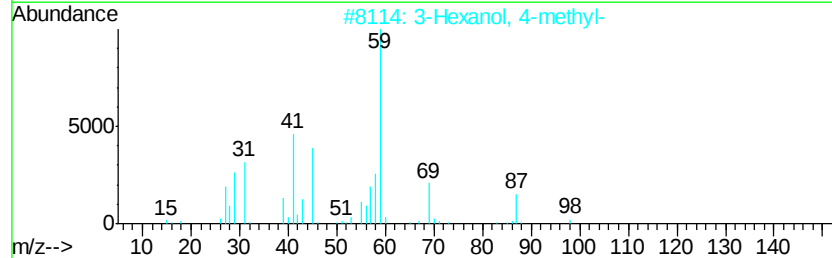
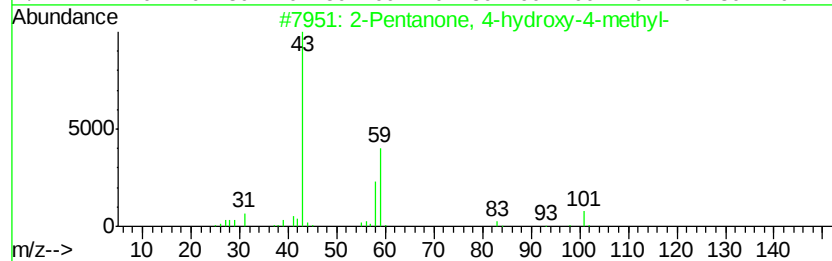
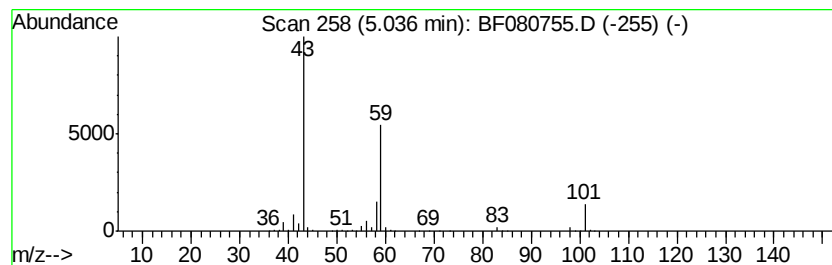
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	44.13 ng	1868440	1,4-Dichlorobenzene-d4	6.85

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	32
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



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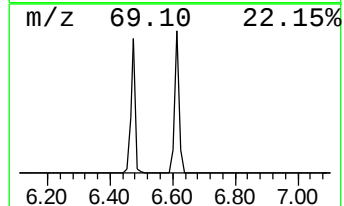
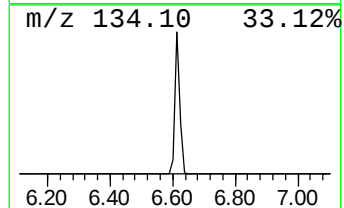
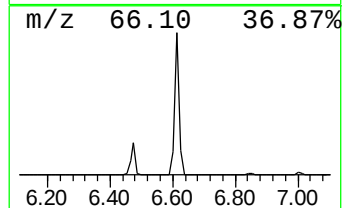
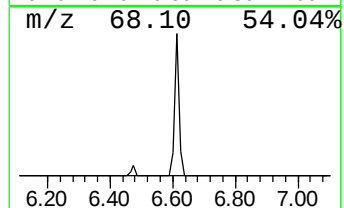
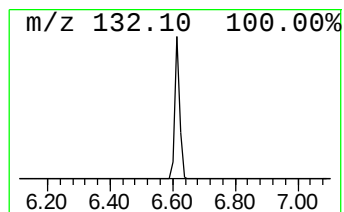
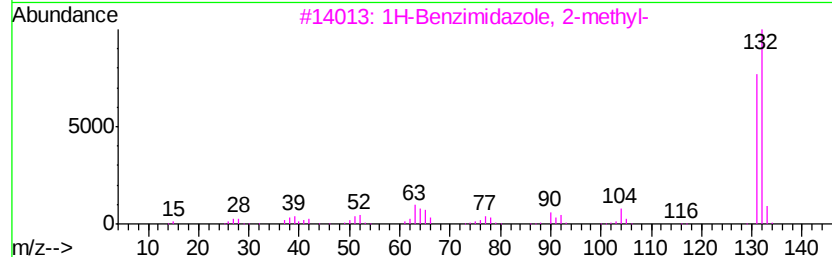
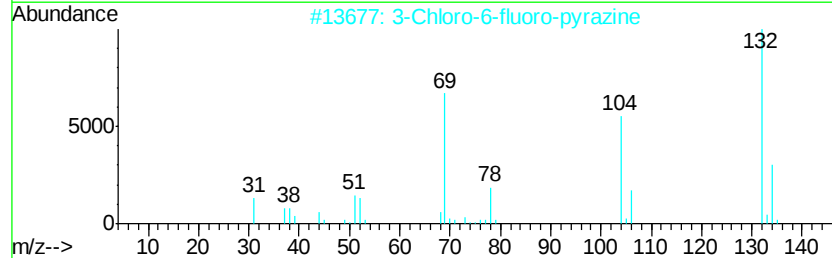
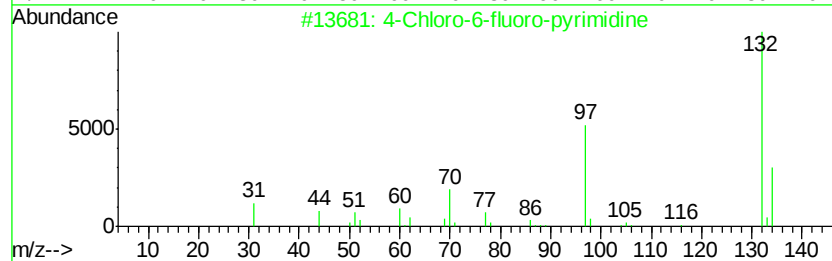
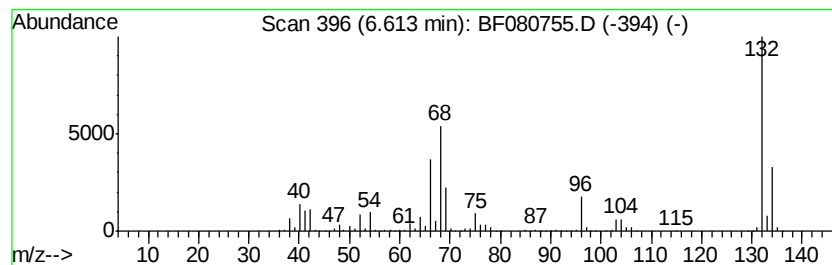
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	48.37 ng	2048240	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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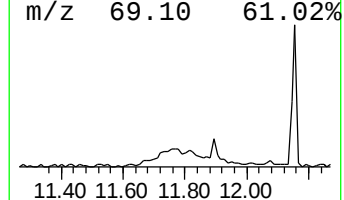
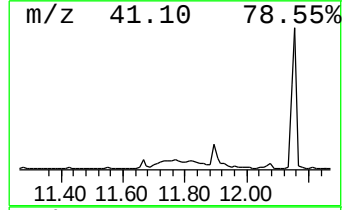
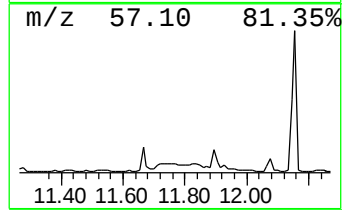
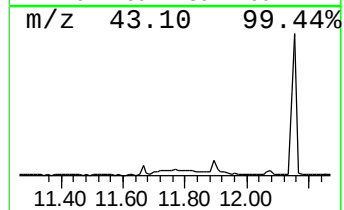
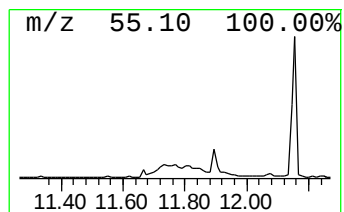
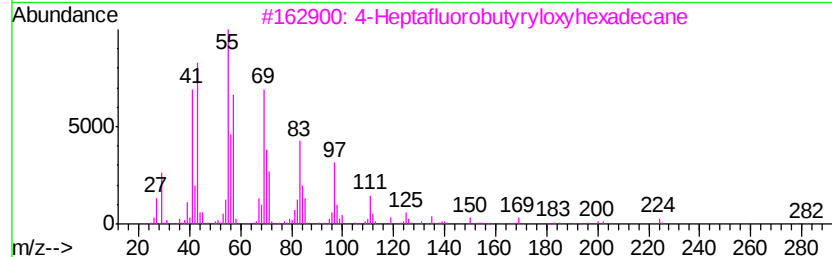
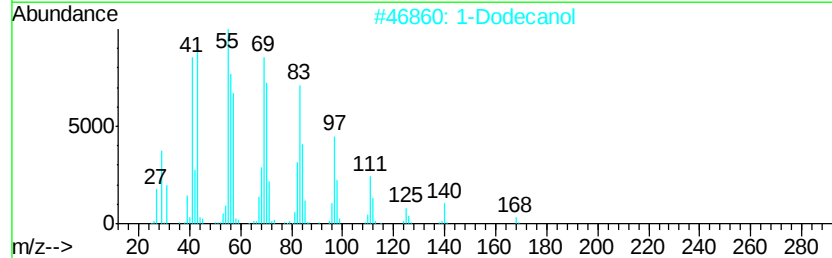
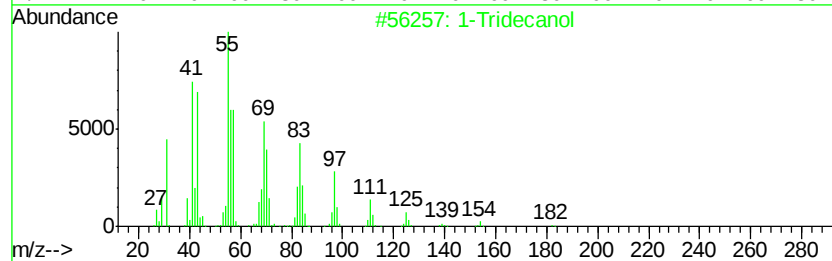
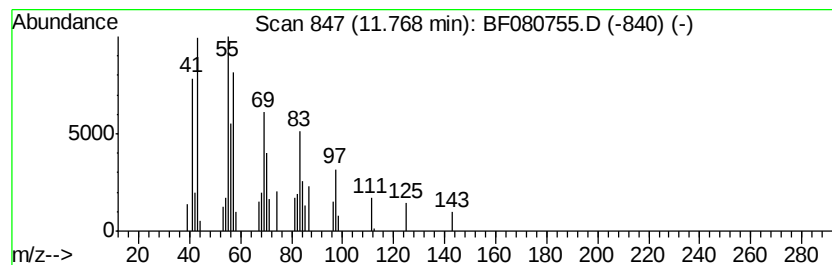
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Peak Number 5 1-Tridecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.92 ng	150047	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecanol		200	C13H28O	000112-70-9	80
2	1-Dodecanol		186	C12H26O	000112-53-8	74
3	4-Heptafluorobutyryloxyhexadecane		438	C20H33F7O2	1000282-97-2	64
4	Cyclopentane, 1-methyl-2-propyl-		126	C9H18	003728-57-2	50
5	1-Hexacosanol		382	C26H54O	000506-52-5	49



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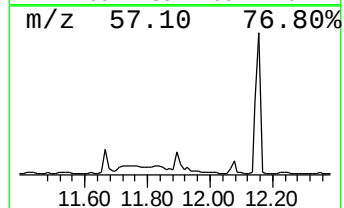
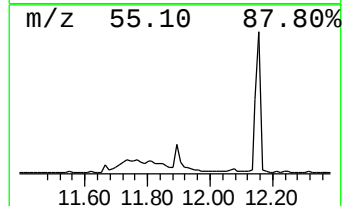
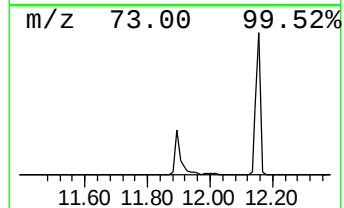
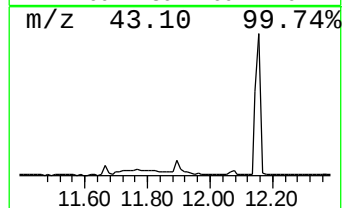
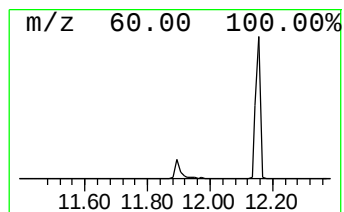
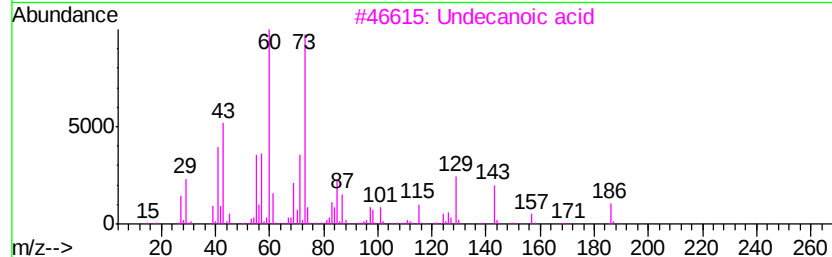
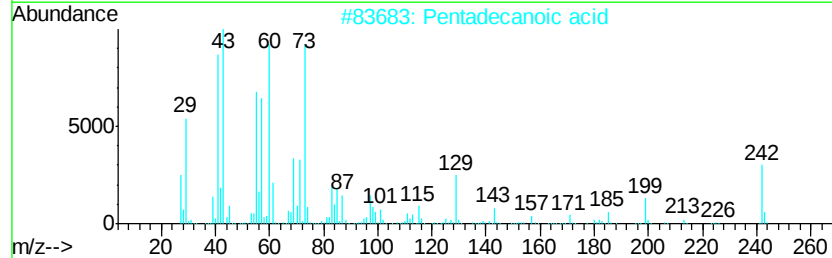
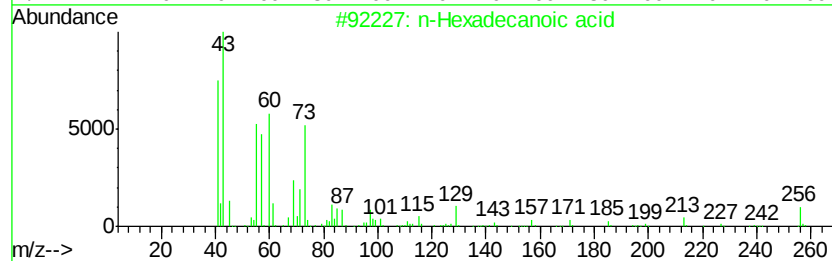
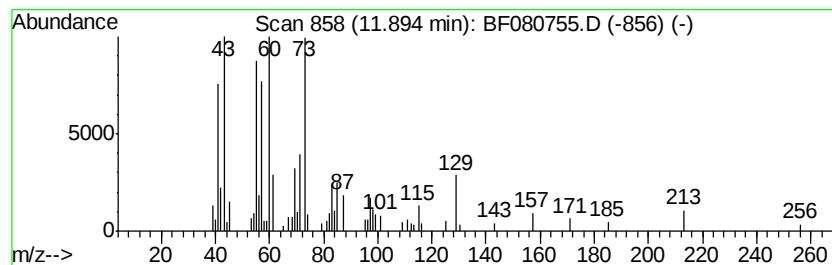
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.85 ng	197902	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	14



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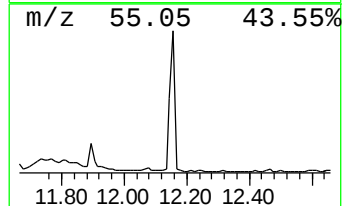
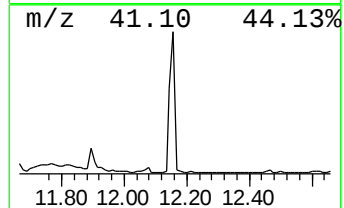
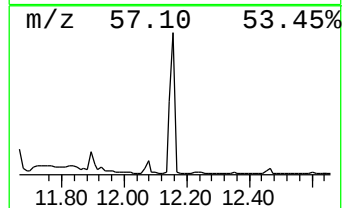
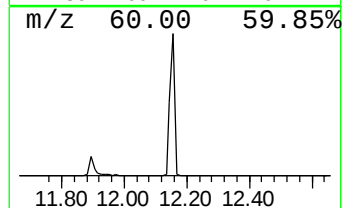
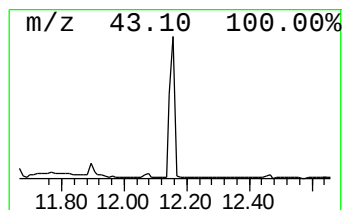
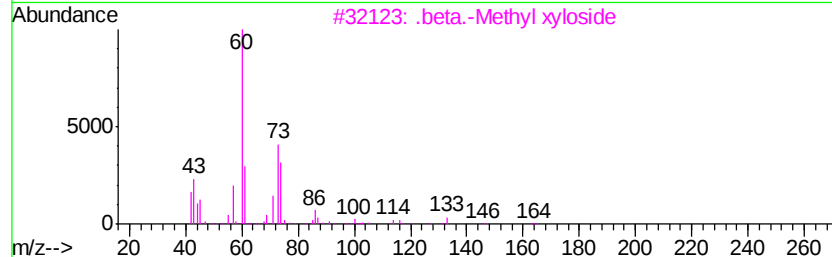
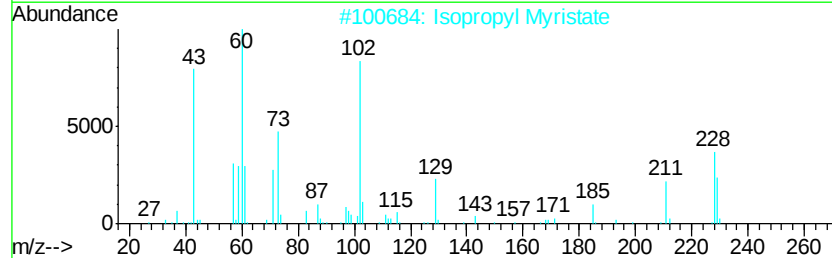
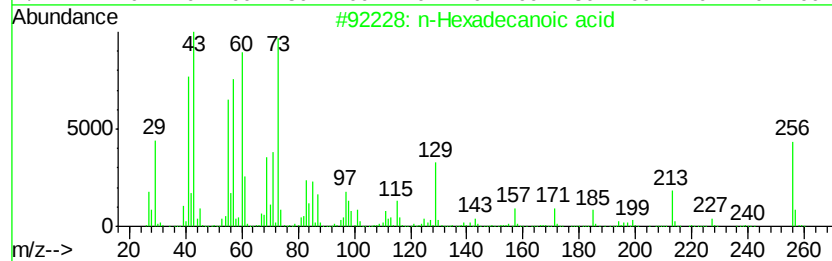
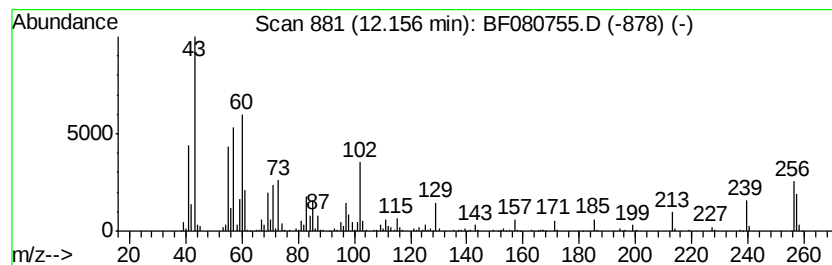
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.16 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	19.77 ng	1015890	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2		Isopropyl Myristate	270	C17H34O2	000110-27-0	49
3		.beta.-Methyl xyloside	164	C6H12O5	1000130-04-0	35
4		.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	35
5		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080755.D
Acq On : 1 Aug 2015 2:03
Operator : TP/UM
Sample : G3127-07
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3RD-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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
3-Hexen-2-one	4.38	2.2	ng	91456	1	6.85	846833	20.0
2-Pentanone, 4-hy...	5.04	44.1	ng	1868440	1	6.85	846833	20.0
unknown6.61	6.61	48.4	ng	2048240	1	6.85	846833	20.0
1-Tridecanol	11.77	2.9	ng	150047	4	11.37	1027470	20.0
n-Hexadecanoic acid	11.89	3.9	ng	197902	4	11.37	1027470	20.0
unknown12.16	12.16	19.8	ng	1015890	4	11.37	1027470	20.0