

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050817\
 Data File : BF094990.D
 Acq On : 8 May 2017 20:37
 Operator : SJ/MA
 Sample : I3010-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-1

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	5.031	521	526	549	rBV	290958	630117	20.71%	2.421%
2	5.660	628	633	659	rBV	1855320	2781026	91.42%	10.685%
3	6.242	728	732	740	rBV2	15167	30933	1.02%	0.119%
4	7.260	899	905	919	rBV	1827641	2771856	91.12%	10.649%
5	7.378	919	925	939	rVB	2292054	2992632	98.37%	11.498%
6	7.713	978	982	994	rVB	463783	533975	17.55%	2.052%
7	7.954	1018	1023	1037	rBV	1840993	2177918	71.59%	8.367%
8	8.613	1130	1135	1157	rBV	1242155	1770100	58.19%	6.801%
9	9.736	1321	1326	1344	rBV	520602	734155	24.13%	2.821%
10	11.507	1622	1627	1643	rBV	2375670	3042110	100.00%	11.688%
11	12.201	1740	1745	1757	rBV	251042	333580	10.97%	1.282%
12	12.560	1801	1806	1819	rBV2	580930	853817	28.07%	3.280%
13	13.407	1945	1950	1956	rBV	35043	40587	1.33%	0.156%
14	13.860	2021	2027	2040	rBV	1267541	1855599	61.00%	7.129%
15	14.177	2077	2081	2092	rVB	31696	45026	1.48%	0.173%
16	14.965	2210	2215	2230	rBV	546292	765301	25.16%	2.940%
17	15.936	2375	2380	2396	rBV	167510	238834	7.85%	0.918%
18	17.018	2559	2564	2570	rBV2	64106	89299	2.94%	0.343%
19	17.295	2605	2611	2614	rBV	2078798	2544882	83.66%	9.777%
20	18.577	2820	2829	2834	rBV5	39925	126284	4.15%	0.485%
21	18.630	2834	2838	2846	rVV	532972	666224	21.90%	2.560%
22	18.695	2846	2849	2853	rVB	39576	44172	1.45%	0.170%
23	20.047	3075	3079	3084	rBV	44650	52158	1.71%	0.200%
24	20.300	3117	3122	3134	rVB	401190	527915	17.35%	2.028%
25	20.771	3197	3202	3208	rVB2	27468	43568	1.43%	0.167%
26	20.871	3212	3219	3221	rBV5	19548	39930	1.31%	0.153%
27	23.729	3696	3705	3715	rVB7	105687	296505	9.75%	1.139%

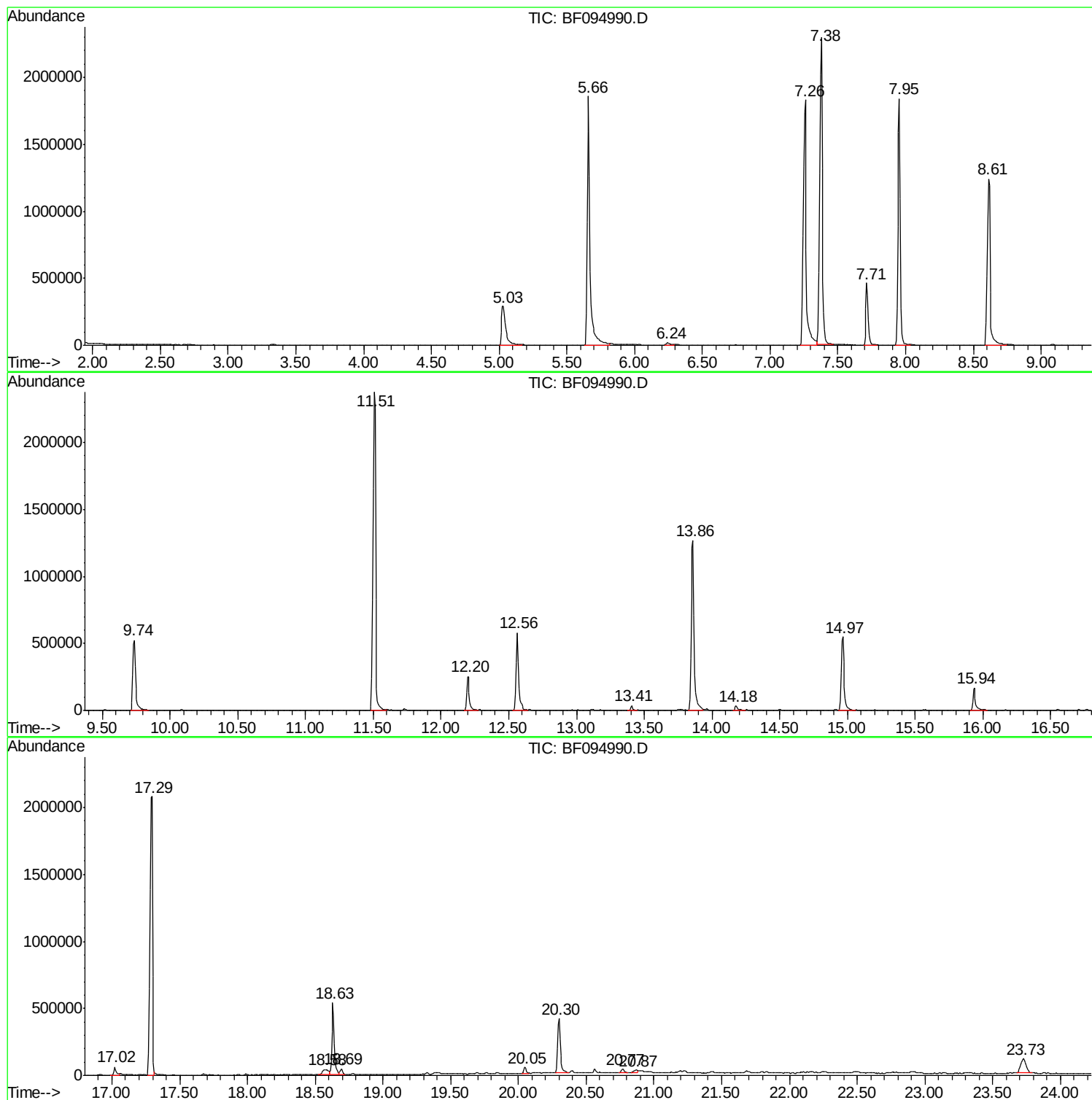
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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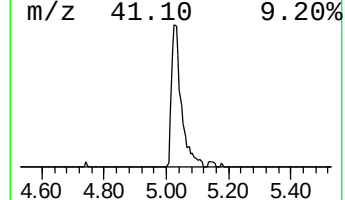
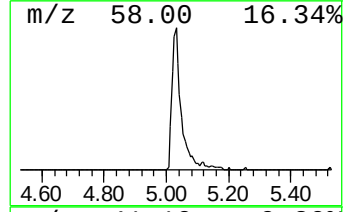
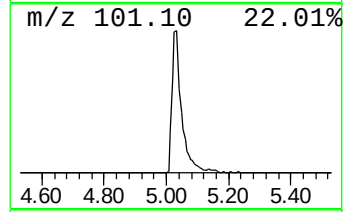
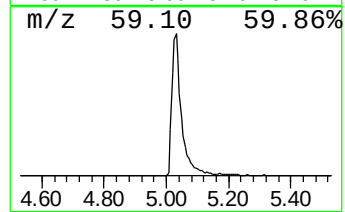
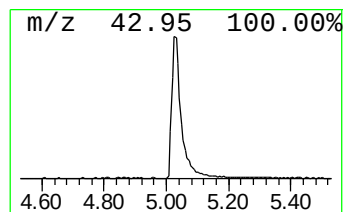
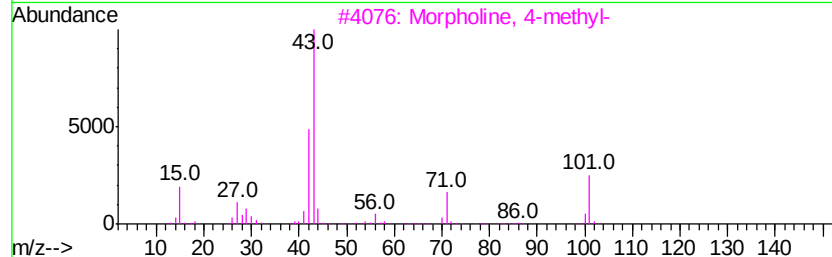
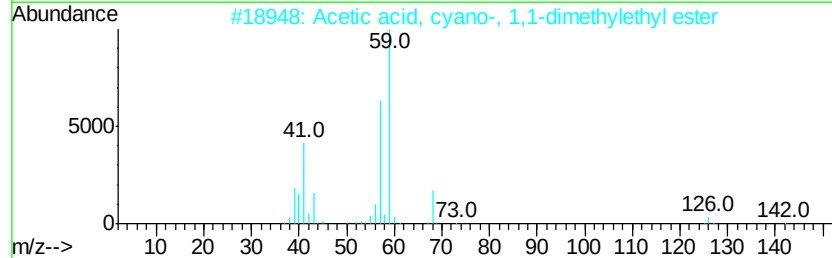
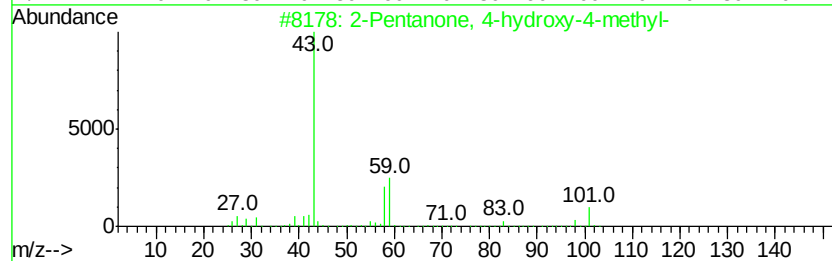
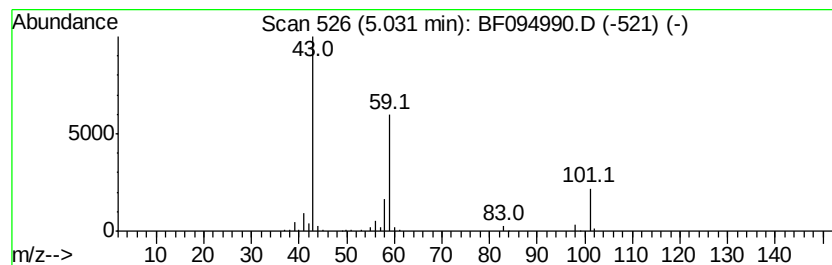
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.03	23.60 ng	630117	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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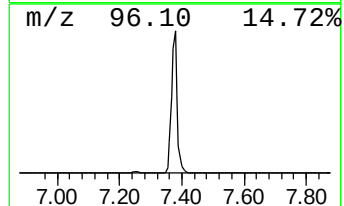
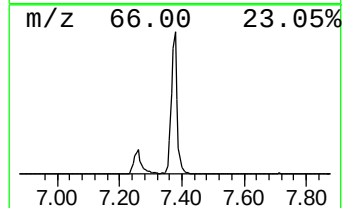
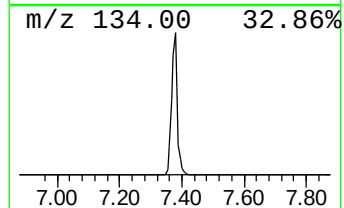
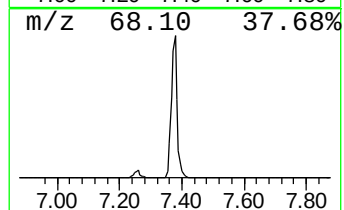
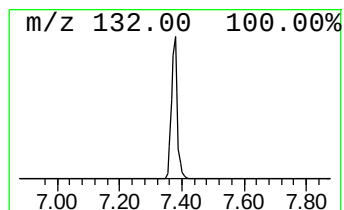
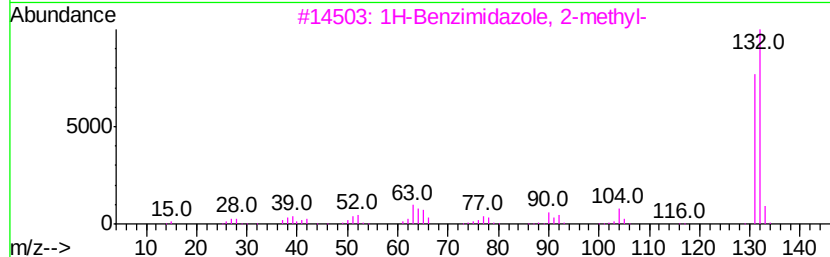
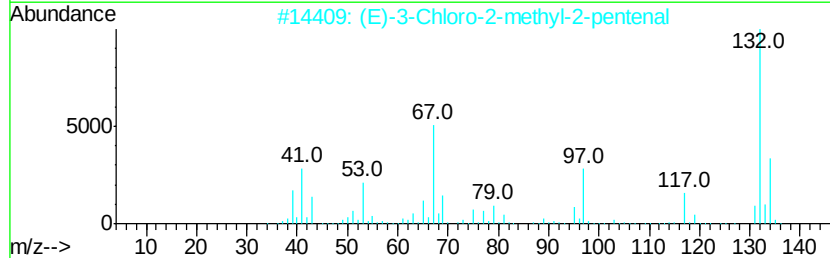
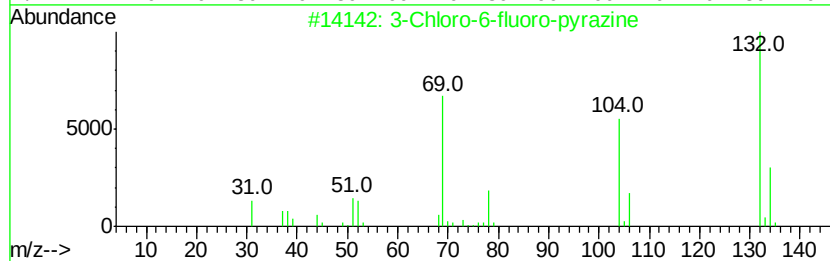
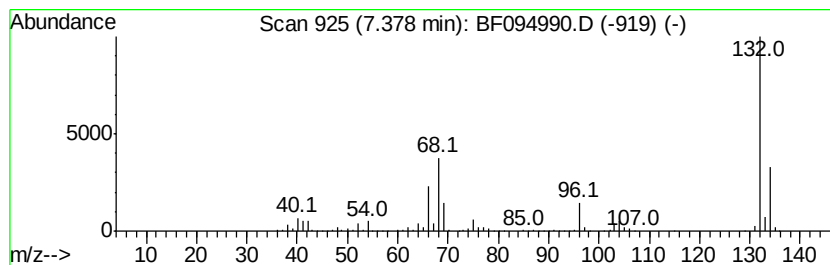
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	112.09 ng	2992630	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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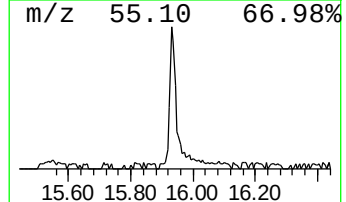
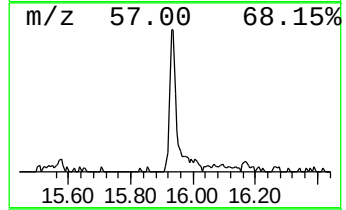
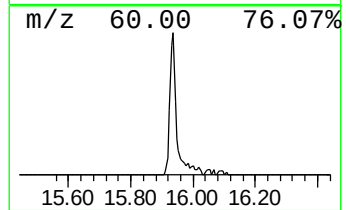
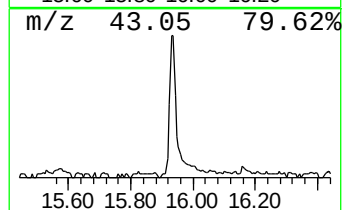
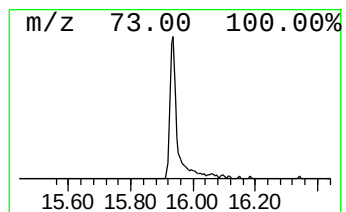
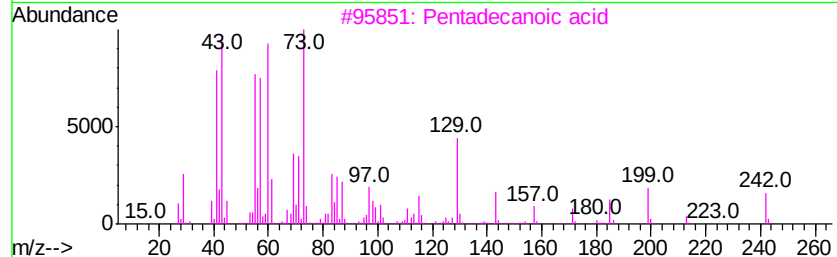
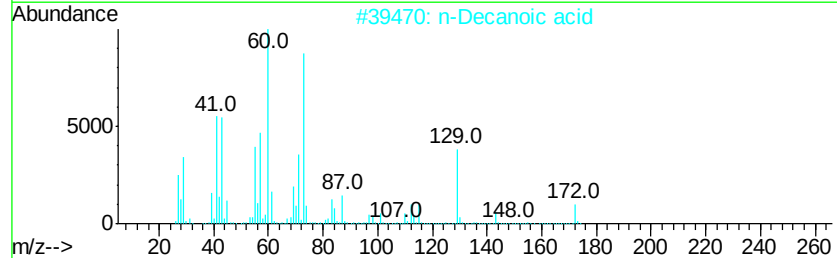
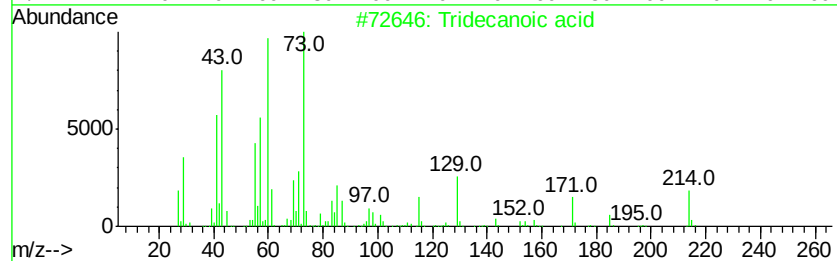
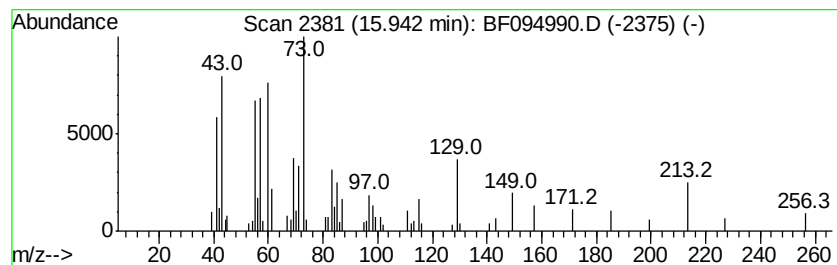
Instrument :
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Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.94	6.24 ng	238834	Phenanthrene-d10		14.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	81
2	n-Decanoic acid	172	C10H20O2	000334-48-5	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



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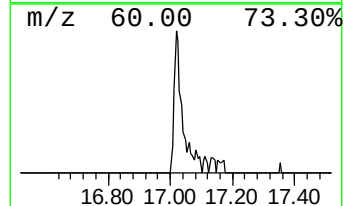
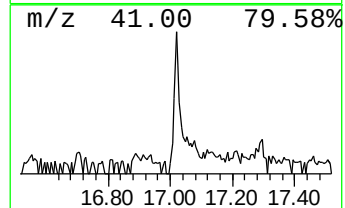
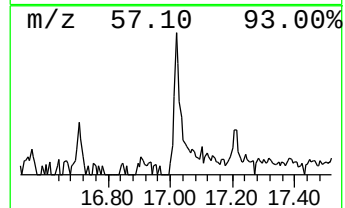
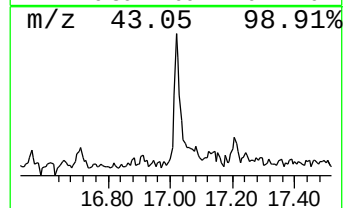
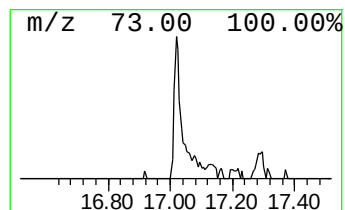
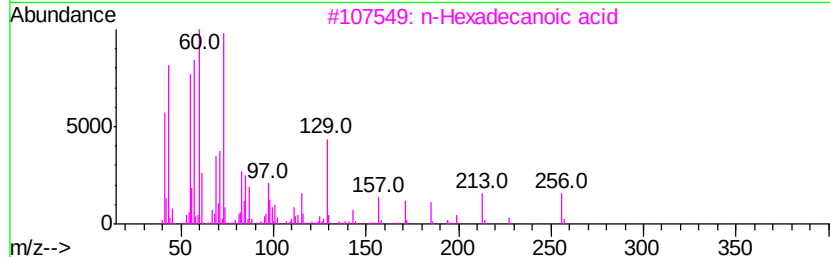
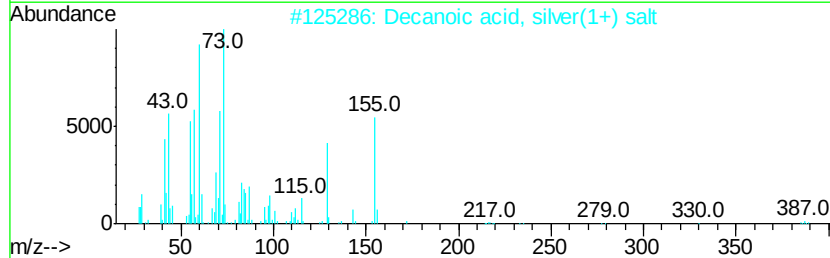
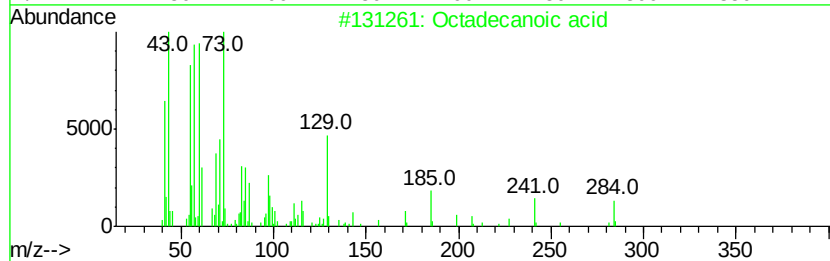
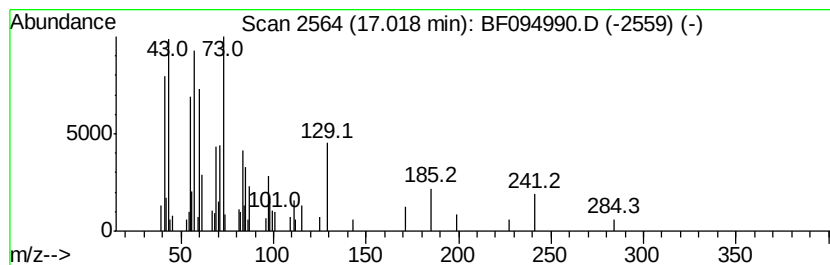
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	2.68 ng	89299	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
4		Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	30
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	30



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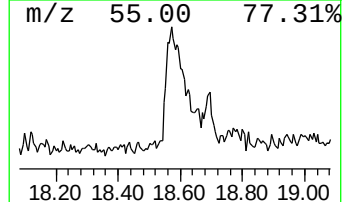
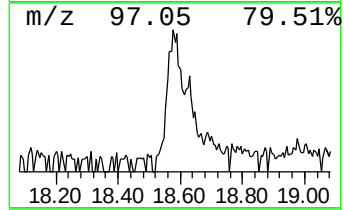
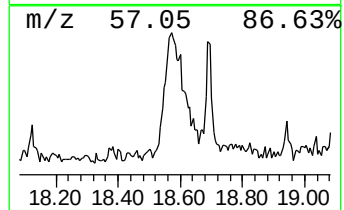
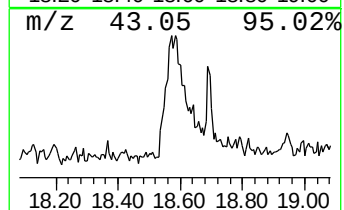
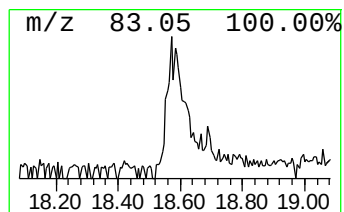
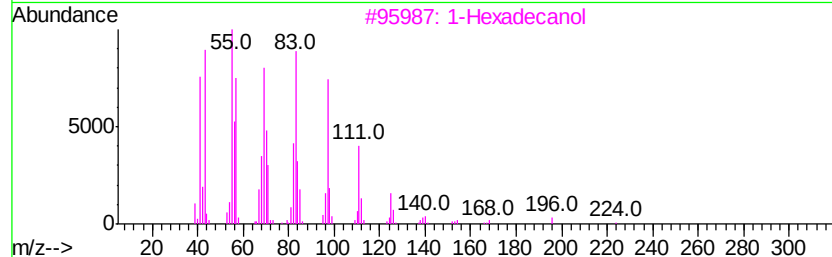
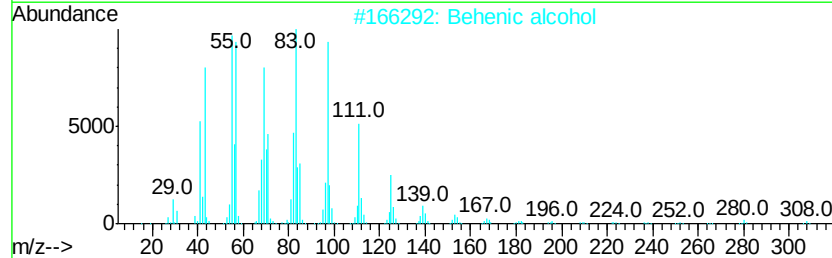
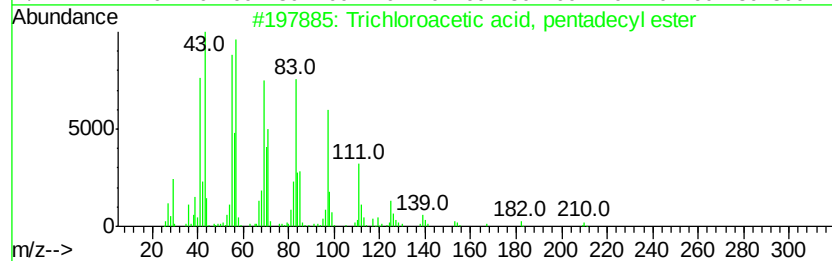
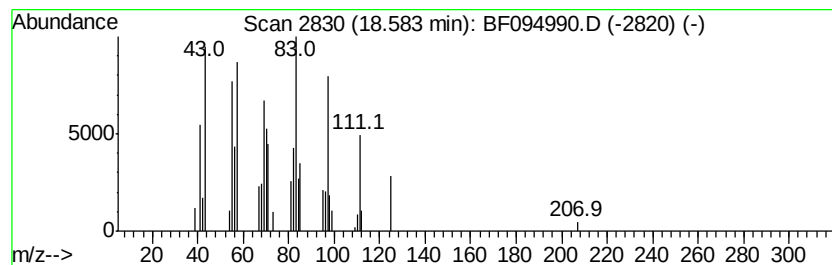
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	3.79 ng	126284	Chrysene-d12	18.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2		Behenic alcohol	326	C22H46O	000661-19-8	87
3		1-Hexadecanol	242	C16H34O	036653-82-4	87
4		1-Heneicosanol	312	C21H44O	015594-90-8	87
5		1-Nonadecene	266	C19H38	018435-45-5	87



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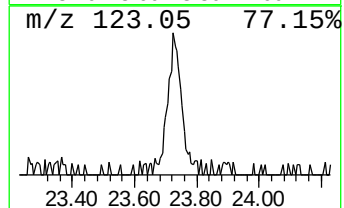
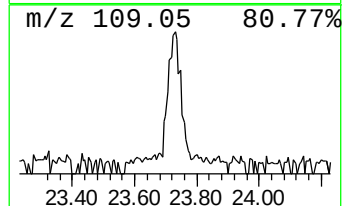
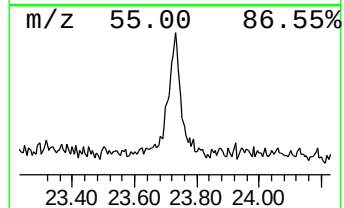
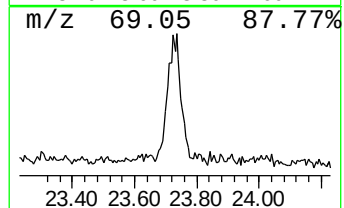
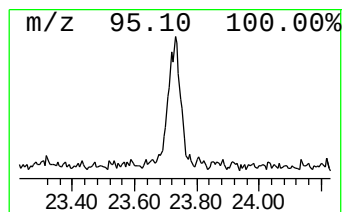
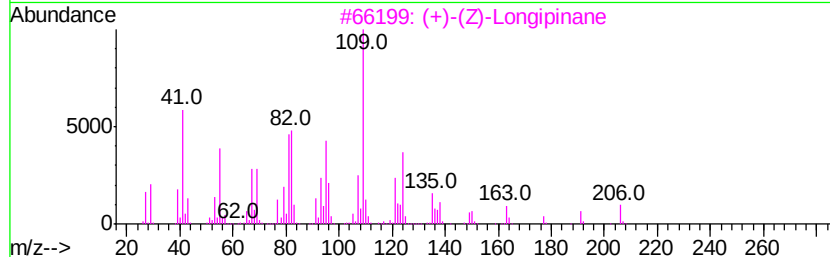
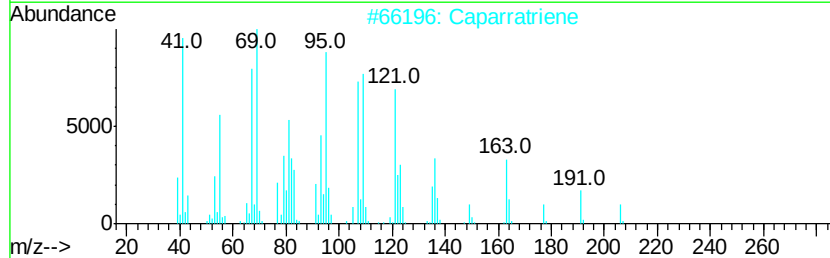
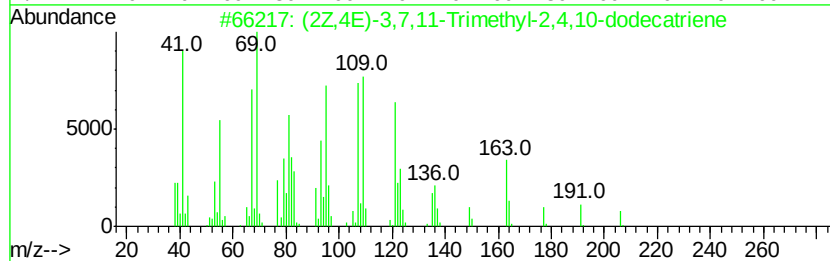
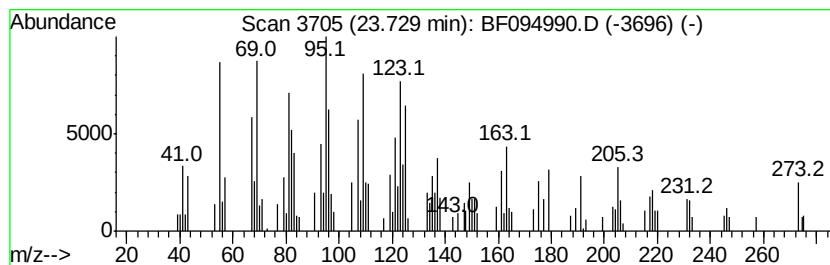
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (2Z,4E)-3,7,11-Trimethyl-2,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.73	11.23 ng	296505	Perylene-d12	20.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	60	
2	Caparratriene	206	C15H26	1000374-08-7	49	
3	(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	47	
4	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	45	
5	1H-Cycloprop[e]azulene, decahydr...	206	C15H26	028580-43-0	42	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050817\
Data File : BF094990.D
Acq On : 8 May 2017 20:37
Operator : SJ/MA
Sample : I3010-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1

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...	5.03	23.6	ng	630117	1	7.71	533975	20.0
unknown7.38	7.38	112.1	ng	2992630	1	7.71	533975	20.0
Tridecanoic acid	15.94	6.2	ng	238834	4	14.97	765301	20.0
Octadecanoic acid	17.02	2.7	ng	89299	5	18.63	666224	20.0
Trichloroacetic a...	18.58	3.8	ng	126284	5	18.63	666224	20.0
(2Z,4E)-3,7,11-Tr...	23.73	11.2	ng	296505	6	20.30	527915	20.0