

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060217\
 Data File : BF095659.D
 Acq On : 3 Jun 2017 5:57
 Operator : SJ/MA
 Sample : I3414-01
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-PMW-11S

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-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	4.781	522	526	541	rBV	24574	66466	2.40%	0.423%
2	5.463	639	642	668	rBV	249747	690810	24.90%	4.396%
3	7.110	919	922	933	rBV	144467	356086	12.83%	2.266%
4	7.198	933	937	955	rVB	847425	1524185	54.94%	9.699%
5	7.534	991	994	1010	rBV	344401	463292	16.70%	2.948%
6	7.775	1030	1035	1056	rBV	1529250	2017059	72.70%	12.835%
7	8.451	1145	1150	1177	rBV	961385	1468506	52.93%	9.344%
8	9.569	1336	1340	1357	rBV	437653	609828	21.98%	3.880%
9	11.345	1636	1642	1663	rBV	2047613	2774455	100.00%	17.655%
10	12.045	1756	1761	1771	rBV	45723	70875	2.55%	0.451%
11	12.398	1816	1821	1831	rBV2	439493	604383	21.78%	3.846%
12	12.963	1907	1917	1931	rBV	380839	738175	26.61%	4.697%
13	13.239	1959	1964	1968	rVB	24697	28596	1.03%	0.182%
14	13.692	2037	2041	2054	rBV	487746	729271	26.29%	4.641%
15	14.010	2091	2095	2103	rBV	20077	27757	1.00%	0.177%
16	14.798	2224	2229	2243	rVB	328777	449221	16.19%	2.859%
17	15.792	2392	2398	2409	rBV	196584	260093	9.37%	1.655%
18	16.886	2579	2584	2597	rBV	167439	232673	8.39%	1.481%
19	16.992	2599	2602	2608	rVB	28503	32037	1.15%	0.204%
20	17.151	2623	2629	2633	rBV	1503657	1770562	63.82%	11.267%
21	18.392	2836	2840	2848	rBV3	40312	69433	2.50%	0.442%
22	18.498	2854	2858	2865	rBV	354191	438564	15.81%	2.791%
23	20.174	3139	3143	3150	rBV	217572	292874	10.56%	1.864%

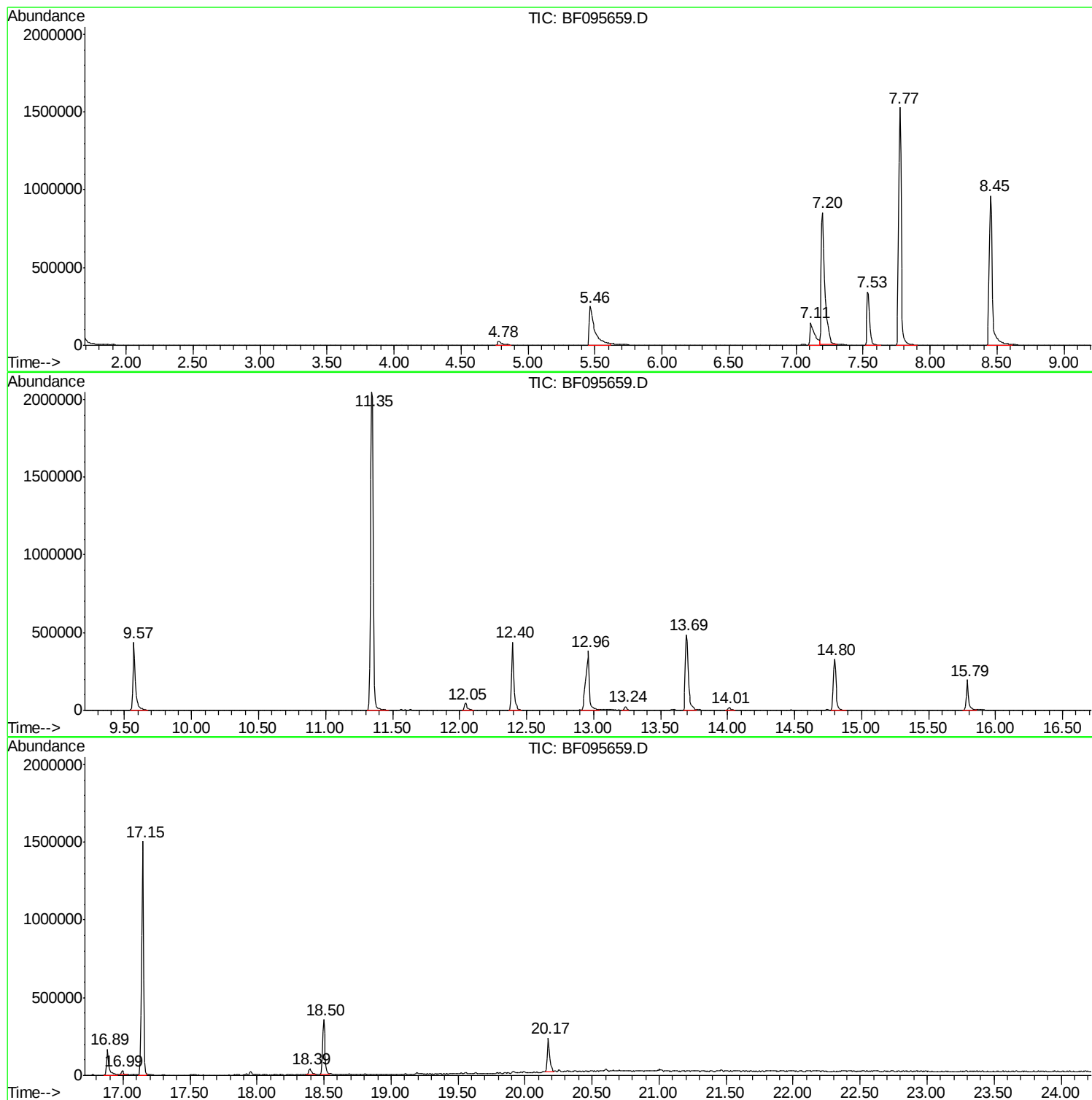
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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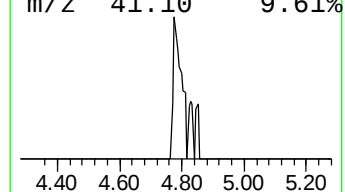
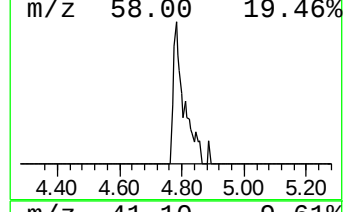
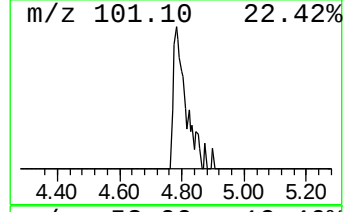
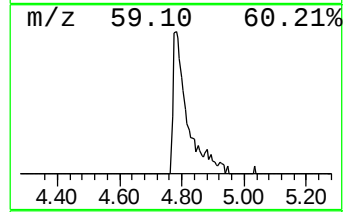
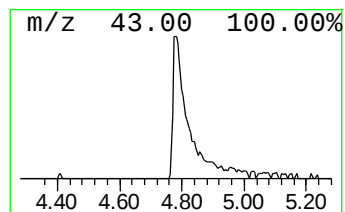
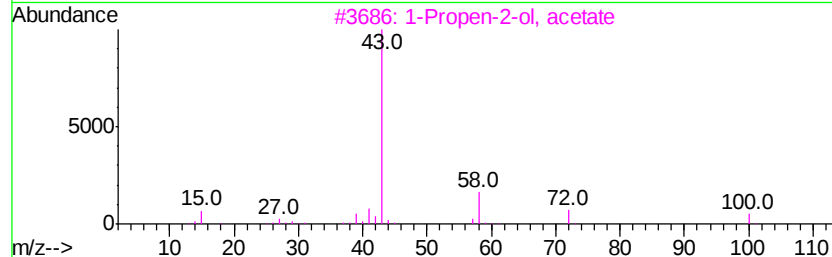
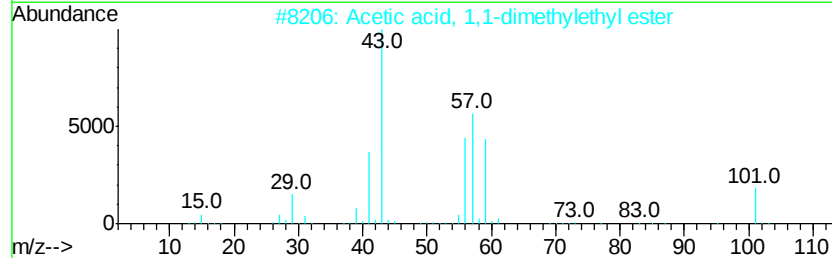
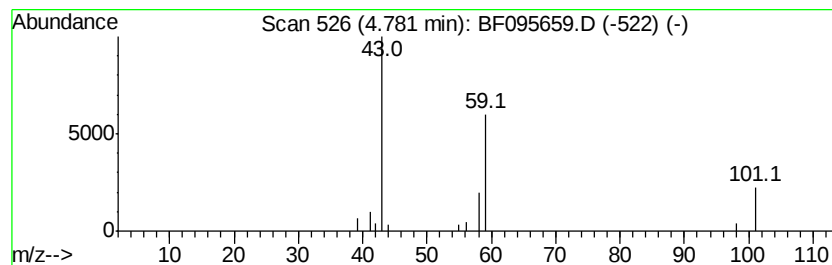
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	2.87 ng	66466	1,4-Dichlorobenzene-d4	7.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			Acetone	58	C3H6O	000067-64-1	7
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7



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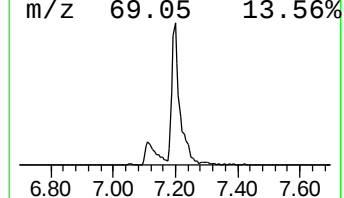
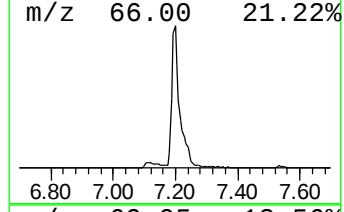
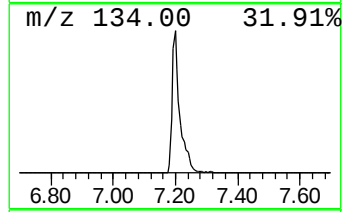
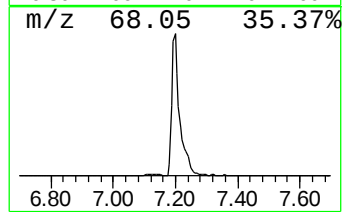
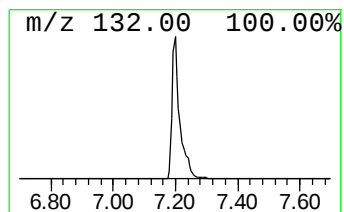
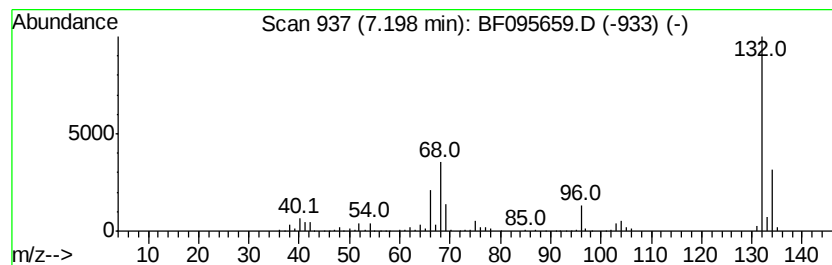
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.20 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	65.80 ng	1524190	1,4-Dichlorobenzene-d4	7.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3		Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5		Aminoindole	132	C8H8N2	005192-03-0	12
4	1H		Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5	5		Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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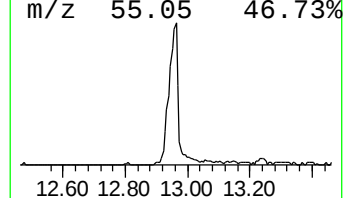
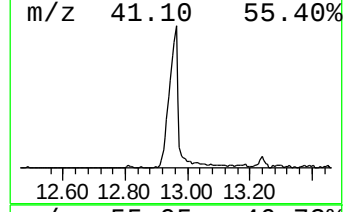
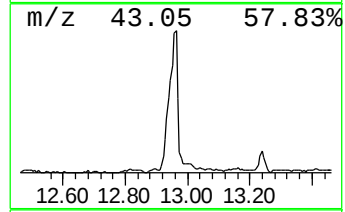
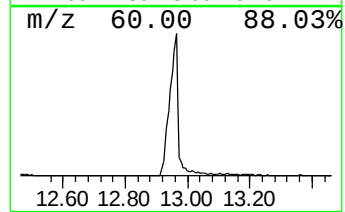
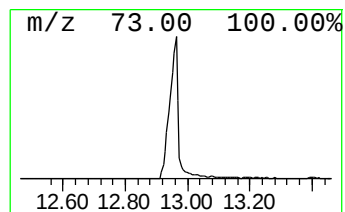
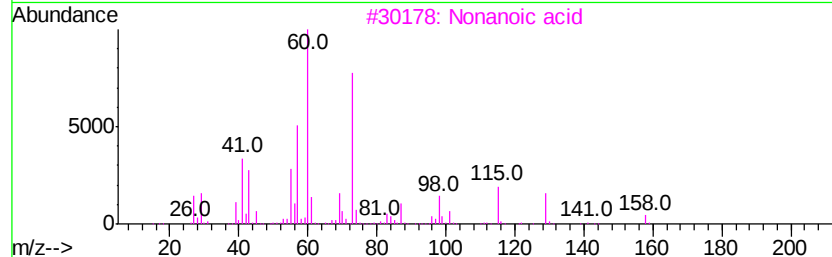
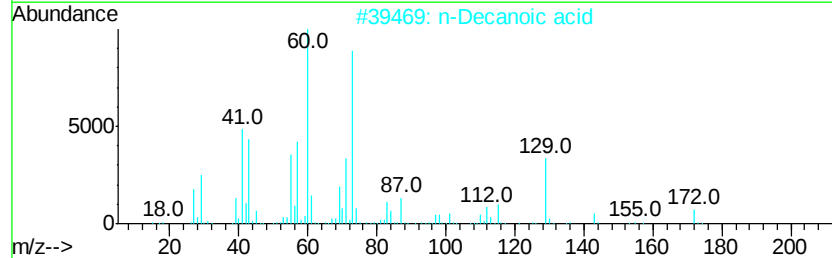
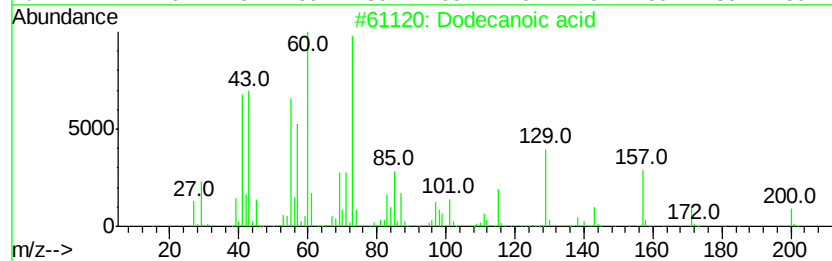
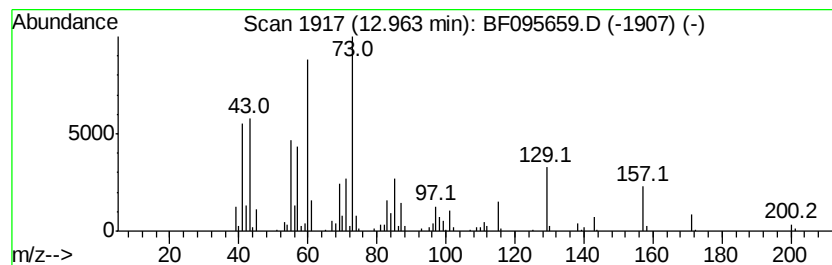
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Peak Number 4 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.96	24.43 ng	738175	Acenaphthene-d10		12.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			n-Decanoic acid	172	C10H20O2	000334-48-5	59
3			Nonanoic acid	158	C9H18O2	000112-05-0	53
4			Hexanoic acid	116	C6H12O2	000142-62-1	38
5			Octanoic acid	144	C8H16O2	000124-07-2	27



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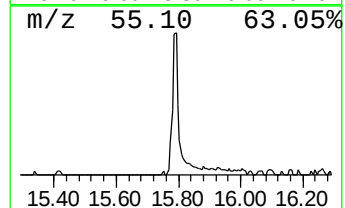
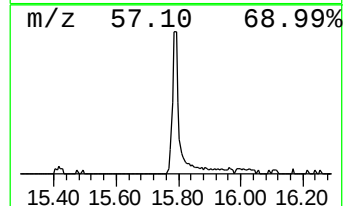
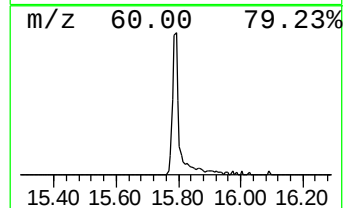
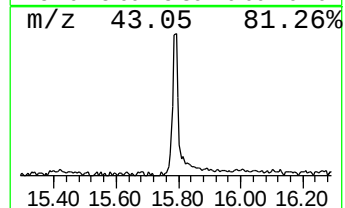
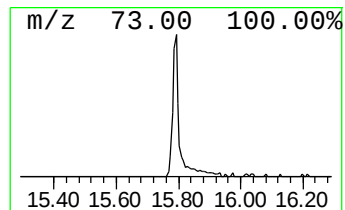
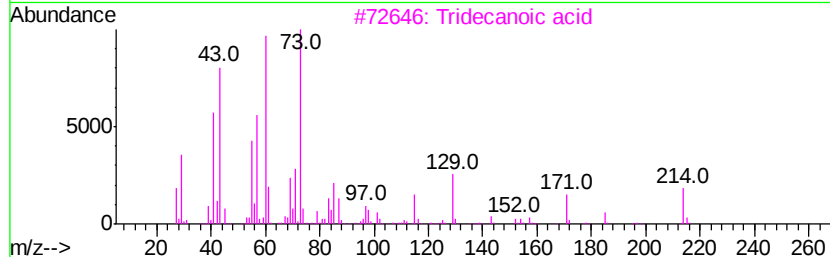
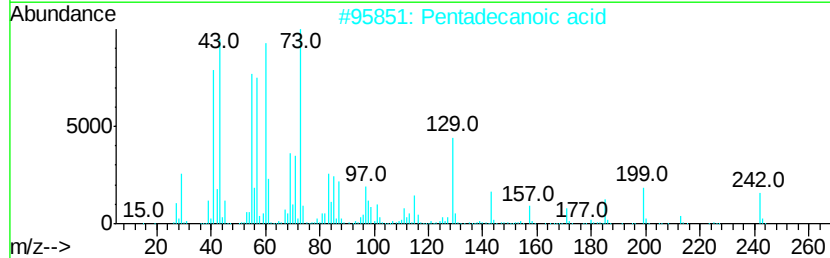
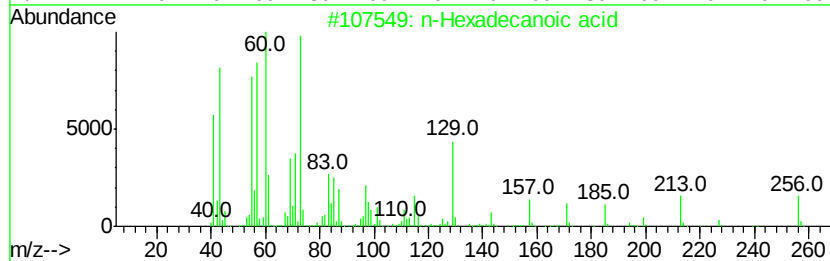
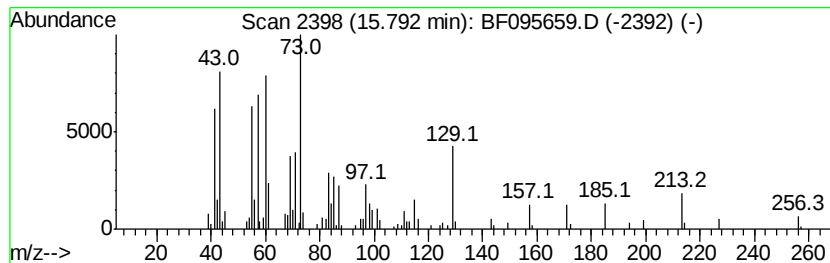
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	11.58 ng	260093	Phenanthrene-d10	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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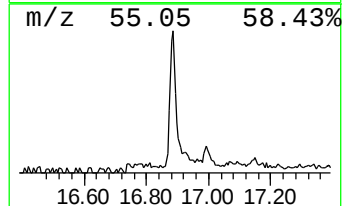
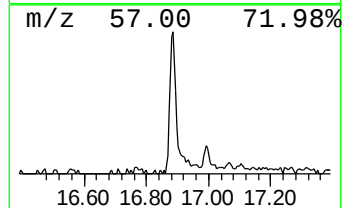
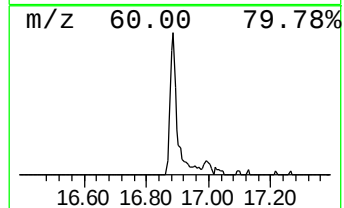
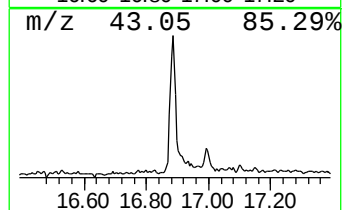
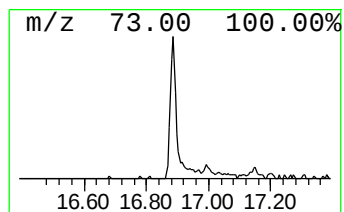
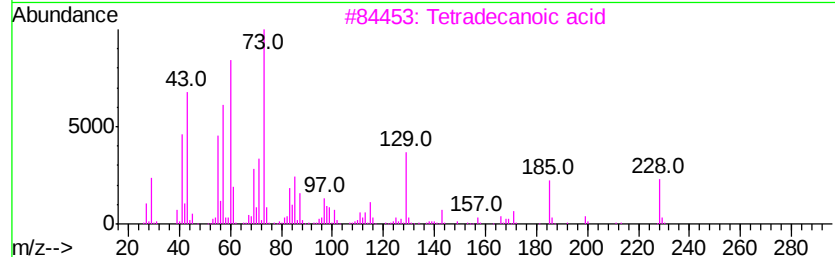
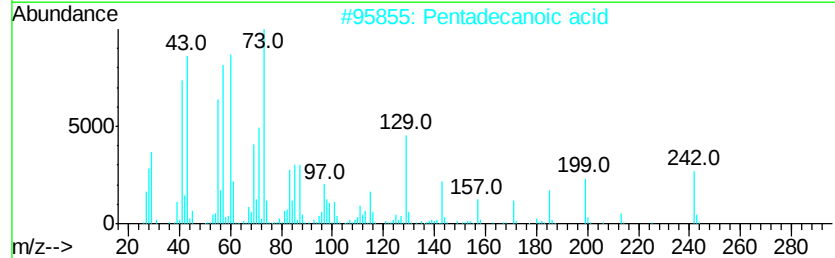
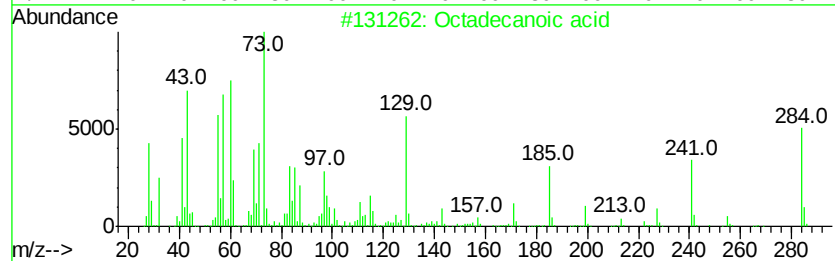
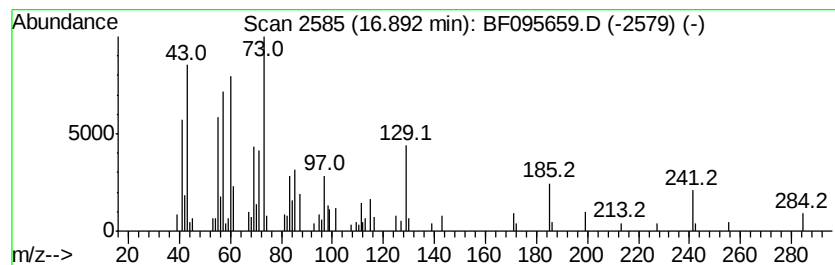
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Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	10.61 ng	232673	Chrysene-d12	18.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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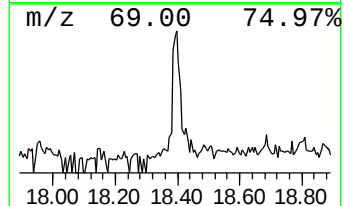
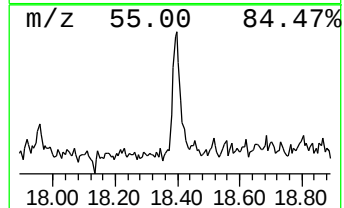
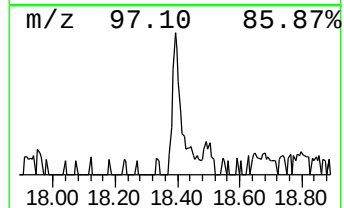
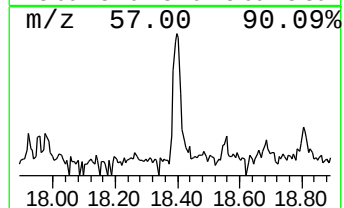
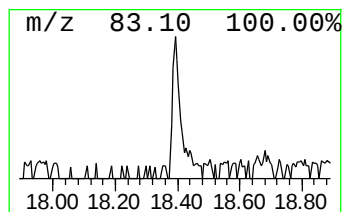
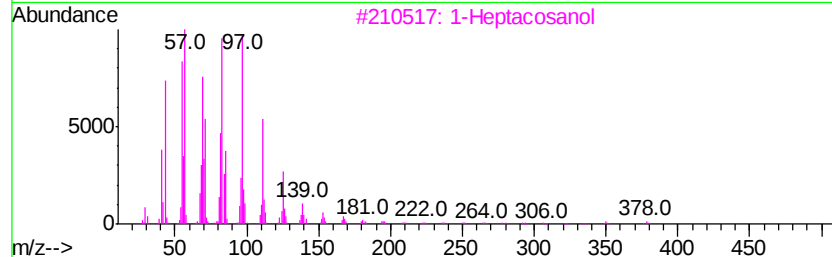
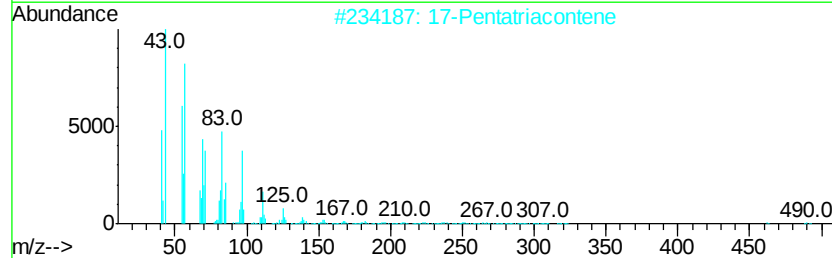
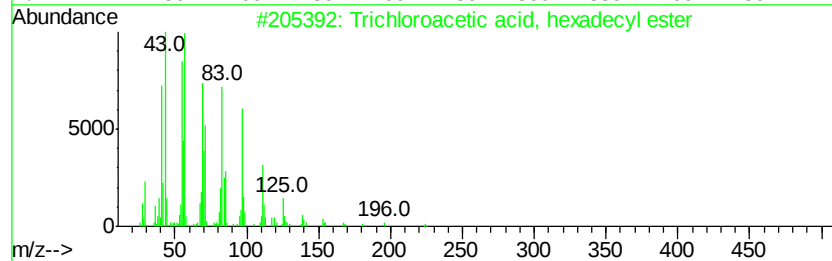
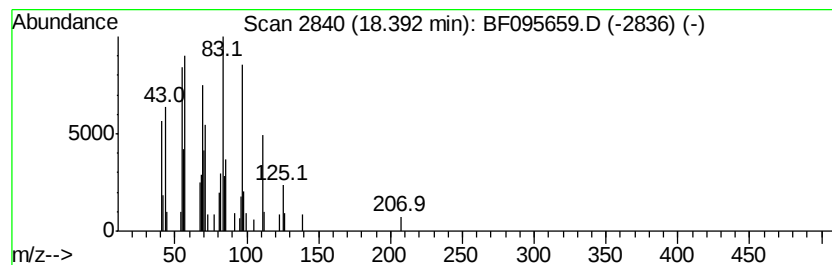
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Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	3.17 ng	69433	Chrysene-d12	18.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	90
3		1-Heptacosanol	396	C27H56O	002004-39-9	90
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	83
5		1-Docosene	308	C22H44	001599-67-3	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060217\
Data File : BF095659.D
Acq On : 3 Jun 2017 5:57
Operator : SJ/MA
Sample : I3414-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-PMW-11S

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...	4.78	2.9	ng	66466	1	7.53	463292	20.0
unknown7.20	7.20	65.8	ng	1524190	1	7.53	463292	20.0
Dodecanoic acid	12.96	24.4	ng	738175	3	12.40	604383	20.0
n-Hexadecanoic acid	15.79	11.6	ng	260093	4	14.80	449221	20.0
Octadecanoic acid	16.89	10.6	ng	232673	5	18.50	438564	20.0
Trichloroacetic a...	18.39	3.2	ng	69433	5	18.50	438564	20.0