

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
 Data File : BF094966.D
 Acq On : 8 May 2017 3:35
 Operator : SJ/MA
 Sample : I3007-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EME-BW

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-BF050217.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	5.048	524	529	546	rBV	310721	664491	18.92%	2.369%
2	5.672	630	635	664	rBV	1968672	2916699	83.03%	10.400%
3	6.254	729	734	746	rBV3	18631	36998	1.05%	0.132%
4	7.266	900	906	921	rBV	1968386	2994738	85.25%	10.679%
5	7.384	921	926	939	rVB	2377891	3206194	91.27%	11.433%
6	7.719	979	983	1001	rVB	504915	614615	17.50%	2.192%
7	7.960	1019	1024	1037	rBV	2066536	2456131	69.92%	8.758%
8	8.625	1131	1137	1158	rBV	1420548	1960719	55.82%	6.992%
9	9.742	1322	1327	1338	rBV	570990	807398	22.98%	2.879%
10	11.519	1623	1629	1643	rBV	2663139	3512861	100.00%	12.526%
11	12.207	1741	1746	1758	rBV	269383	359234	10.23%	1.281%
12	12.572	1803	1808	1821	rBV2	648045	925504	26.35%	3.300%
13	13.413	1947	1951	1956	rBV	42228	44193	1.26%	0.158%
14	13.866	2022	2028	2043	rBV	1335677	2028547	57.75%	7.233%
15	14.183	2073	2082	2085	rBV	36311	47571	1.35%	0.170%
16	14.971	2211	2216	2231	rBV	596825	828202	23.58%	2.953%
17	15.936	2376	2380	2390	rBV3	74220	102287	2.91%	0.365%
18	17.142	2581	2585	2590	rBV2	121715	123409	3.51%	0.440%
19	17.301	2606	2612	2615	rBV	2479207	2963286	84.36%	10.567%
20	18.065	2738	2742	2746	rBV	78118	75845	2.16%	0.270%
21	18.601	2826	2833	2835	rBV5	19739	43828	1.25%	0.156%
22	18.636	2835	2839	2855	rVB	538980	722872	20.58%	2.578%
23	20.300	3118	3122	3135	rBV	378385	550151	15.66%	1.962%
24	23.736	3699	3706	3717	rVB	19405	58213	1.66%	0.208%

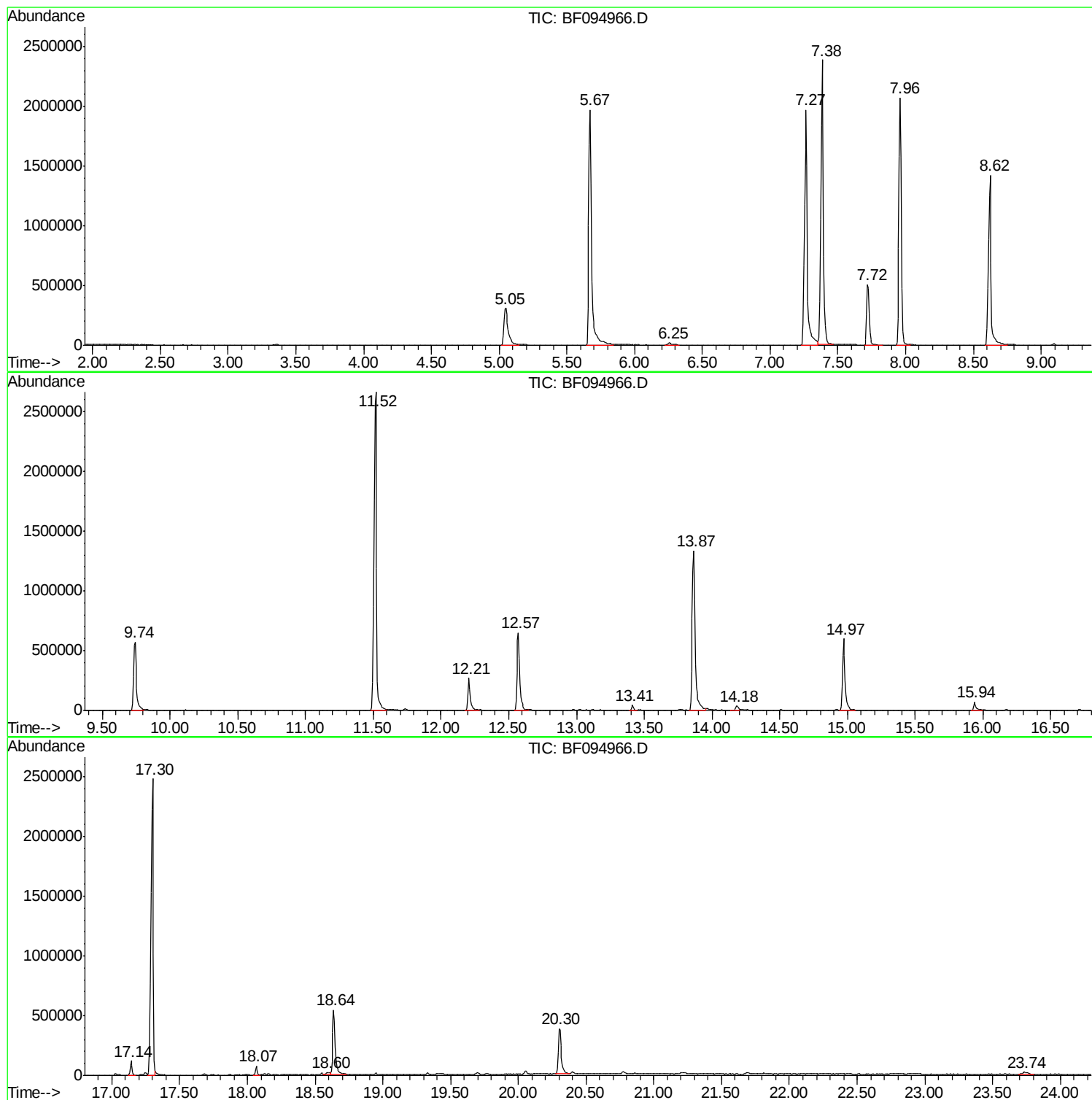
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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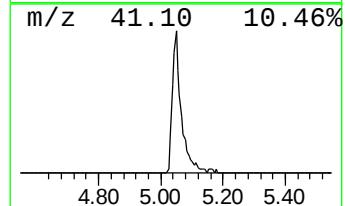
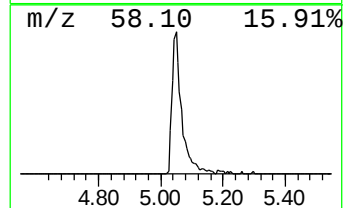
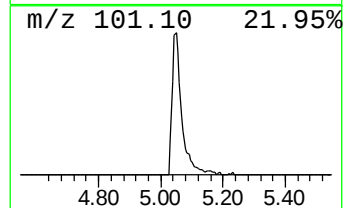
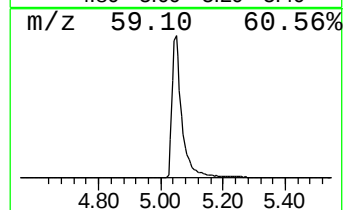
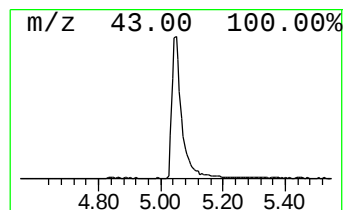
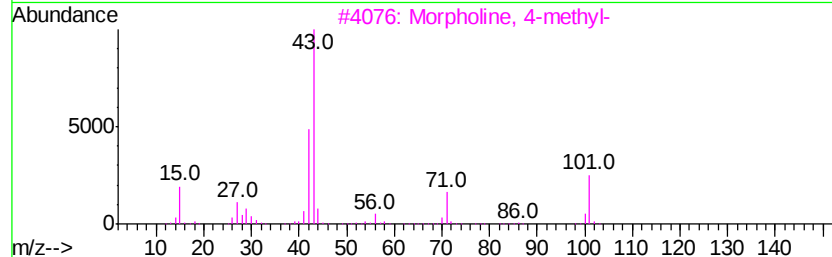
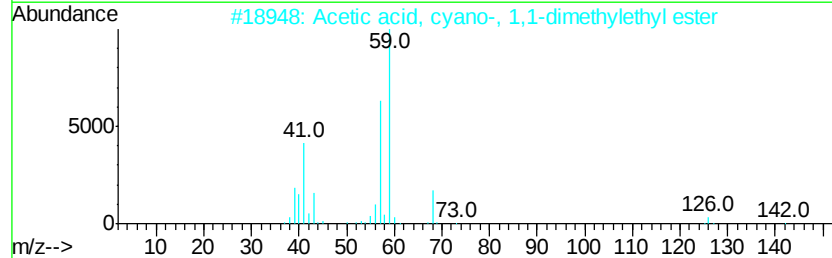
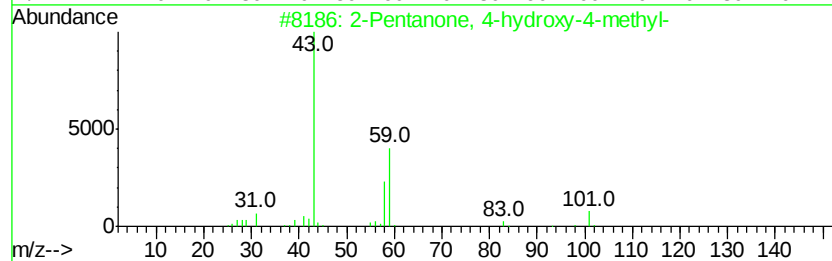
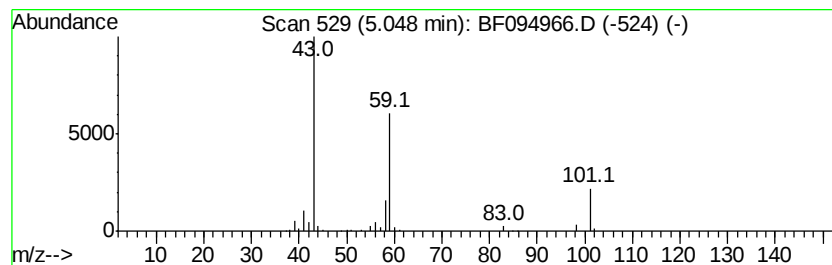
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	21.62 ng	664491	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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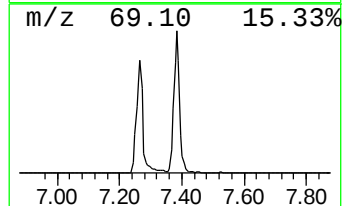
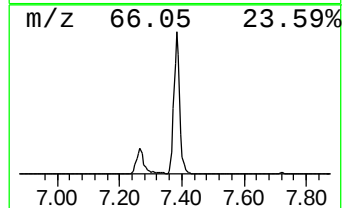
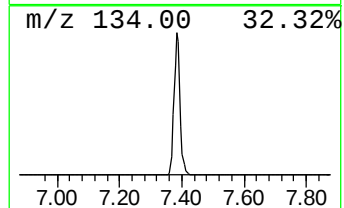
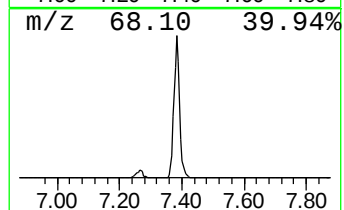
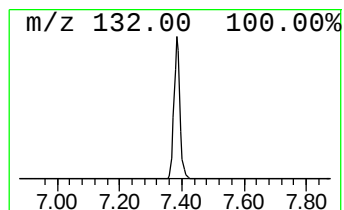
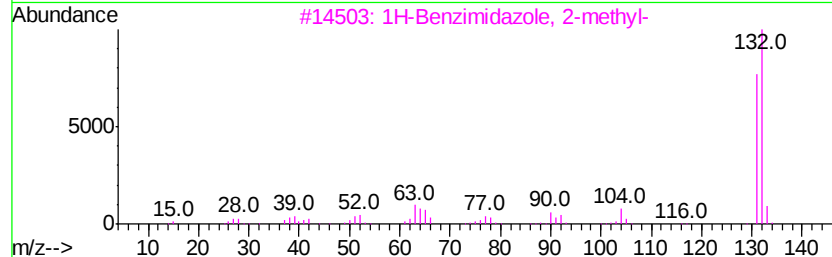
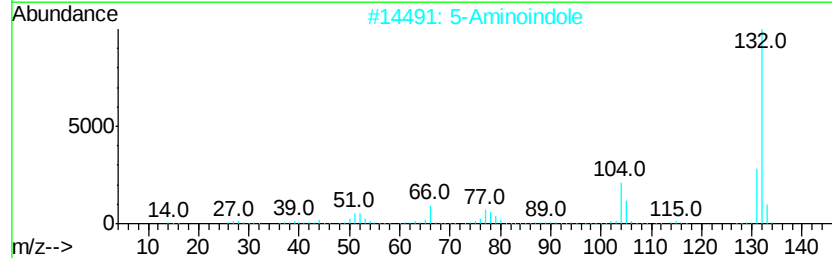
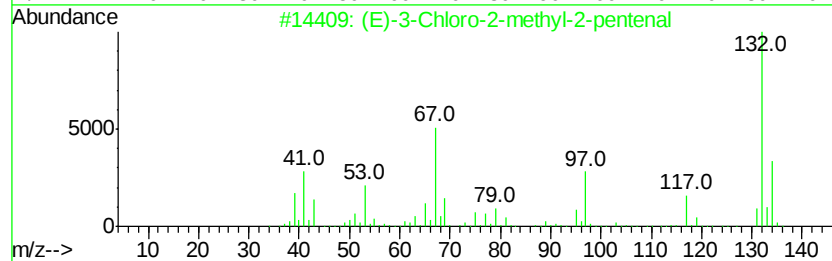
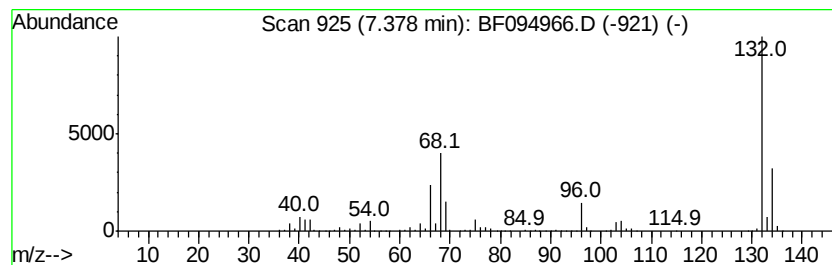
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	104.33 ng	3206190	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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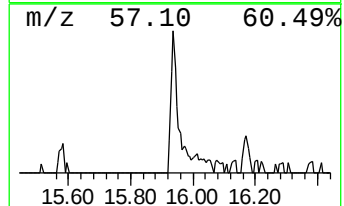
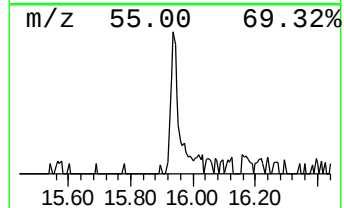
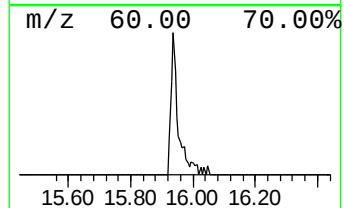
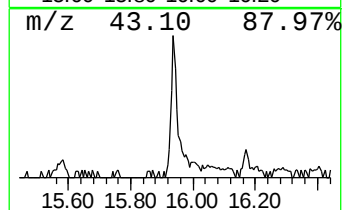
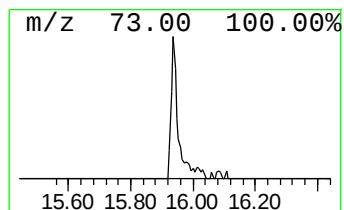
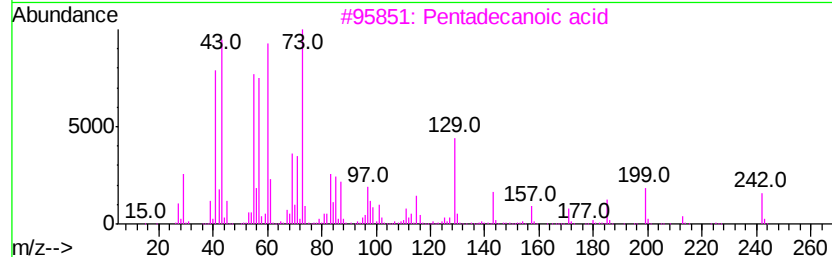
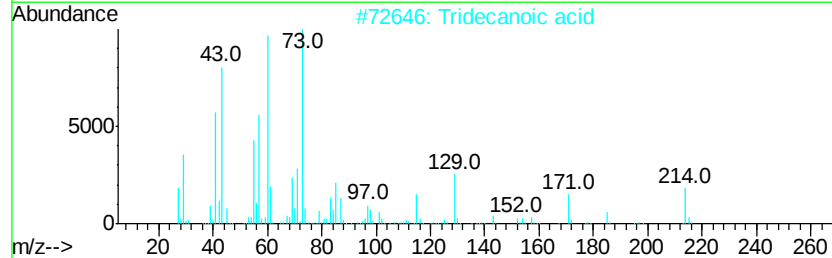
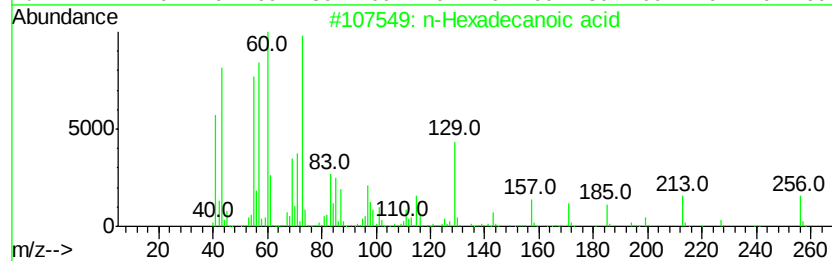
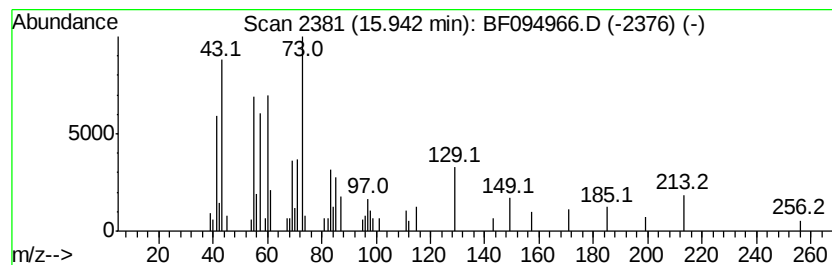
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.47 ng	102287	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	72



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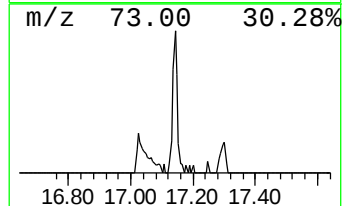
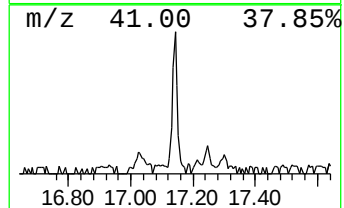
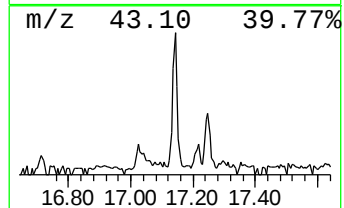
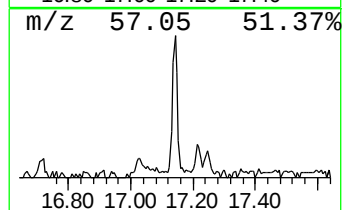
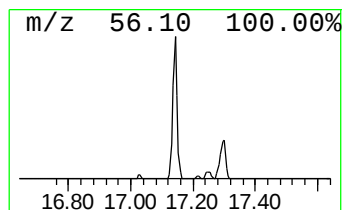
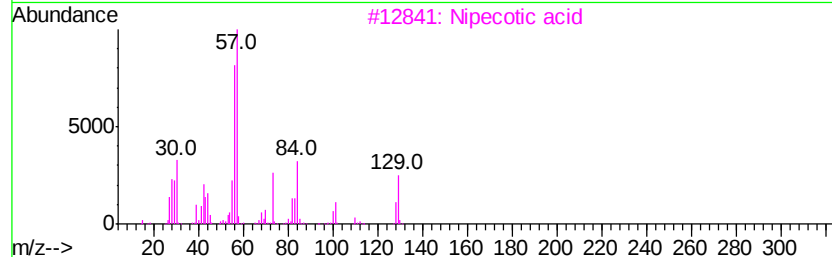
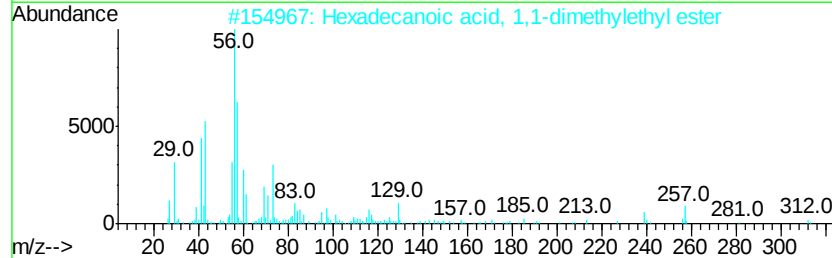
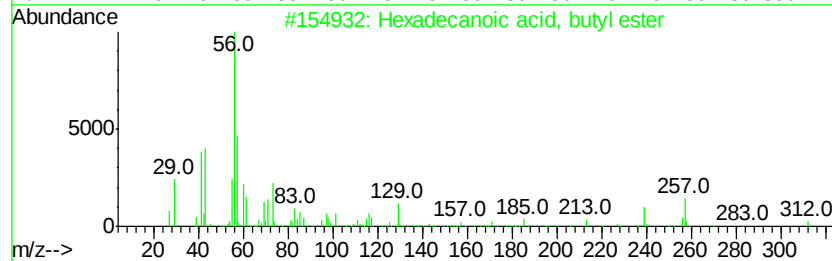
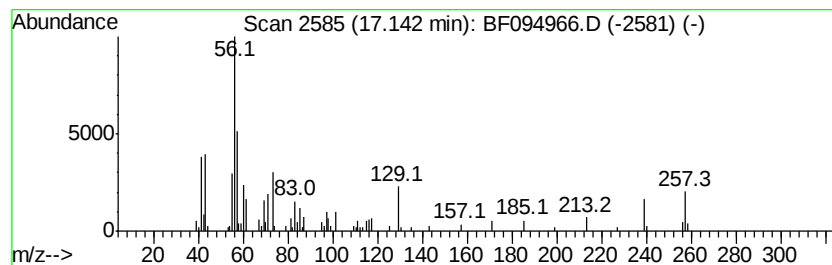
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	3.41 ng	123409	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27



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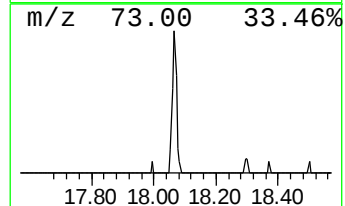
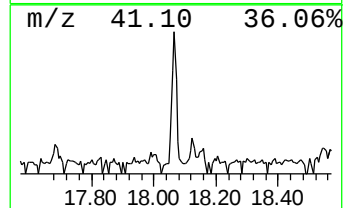
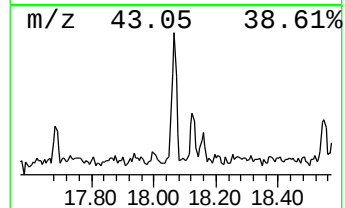
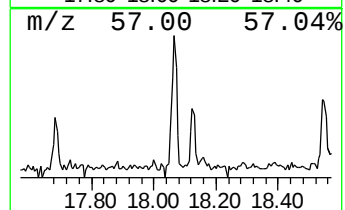
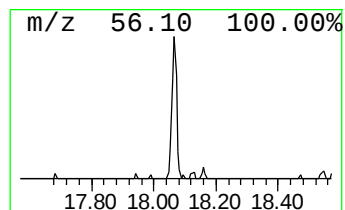
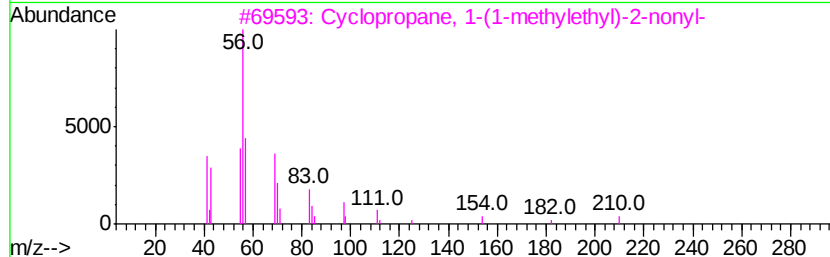
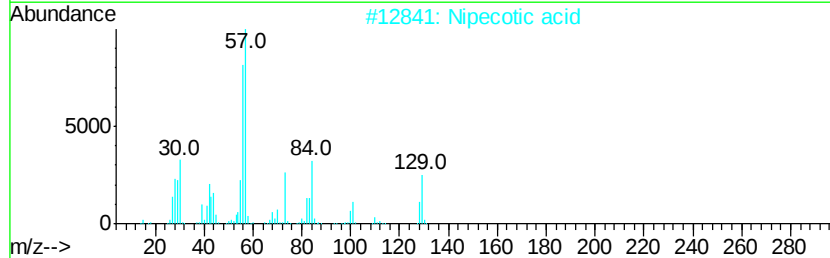
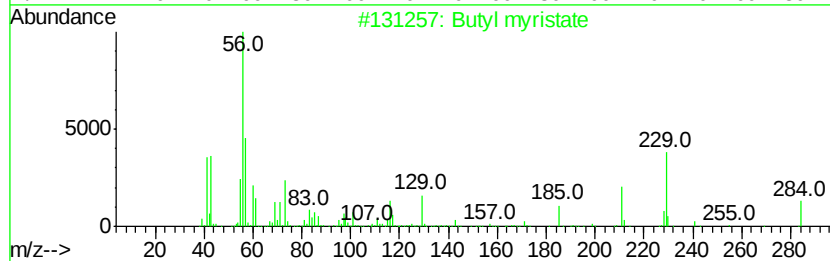
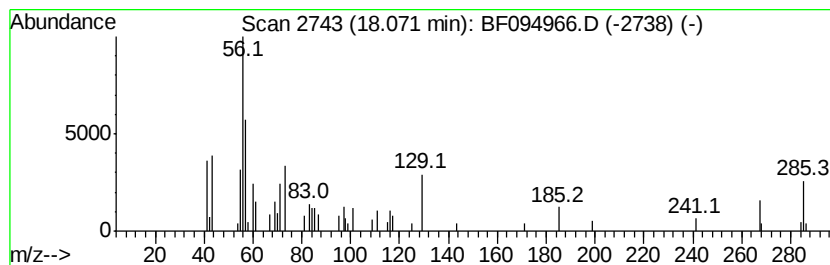
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown18.07 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	2.10 ng	75845	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl myristate	284	C18H36O2	000110-36-1	42
2		Nipecotic acid	129	C6H11NO2	000498-95-3	38
3		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27
5		2-Methyl-1-octadecene	266	C19H38	061868-20-0	27



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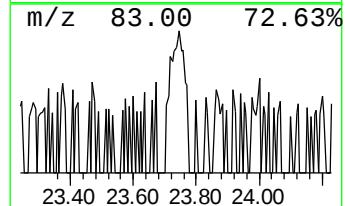
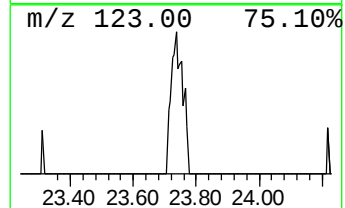
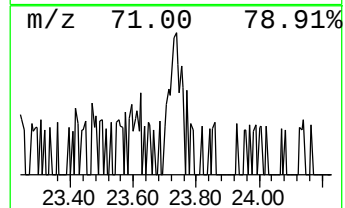
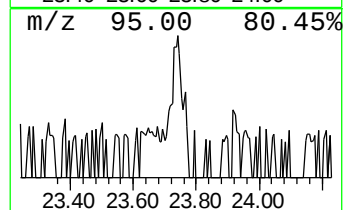
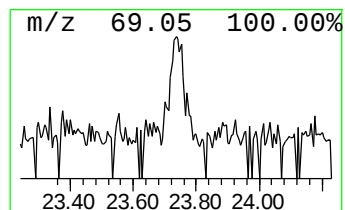
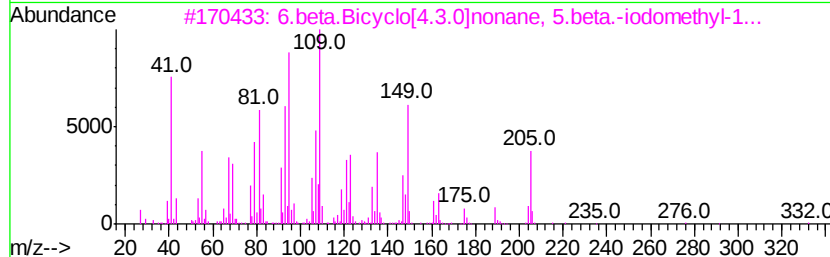
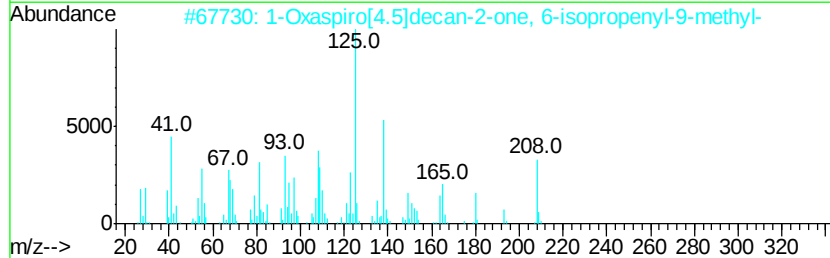
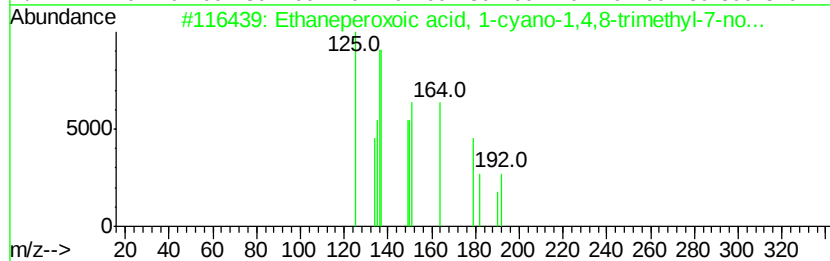
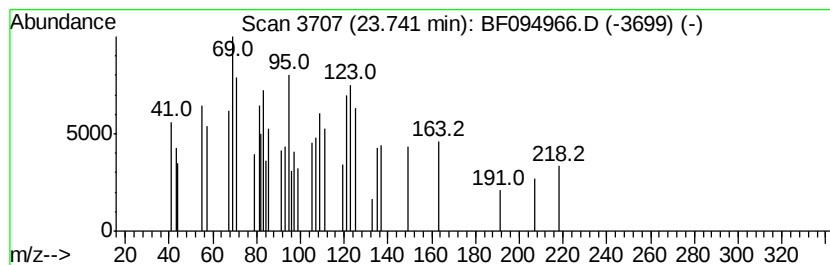
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown23.74 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.74	2.12 ng	58213	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethaneperoxoic acid, 1-cvano-1,4...	267	C15H25N03	058422-65-4	38
2		1-Oxaspiro[4.5]decan-2-one, 6-is...	208	C13H20O2	1000157-58-3	22
3		6.beta.Bicvclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	18
4		4a,5,6,7,8,8a,10,10a-Octahydro-2...	207	C12H17N02	1000194-96-9	14
5		2,4,5,5,8a-Pentamethyl-4a,5,6,7,...	208	C14H24O	1000195-30-1	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094966.D
Acq On : 8 May 2017 3:35
Operator : SJ/MA
Sample : I3007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-BW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.05	21.6	ng	664491	1	7.72	614615	20.0
unknown7.38	7.38	104.3	ng	3206190	1	7.72	614615	20.0
n-Hexadecanoic acid	15.94	2.5	ng	102287	4	14.97	828202	20.0
Hexadecanoic acid...	17.14	3.4	ng	123409	5	18.64	722872	20.0
unknown18.07	18.07	2.1	ng	75845	5	18.64	722872	20.0
unknown23.74	23.74	2.1	ng	58213	6	20.31	550151	20.0