

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
 Data File : BF094968.D
 Acq On : 8 May 2017 4:38
 Operator : SJ/MA
 Sample : I2947-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04-6.5-7.0

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	3.325	229	236	249	rBV	32425	70471	3.49%	0.378%
2	5.037	523	527	544	rBV	105743	208748	10.33%	1.118%
3	5.666	630	634	665	rBV	1125863	1873411	92.73%	10.036%
4	7.260	900	905	921	rBV	1218080	1801462	89.17%	9.651%
5	7.378	921	925	935	rVB	1501444	2006428	99.32%	10.749%
6	7.719	979	983	1000	rVB	464217	542225	26.84%	2.905%
7	7.960	1019	1024	1040	rBV	1198987	1508906	74.69%	8.084%
8	8.619	1131	1136	1153	rBV	790262	1126851	55.78%	6.037%
9	9.736	1322	1326	1340	rBV	514340	724255	35.85%	3.880%
10	11.513	1623	1628	1641	rBV	1653808	2020217	100.00%	10.823%
11	12.207	1741	1746	1753	rBV	168944	219044	10.84%	1.173%
12	12.571	1803	1808	1820	rBV2	568717	826434	40.91%	4.427%
13	13.413	1947	1951	1956	rVB	38533	41127	2.04%	0.220%
14	13.865	2023	2028	2042	rBV	769199	1210853	59.94%	6.487%
15	14.183	2078	2082	2086	rBV	31821	42460	2.10%	0.227%
16	14.971	2211	2216	2230	rBV	617581	792044	39.21%	4.243%
17	15.936	2376	2380	2389	rBV	71621	99434	4.92%	0.533%
18	16.759	2518	2520	2529	rVB4	18152	38592	1.91%	0.207%
19	16.836	2529	2533	2538	rVB	125609	132035	6.54%	0.707%
20	17.030	2562	2566	2569	rBV3	15468	24675	1.22%	0.132%
21	17.142	2581	2585	2591	rVB	42166	42546	2.11%	0.228%
22	17.295	2606	2611	2621	rBV	1509134	1674187	82.87%	8.969%
23	18.065	2738	2742	2746	rBV2	29647	29049	1.44%	0.156%
24	18.124	2748	2752	2756	rVV	35935	37122	1.84%	0.199%
25	18.547	2820	2824	2827	rBV	50670	50430	2.50%	0.270%
26	18.600	2827	2833	2835	rVV5	11654	22099	1.09%	0.118%
27	18.636	2835	2839	2852	rVB	471659	622238	30.80%	3.333%
28	18.947	2888	2892	2898	rVB2	34584	36336	1.80%	0.195%
29	19.330	2953	2957	2963	rVB	41145	45834	2.27%	0.246%
30	20.053	3074	3080	3086	rBV	50561	60985	3.02%	0.327%
31	20.300	3118	3122	3131	rBV	434862	566043	28.02%	3.032%
32	20.400	3135	3139	3142	rBV3	14538	20391	1.01%	0.109%
33	20.777	3198	3203	3212	rVB	50936	92390	4.57%	0.495%
34	21.694	3354	3359	3362	rBV5	15602	22245	1.10%	0.119%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.383	3472	3476	3483	rBV7	16041	34914	1.73%	0.187%
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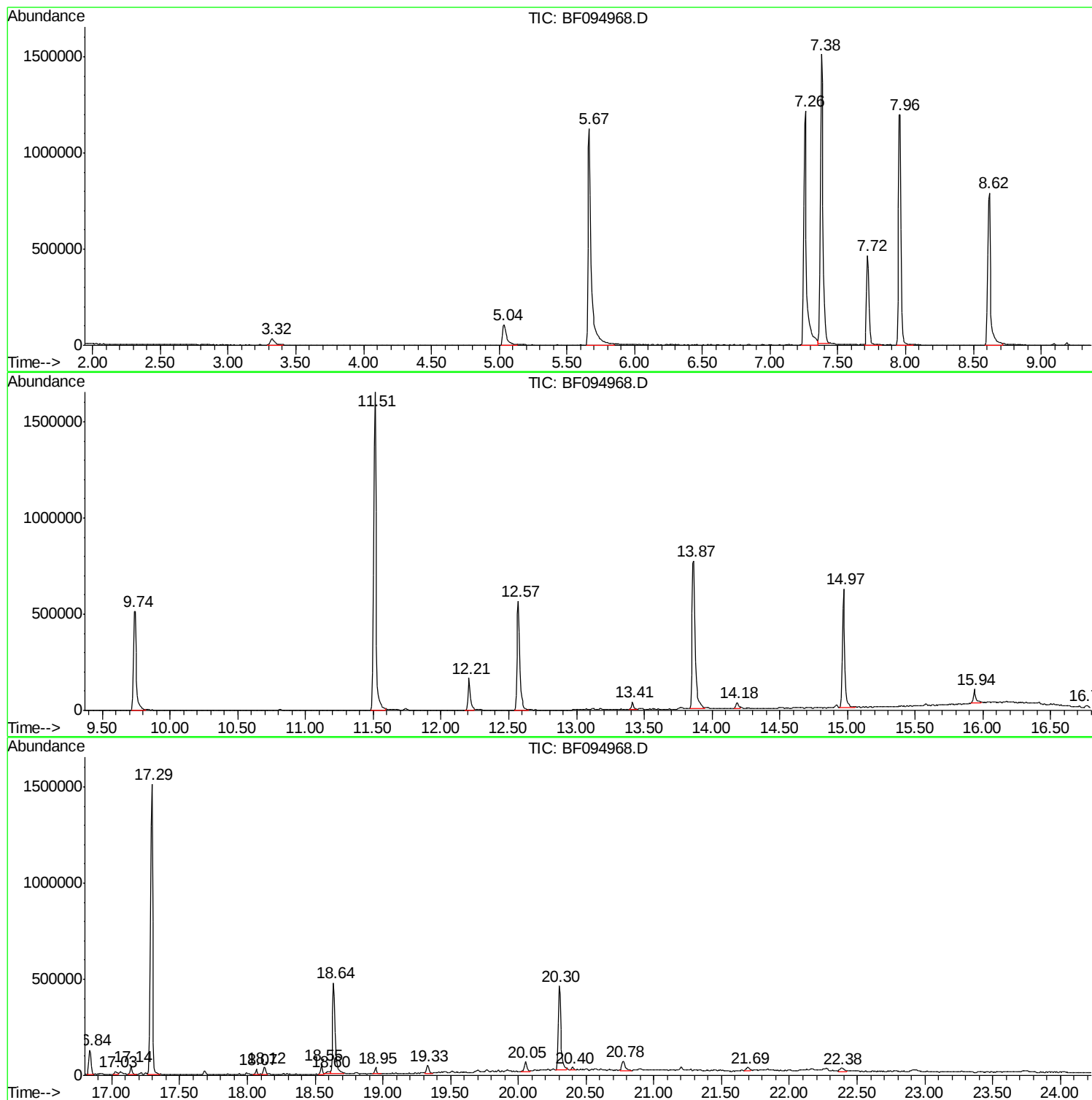
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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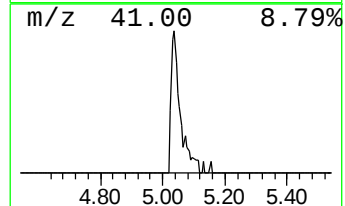
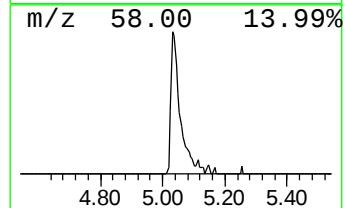
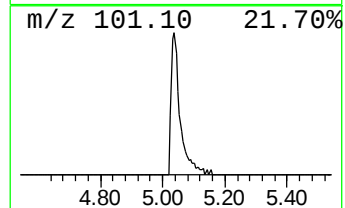
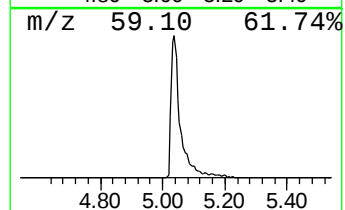
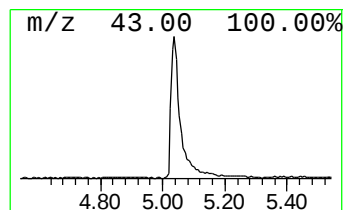
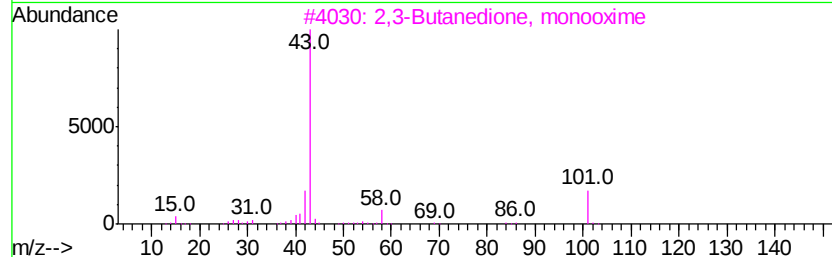
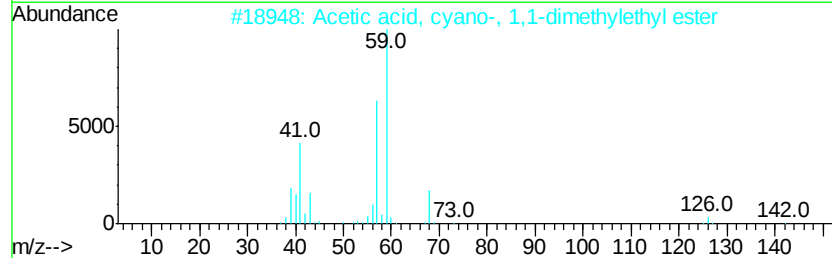
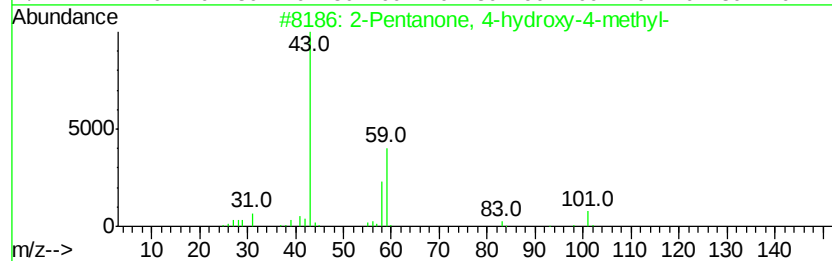
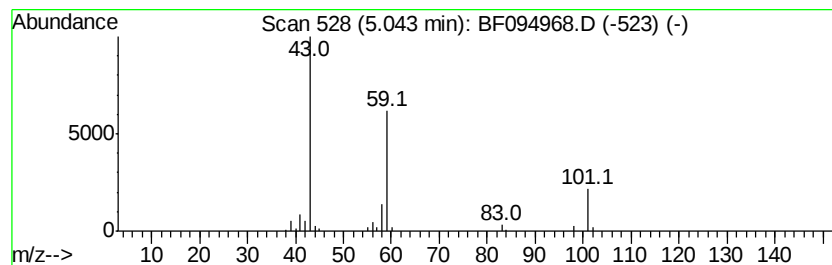
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	7.70 ng	208748	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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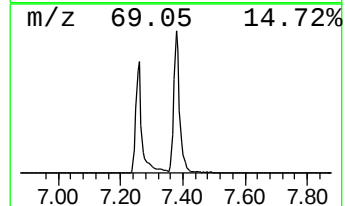
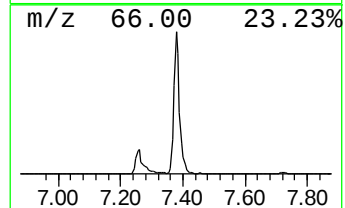
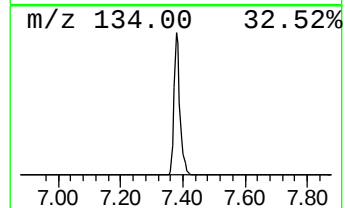
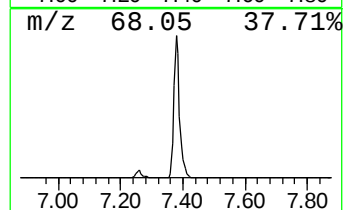
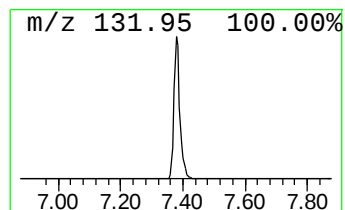
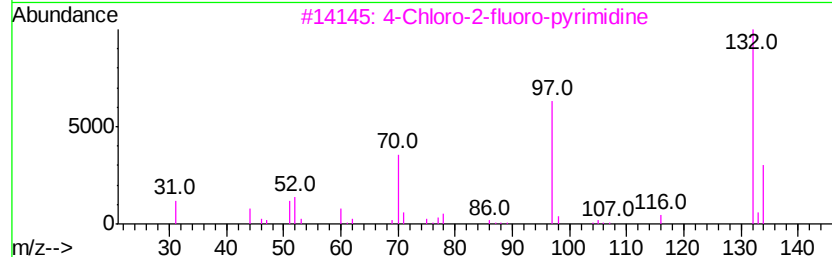
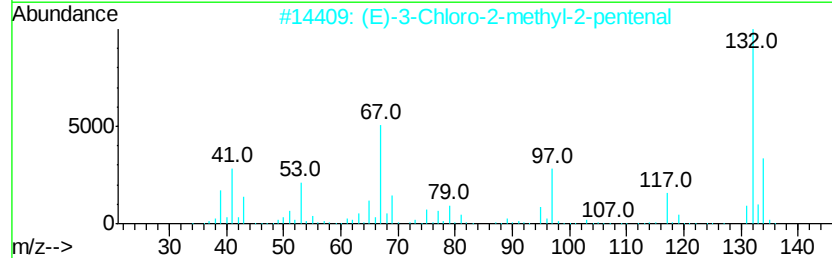
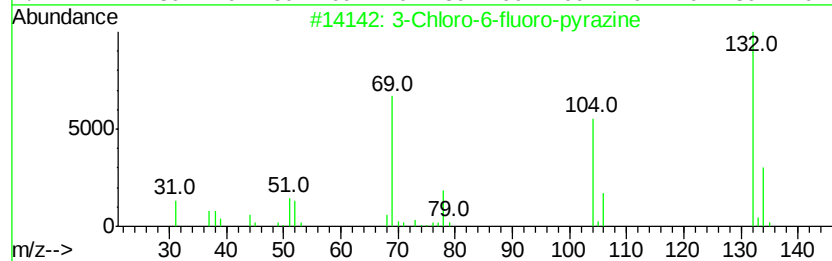
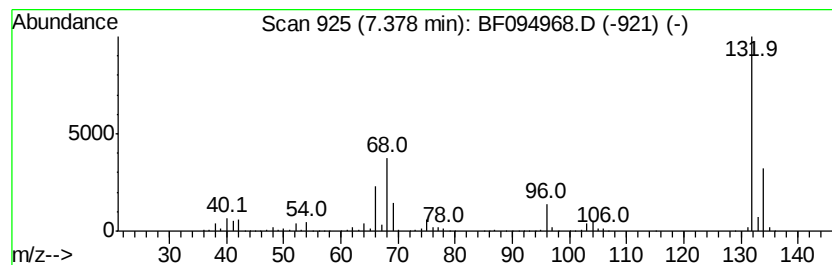
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	74.01 ng	2006430	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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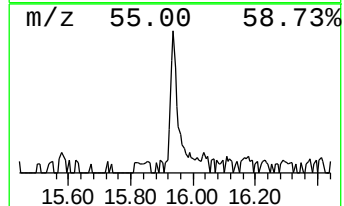
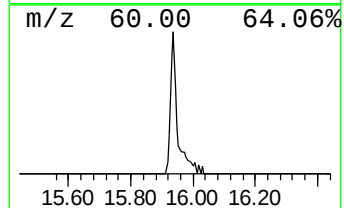
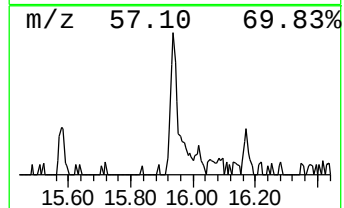
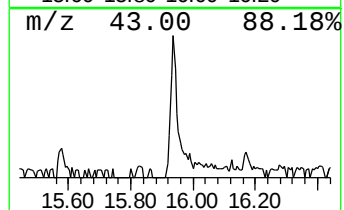
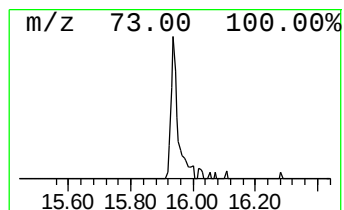
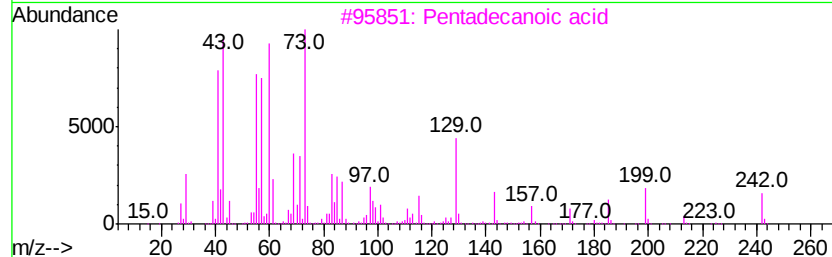
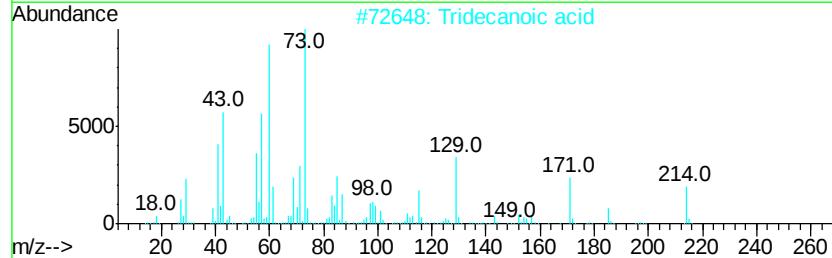
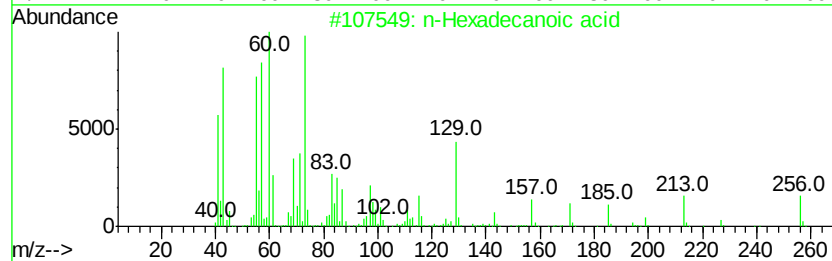
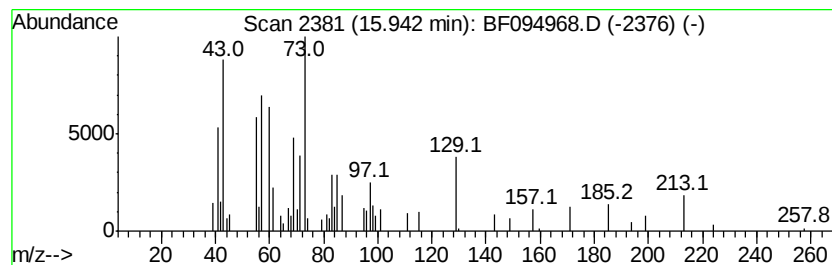
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.94	2.51 ng	99434	Phenanthrene-d10		14.97	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
2		Tridecanoic acid	214	C13H26O2	000638-53-9	72
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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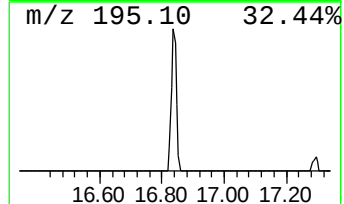
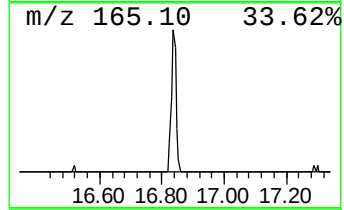
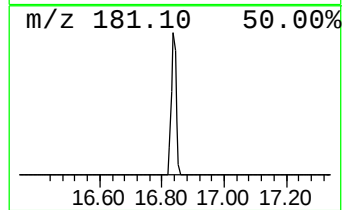
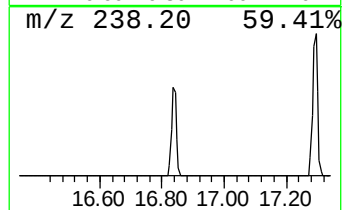
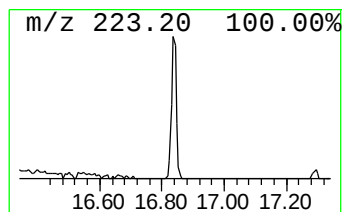
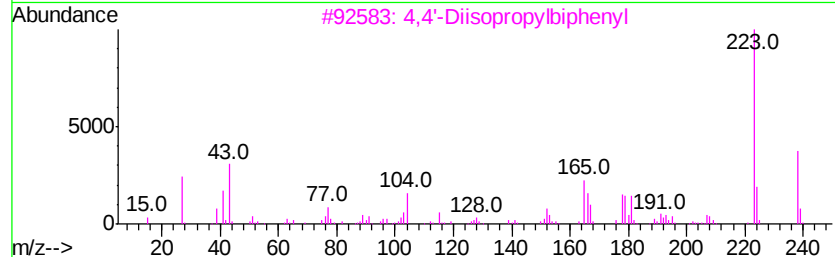
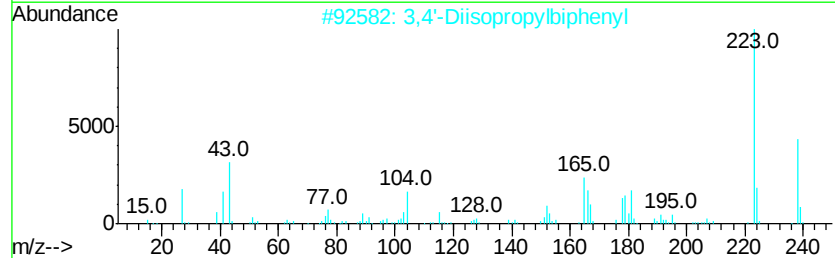
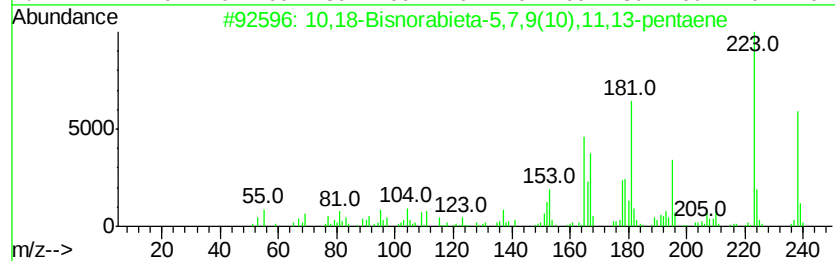
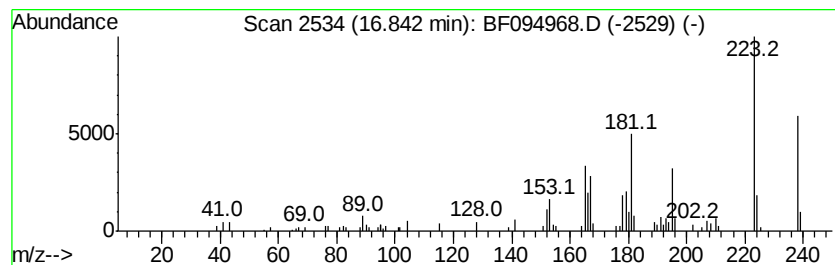
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	4.24 ng	132035	Chrysene-d12	18.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2		3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	68
3		4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	50
4		9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	43
5		Anthracene, 9,10-dimethoxy-	238	C16H14O2	002395-97-3	43



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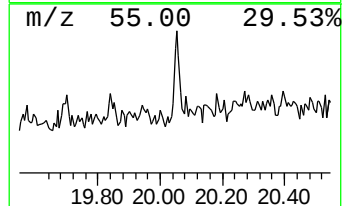
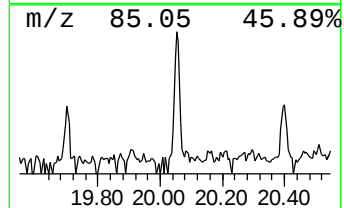
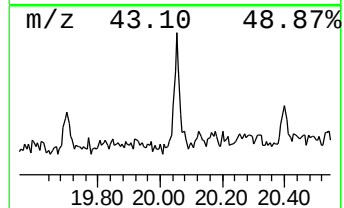
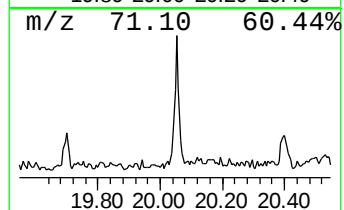
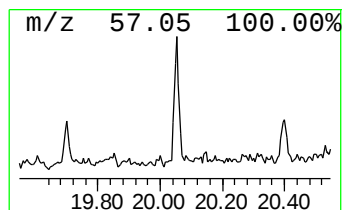
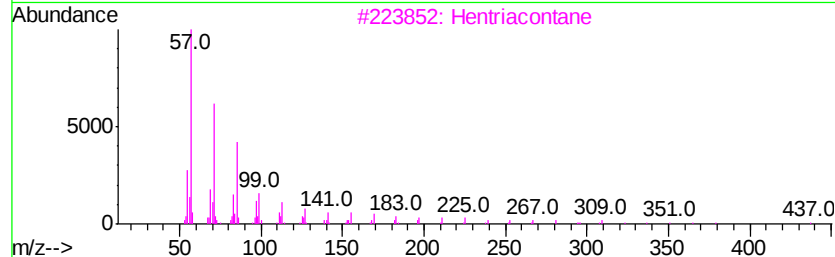
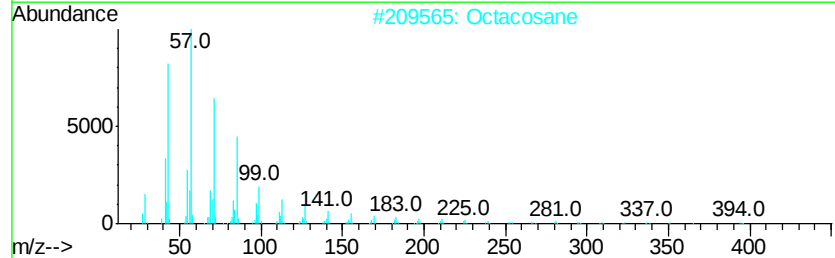
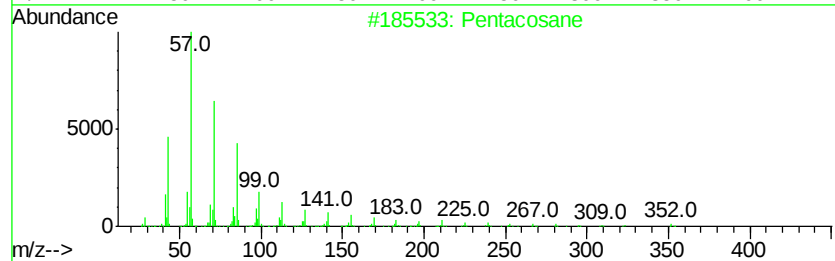
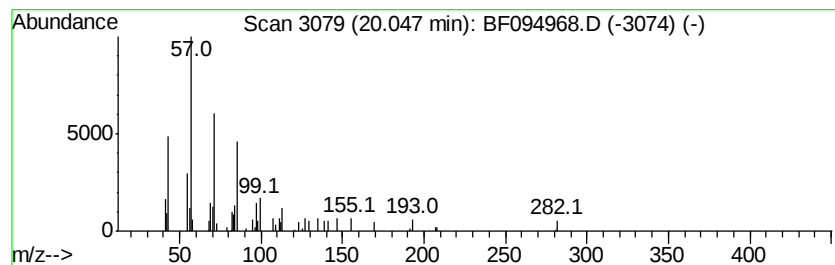
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.05	2.15 ng	60985	Perylene-d12	20.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Hentriacontane		437	C31H64	000630-04-6	91
4	Hexacosane		366	C26H54	000630-01-3	90
5	2-methyloctacosane		408	C29H60	1000376-72-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094968.D
Acq On : 8 May 2017 4:38
Operator : SJ/MA
Sample : I2947-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-6.5-7.0

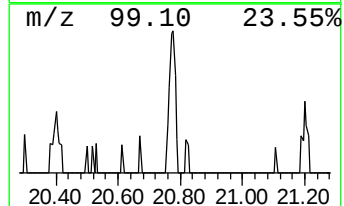
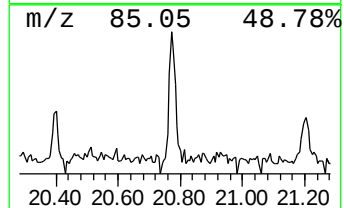
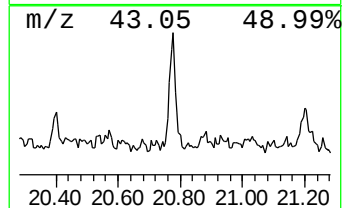
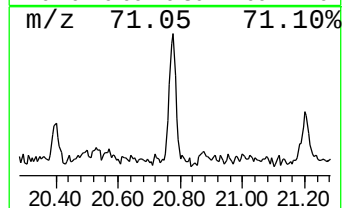
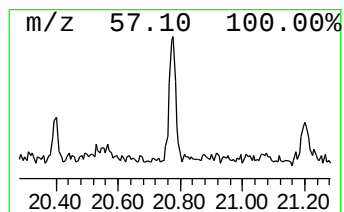
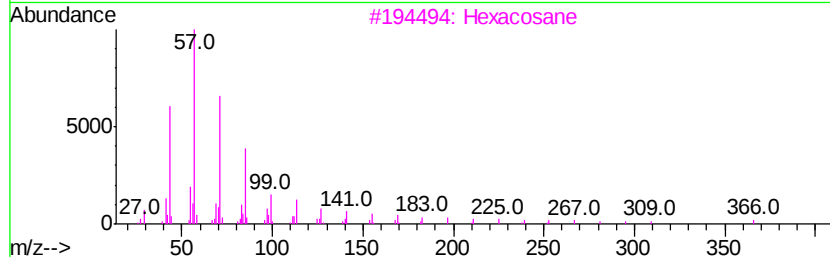
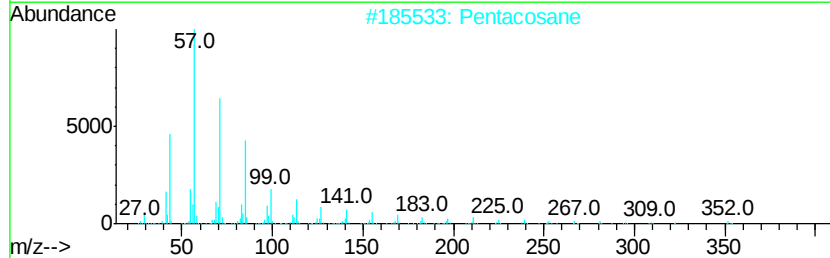
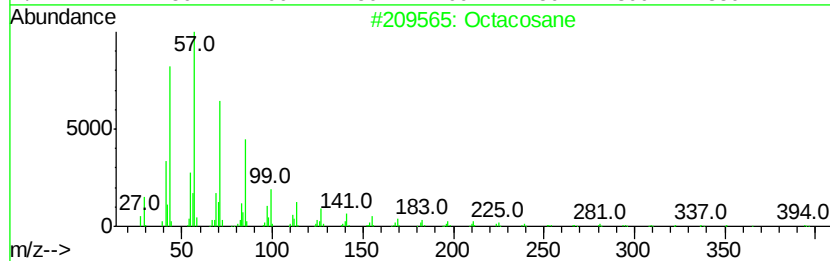
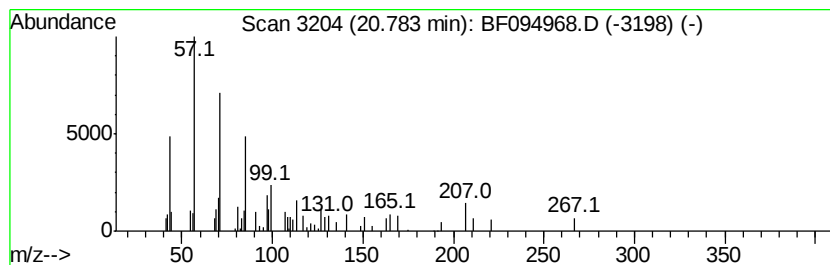
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	3.26 ng	92390	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	86
5		Heptadecane	240	C17H36	000629-78-7	86



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Instrument :
BNA_F
ClientSampleId :
SB-04-6.5-7.0

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...	5.04	7.7	ng	208748	1	7.72	542225	20.0
unknown7.38	7.38	74.0	ng	2006430	1	7.72	542225	20.0
n-Hexadecanoic acid	15.94	2.5	ng	99434	4	14.97	792044	20.0
10,18-Bisnorabiet...	16.84	4.2	ng	132035	5	18.64	622238	20.0
Pentacosane	20.05	2.1	ng	60985	6	20.30	566043	20.0
Octacosane	20.78	3.3	ng	92390	6	20.30	566043	20.0