

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082416\
 Data File : BF089874.D
 Acq On : 24 Aug 2016 15:08
 Operator : UM/SJ
 Sample : H4551-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AST-5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.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	1.655	4	6	14	rBV	1538251	2682559	10.84%	2.204%
2	1.770	14	16	72	rVB	9412027	24743365	100.00%	20.330%
3	4.798	278	281	289	rVB	1650097	2370170	9.58%	1.947%
4	5.244	317	320	322	rBV	8505784	8794180	35.54%	7.225%
5	6.307	409	413	415	rBV	8131567	9414441	38.05%	7.735%
6	6.433	421	424	426	rBV	9324061	9387645	37.94%	7.713%
7	6.662	442	444	447	rBV	2234972	2370549	9.58%	1.948%
8	6.822	456	458	460	rBV	8272557	7120118	28.78%	5.850%
9	7.233	491	494	496	rBV	5851712	5750373	23.24%	4.725%
10	7.347	500	504	513	rVV	244502	482201	1.95%	0.396%
11	7.953	554	557	559	rBV	3965912	3402300	13.75%	2.795%
12	9.039	649	652	654	rBV	8756745	10541302	42.60%	8.661%
13	9.428	684	686	689	rBV	2402821	3110224	12.57%	2.555%
14	9.702	708	710	713	rBV	4032179	3553023	14.36%	2.919%
15	10.490	776	779	781	rBV	5438465	5745134	23.22%	4.720%
16	10.628	789	791	797	rVB	304329	344307	1.39%	0.283%
17	11.176	837	839	842	rBV	3687142	3463887	14.00%	2.846%
18	11.439	859	862	866	rBV	365250	732226	2.96%	0.602%
19	11.736	886	888	896	rBV2	359877	452281	1.83%	0.372%
20	12.776	976	979	982	rBV	7845780	9052342	36.58%	7.438%
21	13.759	1063	1065	1072	rBV	161402	424895	1.72%	0.349%
22	13.874	1072	1075	1079	rVV2	3826187	4648583	18.79%	3.819%
23	14.891	1161	1164	1166	rBV	565861	647889	2.62%	0.532%
24	15.405	1206	1209	1212	rBV	2032516	2477484	10.01%	2.036%

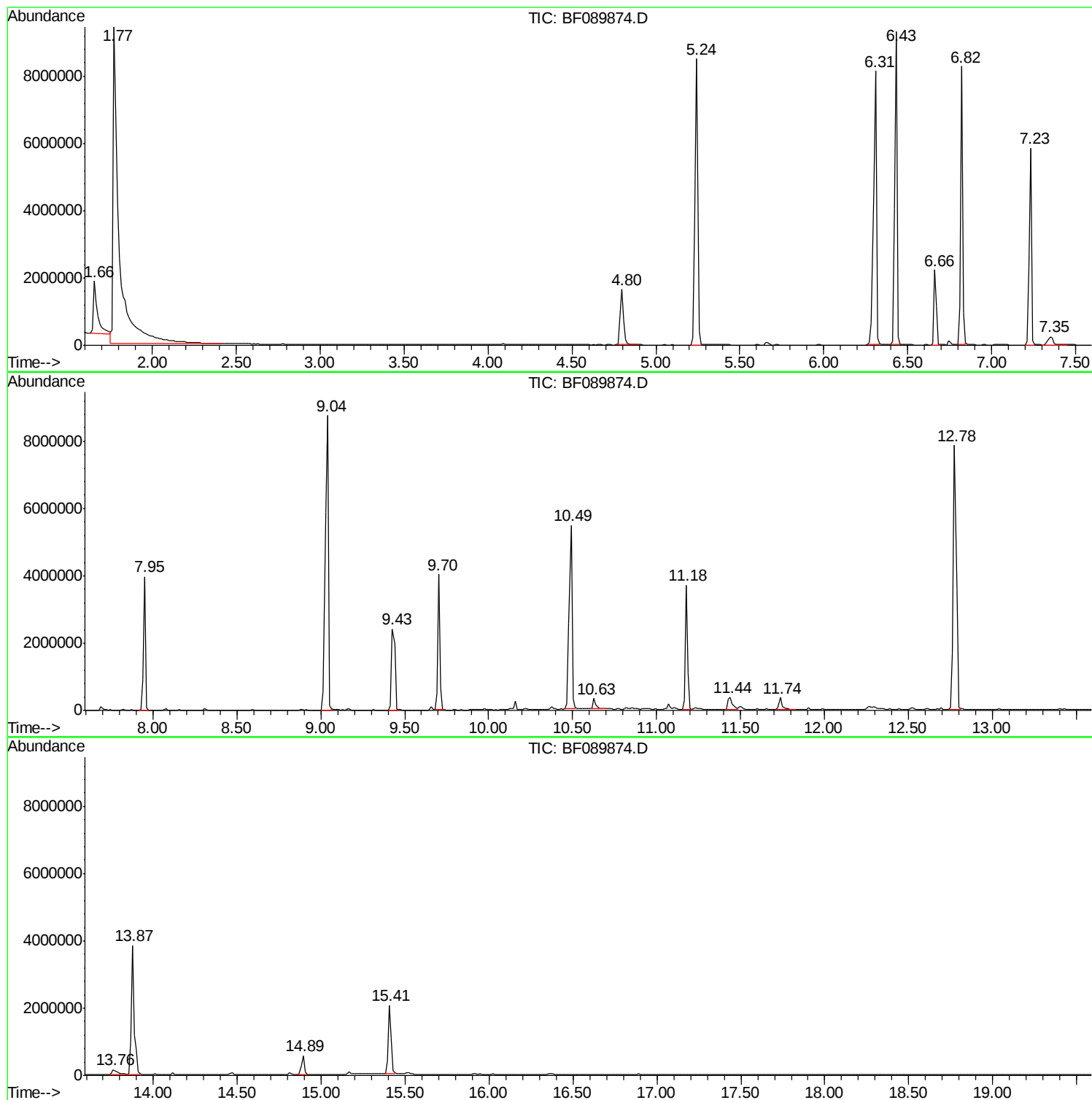
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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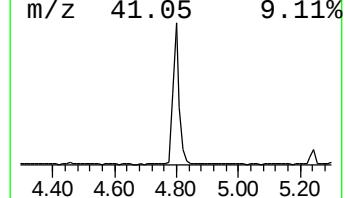
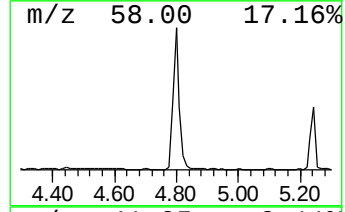
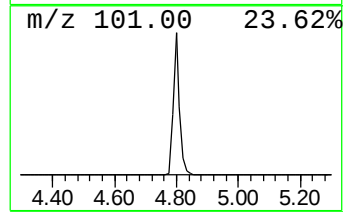
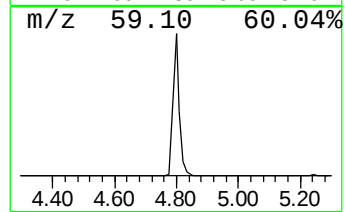
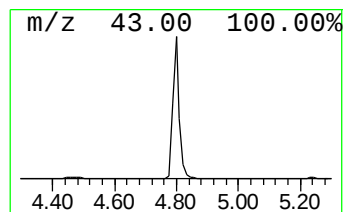
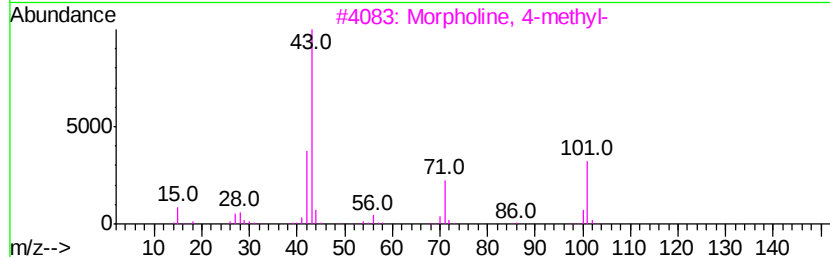
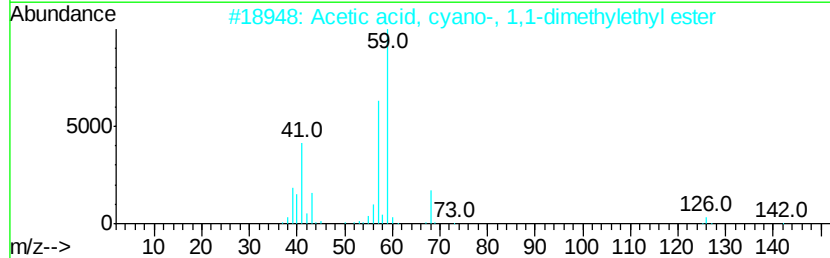
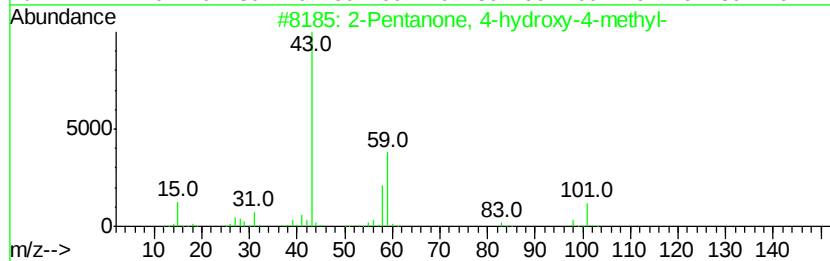
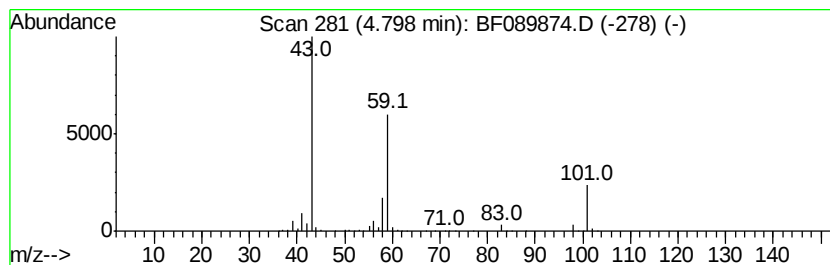
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	20.00 ng	2370170	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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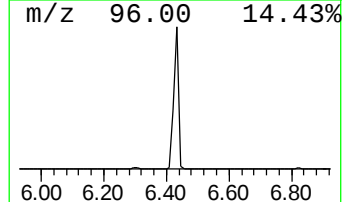
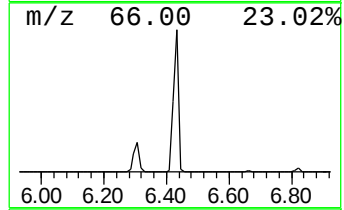
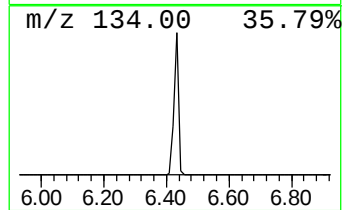
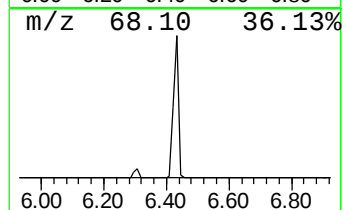
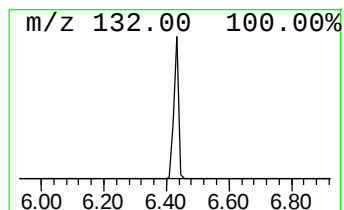
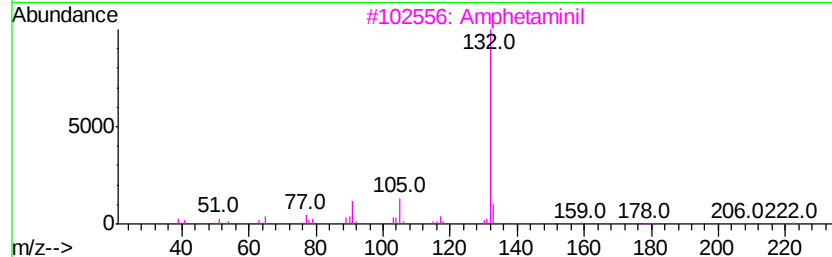
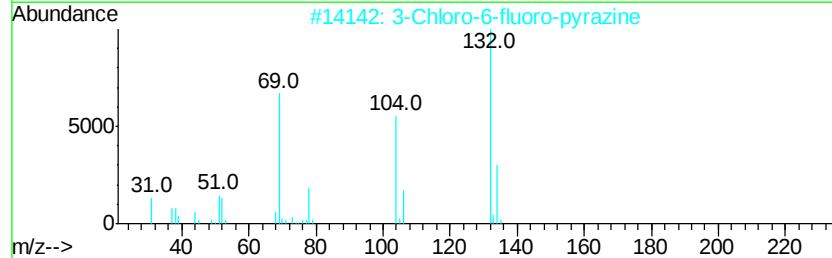
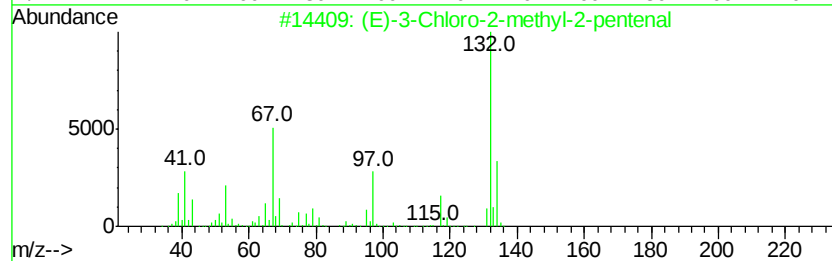
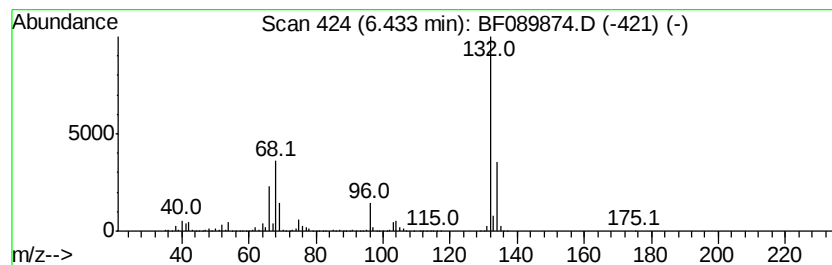
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Peak Number 4 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	79.20 ng	9387650	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Xenon	132	Xe	007440-63-3	9



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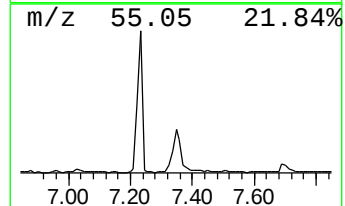
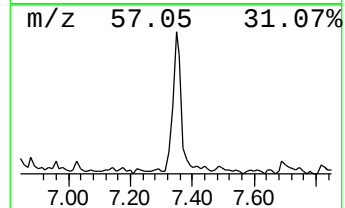
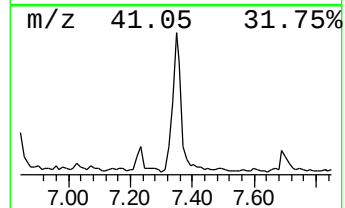
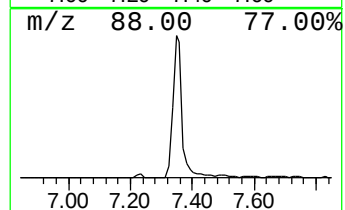
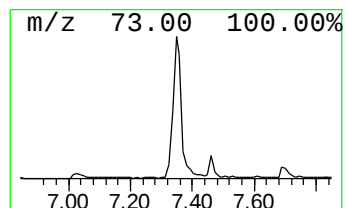
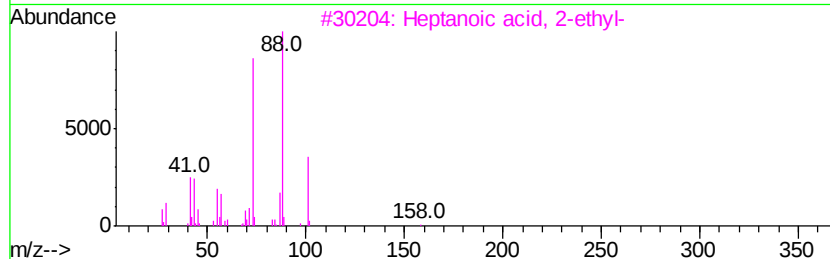
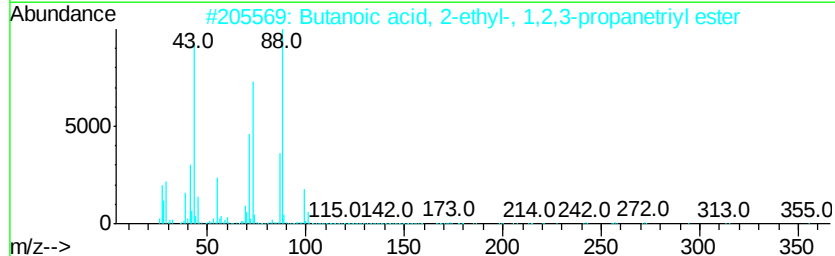
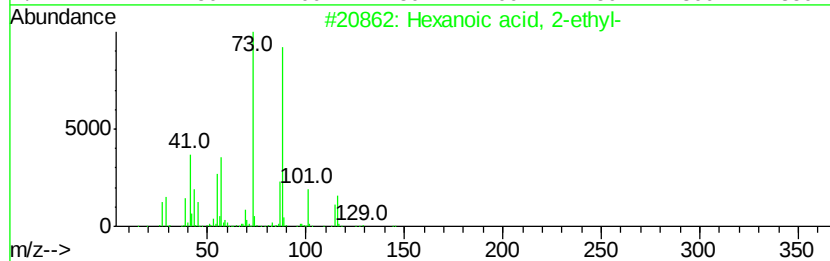
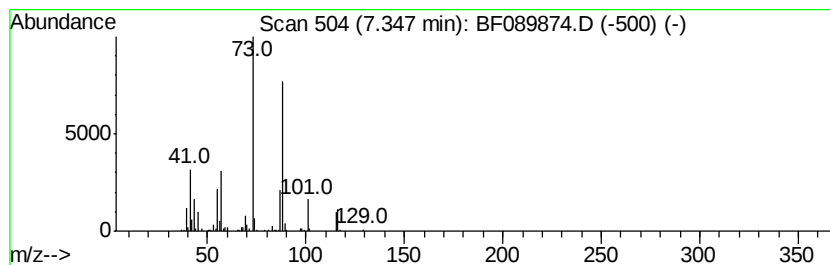
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Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	2.83 ng	482201	Naphthalene-d8	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
4		L(-)-Fucose, tetramethyl ether	220	C10H20O5	1000332-75-0	42
5		Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38



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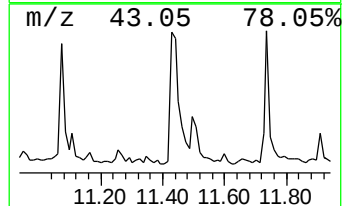
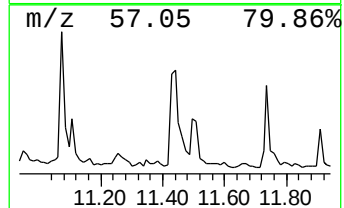
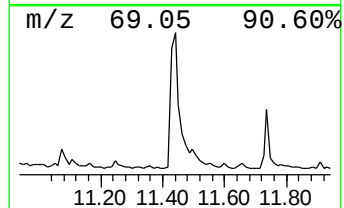
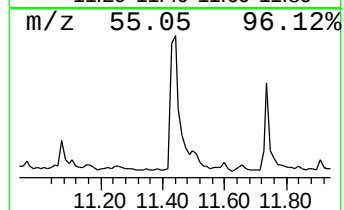
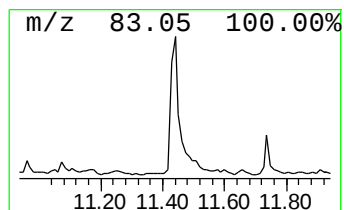
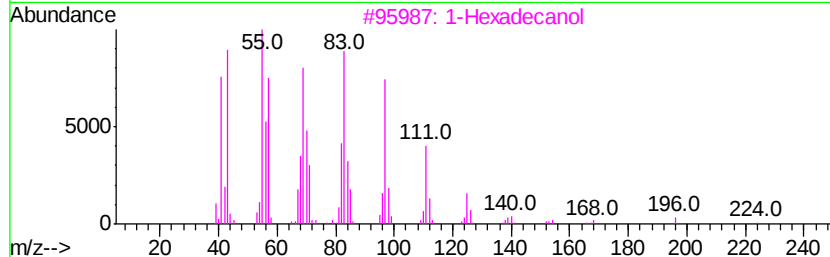
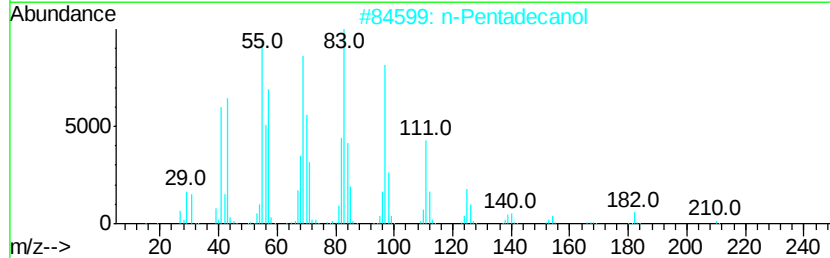
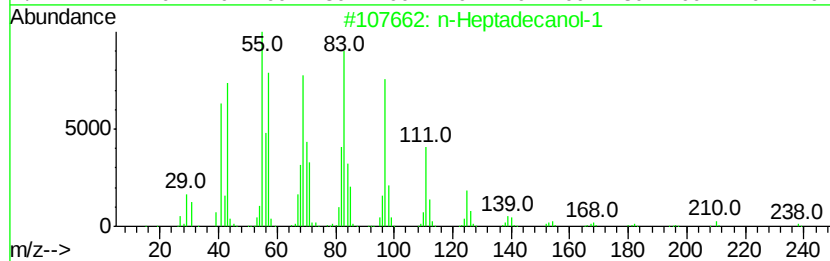
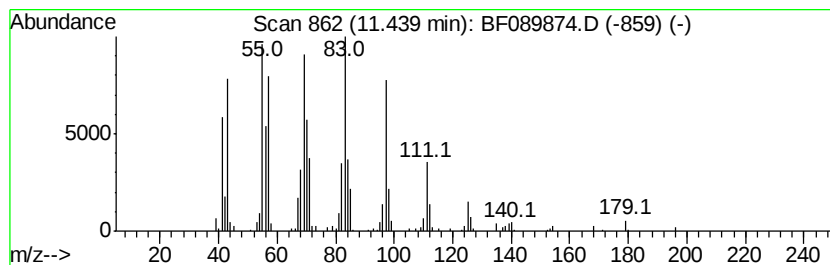
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Peak Number 7 n-Heptadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	4.23 ng	732226	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2		n-Pentadecanol	228	C15H32O	000629-76-5	94
3		1-Hexadecanol	242	C16H34O	036653-82-4	94
4		9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5		Cyclotetradecane	196	C14H28	000295-17-0	91



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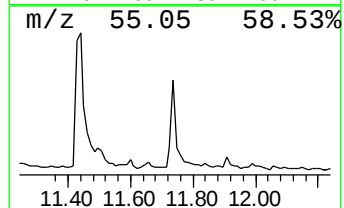
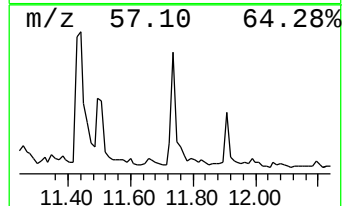
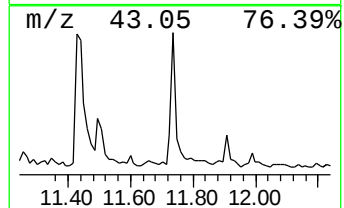
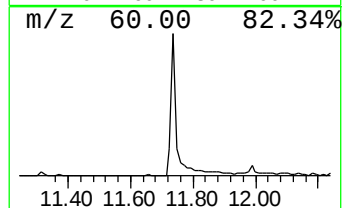
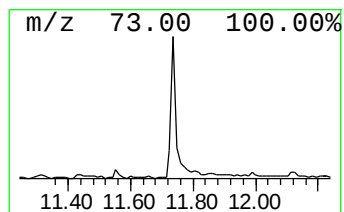
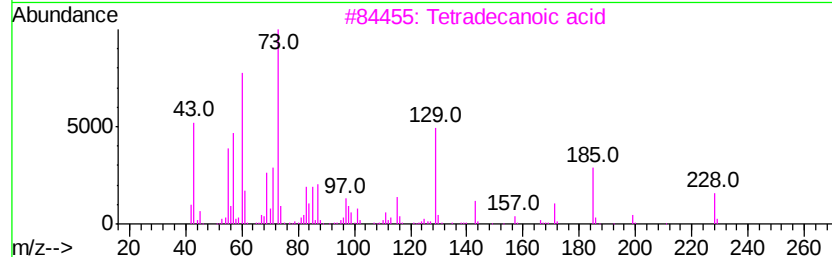
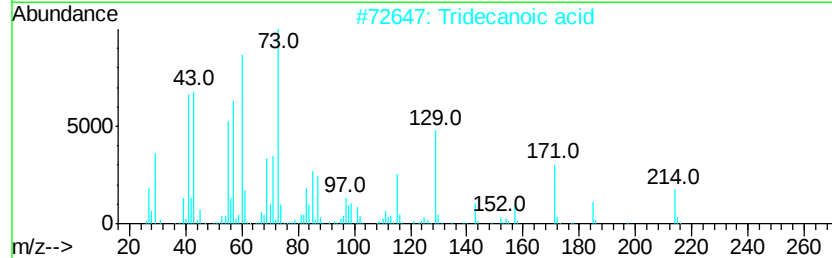
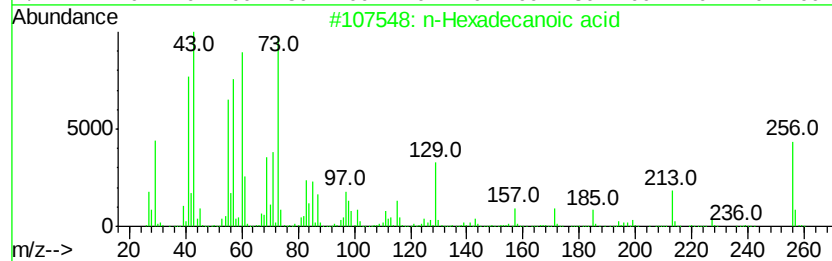
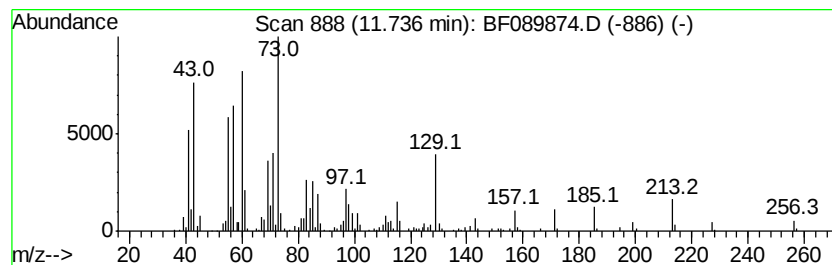
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.61 ng	452281	Phenanthrene-d10	11.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
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	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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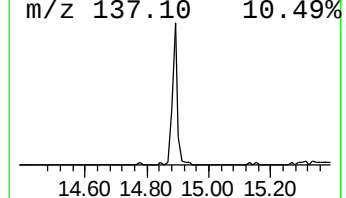
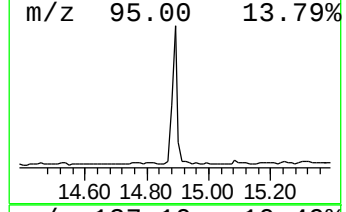
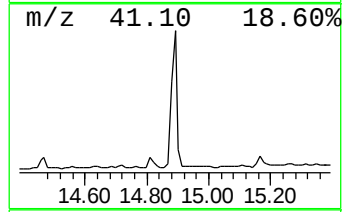
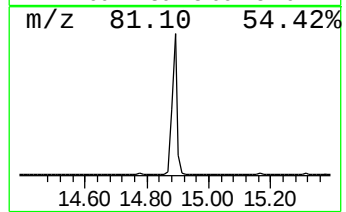
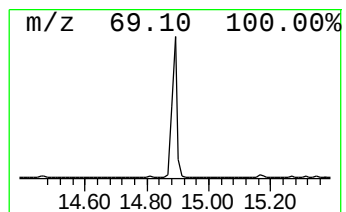
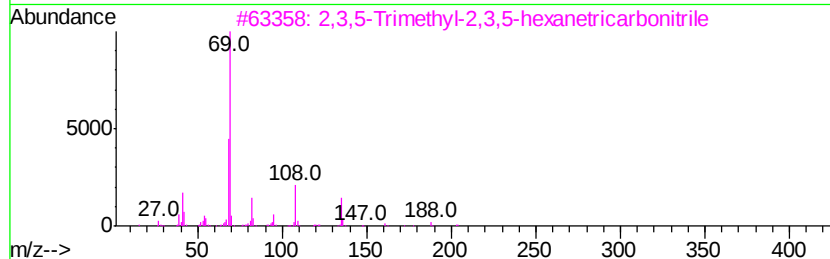
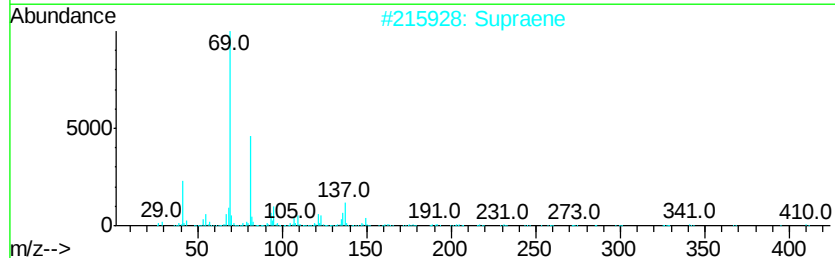
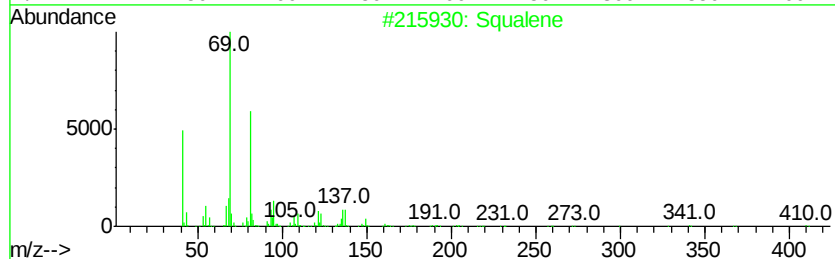
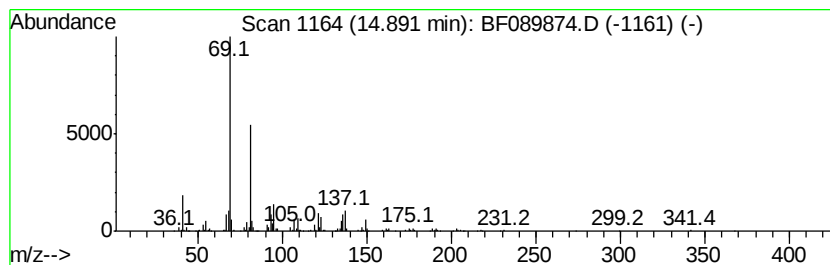
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	5.23 ng	647889	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
4		Butanoic acid, 4-cyano-2-ethyl-2...	290	C15H18N2O4	203808-68-8	43
5		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082416\
Data File : BF089874.D
Acq On : 24 Aug 2016 15:08
Operator : UM/SJ
Sample : H4551-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AST-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	20.0	ng	2370170	1	6.66	2370550	20.0
unknown6.43	6.43	79.2	ng	9387650	1	6.66	2370550	20.0
Hexanoic acid, 2-...	7.35	2.8	ng	482201	2	7.95	3402300	20.0
n-Heptadecanol-1	11.44	4.2	ng	732226	4	11.18	3463890	20.0
n-Hexadecanoic acid	11.74	2.6	ng	452281	4	11.18	3463890	20.0
Squalene	14.89	5.2	ng	647889	6	15.41	2477480	20.0