

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
 Data File : BF094969.D
 Acq On : 8 May 2017 5:10
 Operator : SJ/MA
 Sample : I2947-12
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

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

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	248	rBV	66133	142395	4.72%	0.568%
2	5.043	524	528	552	rBV	142875	302342	10.02%	1.206%
3	5.666	630	634	661	rBV	1638909	2552120	84.58%	10.177%
4	7.266	900	906	921	rBV	1780186	2572749	85.26%	10.259%
5	7.384	921	926	937	rVB	2186565	2800008	92.79%	11.166%
6	7.719	979	983	994	rVB	474501	566732	18.78%	2.260%
7	7.960	1019	1024	1043	rVB	1920189	2240658	74.25%	8.935%
8	8.619	1131	1136	1155	rBV	1248794	1740974	57.69%	6.943%
9	9.189	1228	1233	1240	rVB2	24655	31151	1.03%	0.124%
10	9.736	1322	1326	1338	rBV	562554	778327	25.79%	3.104%
11	11.513	1623	1628	1643	rBV	2362442	3017568	100.00%	12.033%
12	12.201	1741	1745	1753	rBV	301831	400947	13.29%	1.599%
13	12.571	1803	1808	1821	rBV2	597183	889402	29.47%	3.547%
14	13.413	1947	1951	1957	rVB	47962	52791	1.75%	0.211%
15	13.865	2022	2028	2042	rBV	1178316	1707749	56.59%	6.810%
16	14.183	2076	2082	2085	rBV	40730	49886	1.65%	0.199%
17	14.971	2211	2216	2228	rBV	523787	699394	23.18%	2.789%
18	15.936	2373	2380	2391	rBV2	97457	145432	4.82%	0.580%
19	17.059	2568	2571	2581	rVV	19775	35912	1.19%	0.143%
20	17.142	2581	2585	2589	rVV	144739	137138	4.54%	0.547%
21	17.295	2606	2611	2615	rBV2	1897841	2188875	72.54%	8.729%
22	18.065	2738	2742	2746	rBV2	93993	93993	3.11%	0.375%
23	18.130	2748	2753	2755	rBV	30657	34936	1.16%	0.139%
24	18.548	2820	2824	2827	rBV	33825	34771	1.15%	0.139%
25	18.600	2827	2833	2835	rBV3	17235	33669	1.12%	0.134%
26	18.636	2835	2839	2848	rVV	503211	611718	20.27%	2.439%
27	18.948	2886	2892	2898	rBV	23265	32252	1.07%	0.129%
28	19.330	2951	2957	2962	rVB	41439	57165	1.89%	0.228%
29	20.053	3076	3080	3087	rBV	91156	110631	3.67%	0.441%
30	20.300	3118	3122	3130	rBV	435996	574991	19.05%	2.293%
31	20.400	3136	3139	3144	rVB3	35655	46438	1.54%	0.185%
32	20.777	3198	3203	3213	rVB	81804	124810	4.14%	0.498%
33	21.694	3354	3359	3363	rVB5	24076	38558	1.28%	0.154%
34	22.383	3467	3476	3484	rBV5	30222	89997	2.98%	0.359%

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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

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35	22.488	3492	3494	3507	rVB9	26867	79141	2.62%	0.316%
36	22.918	3562	3567	3574	rVB9	25310	61335	2.03%	0.245%

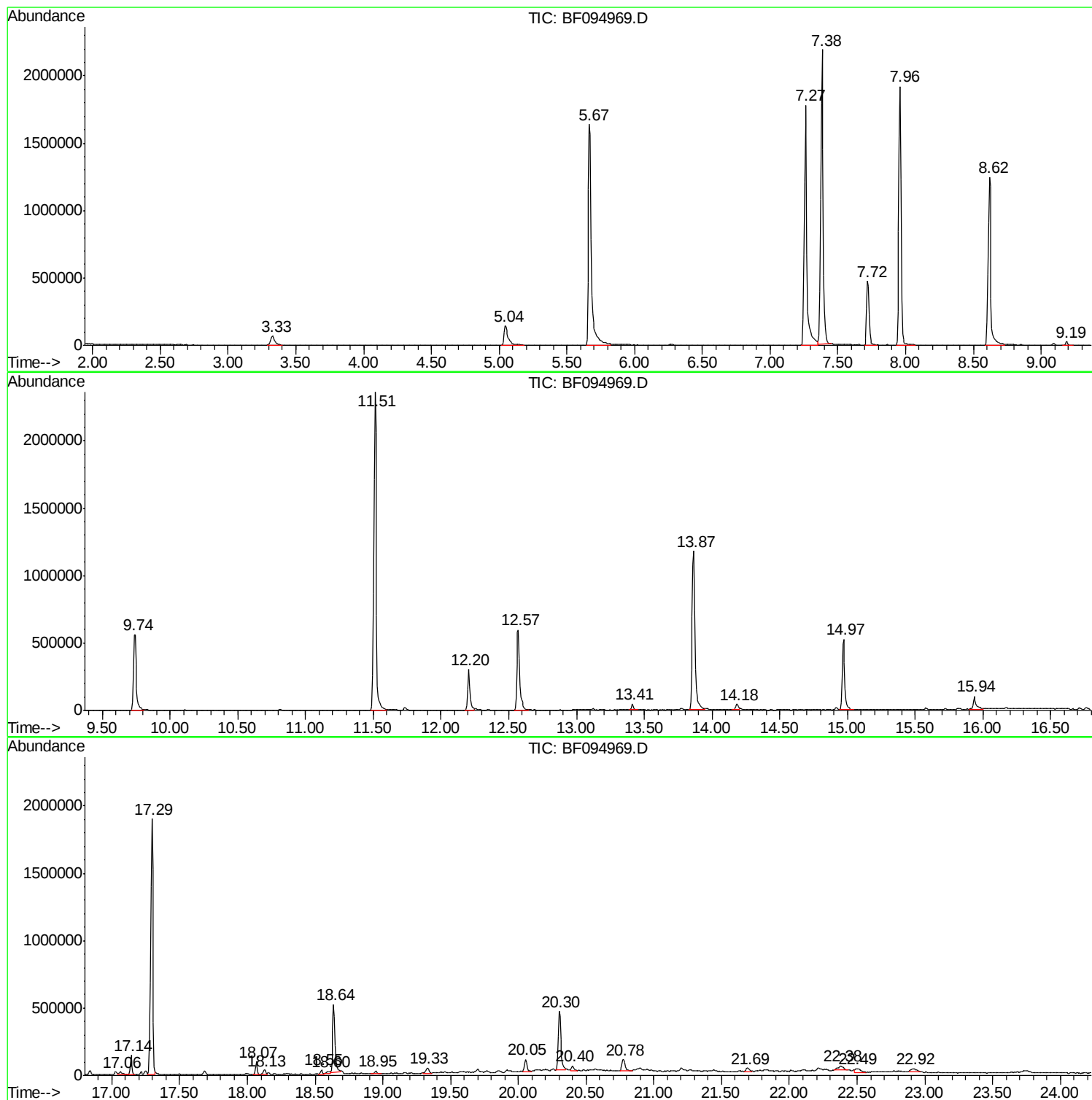
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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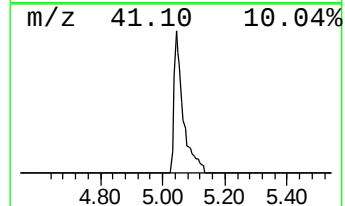
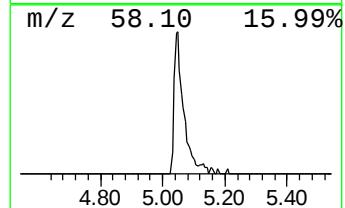
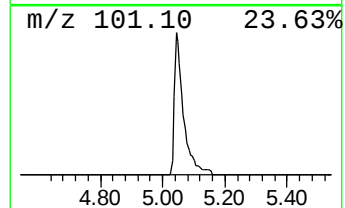
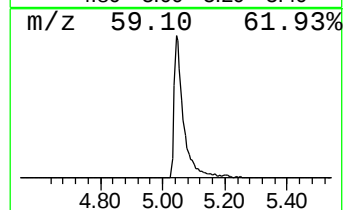
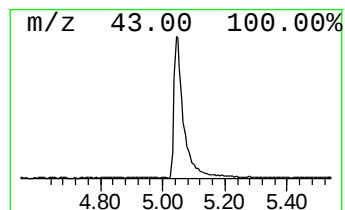
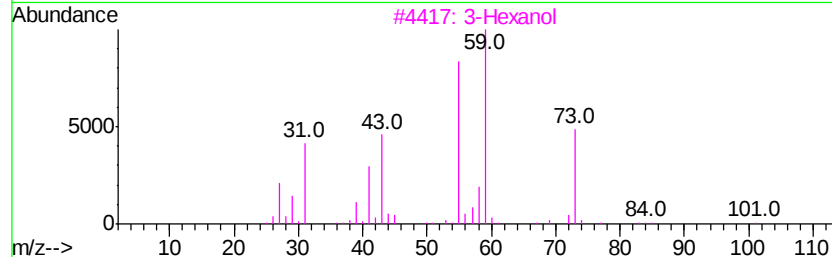
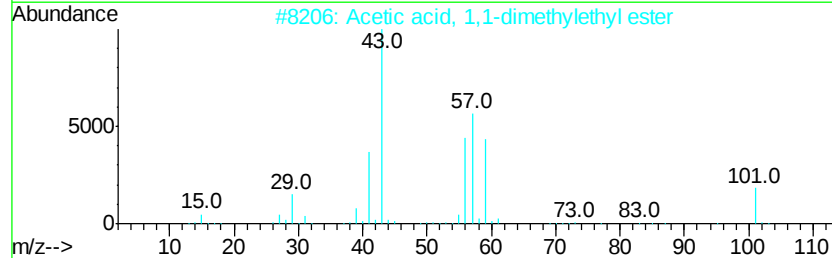
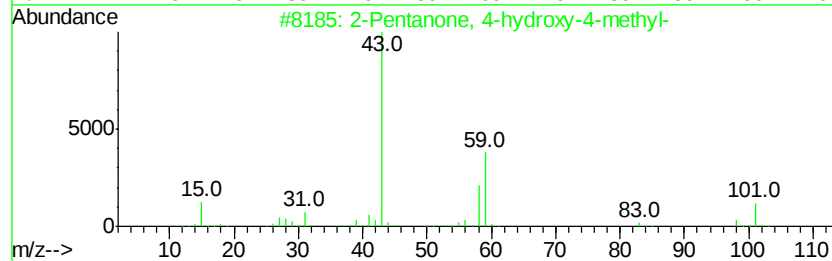
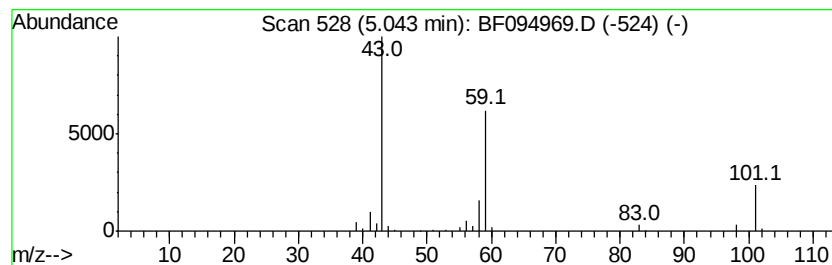
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	10.67 ng	302342	1,4-Dichlorobenzene-d4	7.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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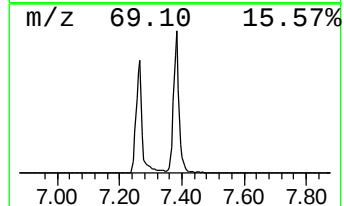
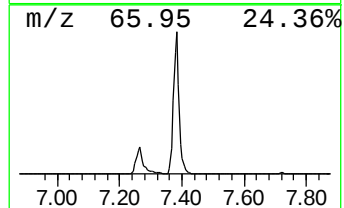
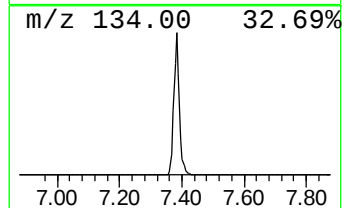
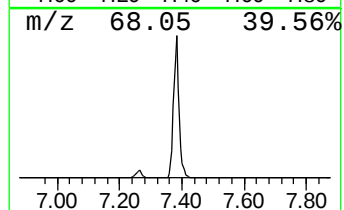
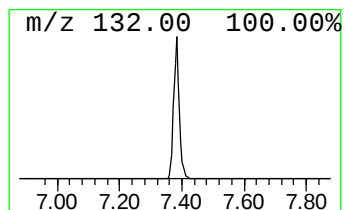
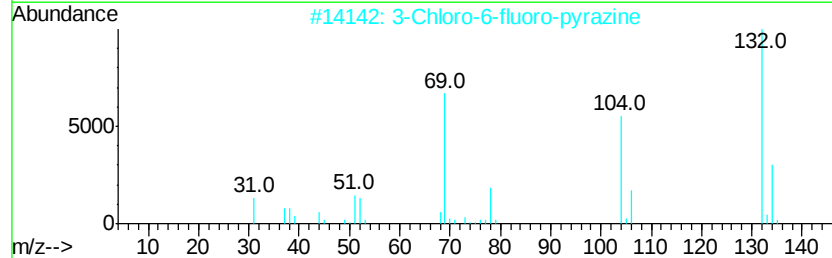
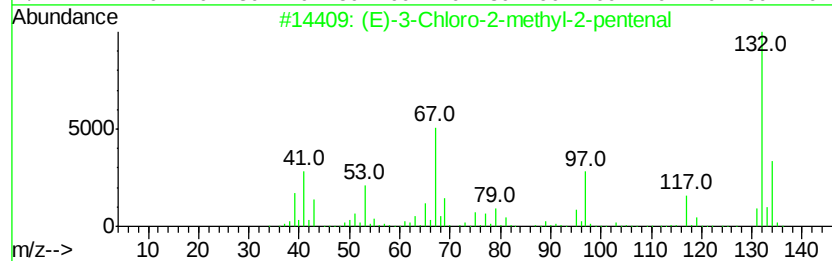
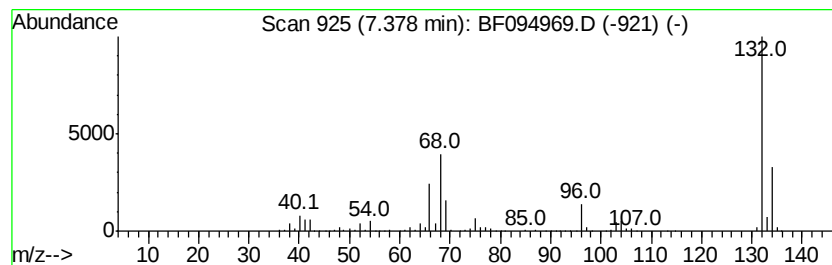
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	98.81 ng	2800010	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		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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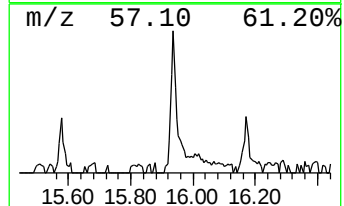
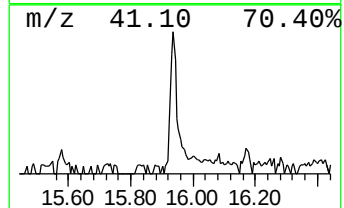
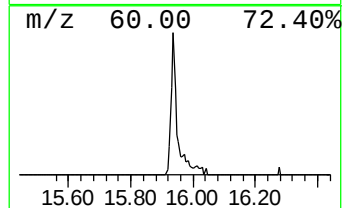
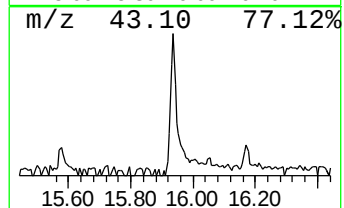
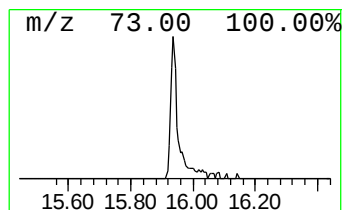
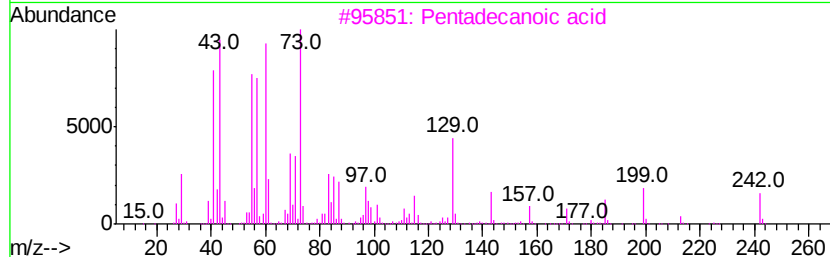
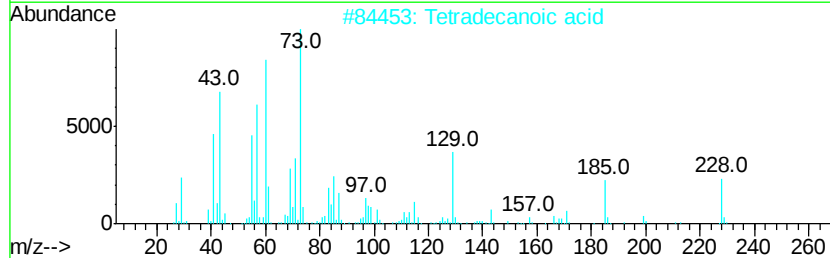
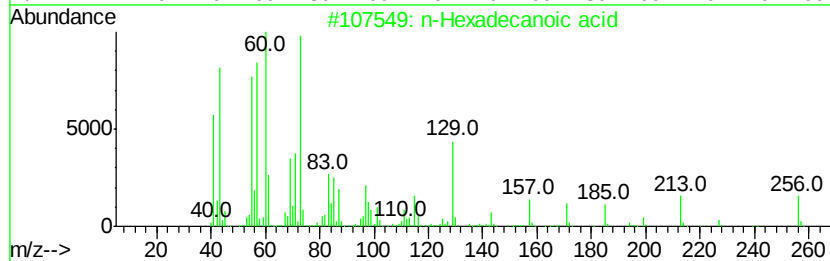
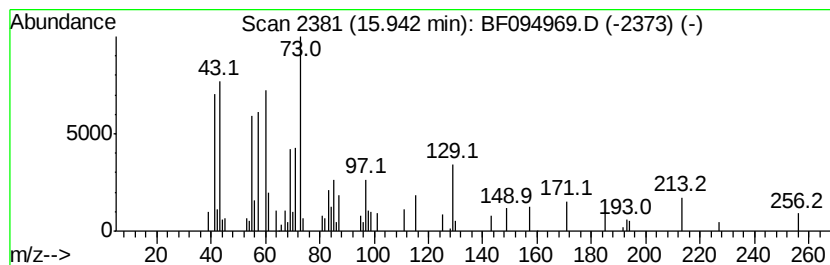
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.16 ng	145432	Phenanthrene-d10	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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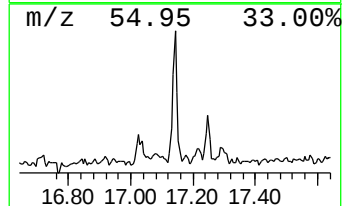
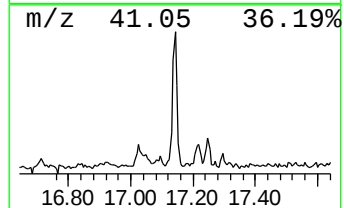
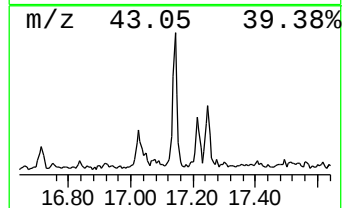
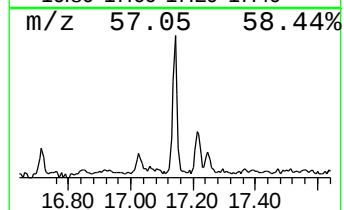
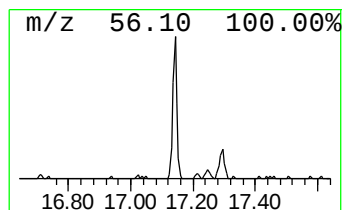
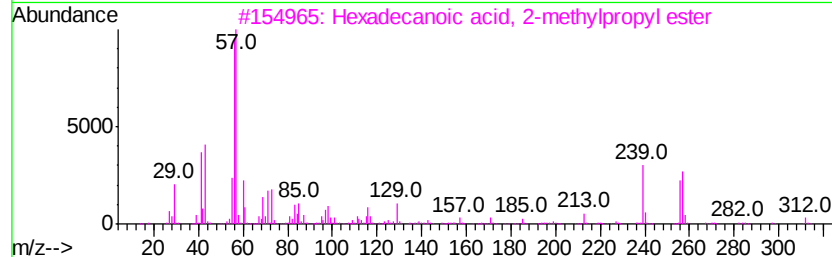
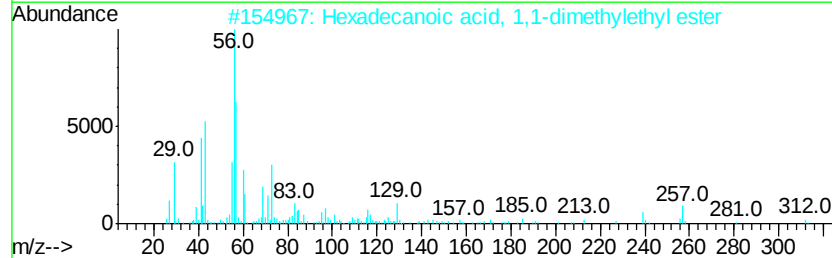
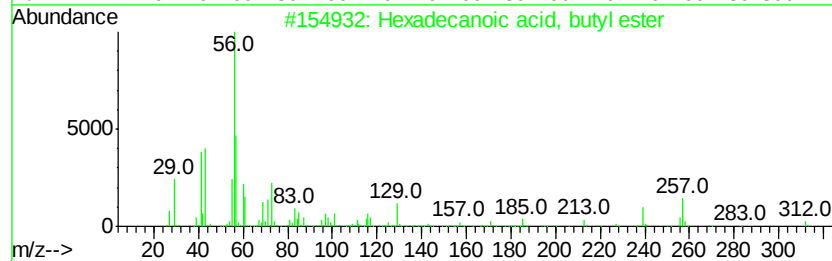
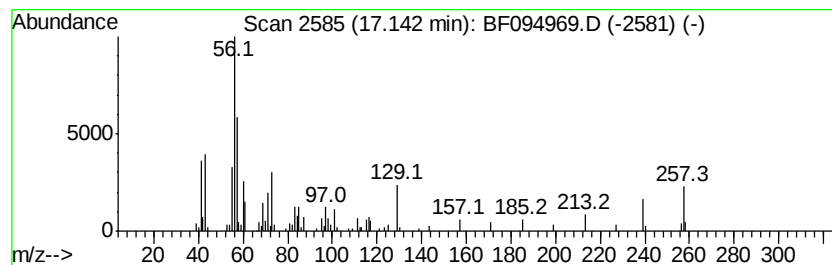
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	4.48 ng	137138	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	68
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	35



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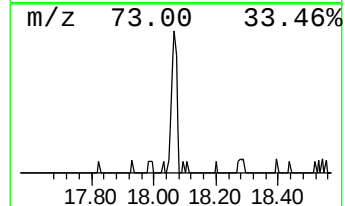
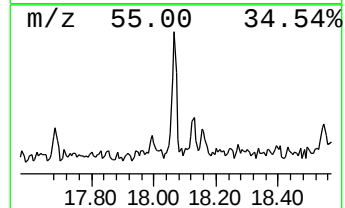
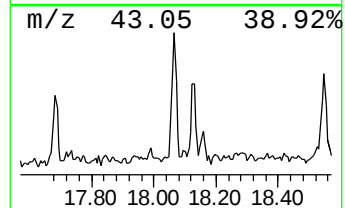
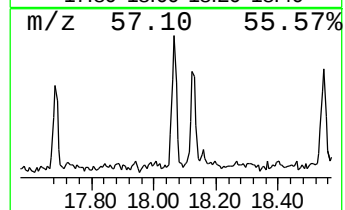
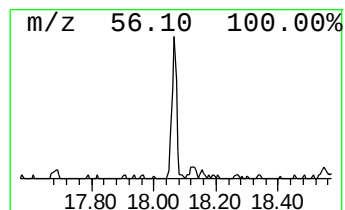
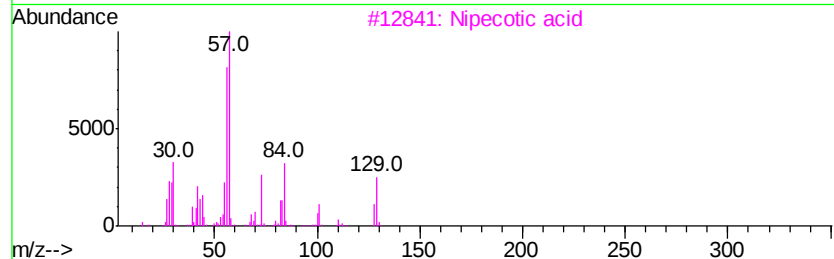
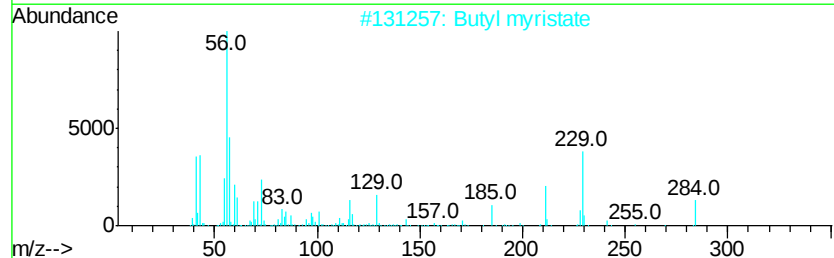
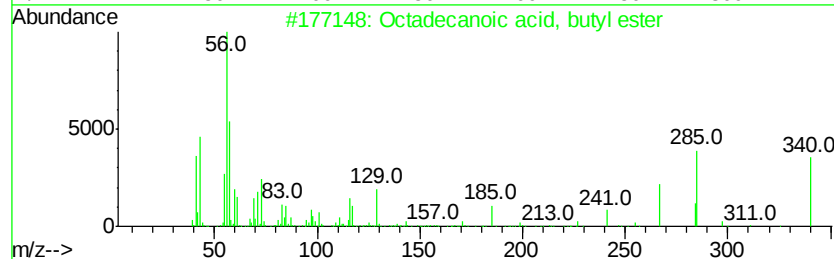
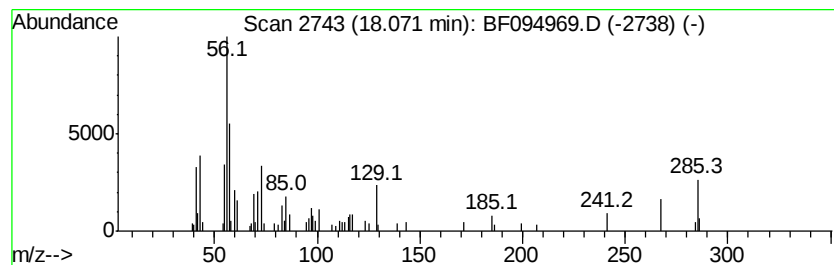
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Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	3.07 ng	93993	Chrysene-d12	18.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		Nipecotic acid	129	C6H11NO2	000498-95-3	40
4		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30
5		4-t-Butylcyclohexylamine	155	C10H21N	005400-88-4	27



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SB-04-6.5-7.0-DUP

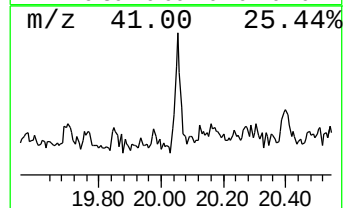
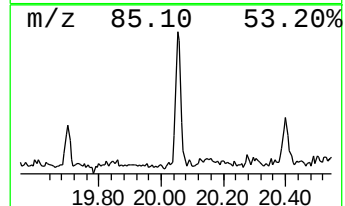
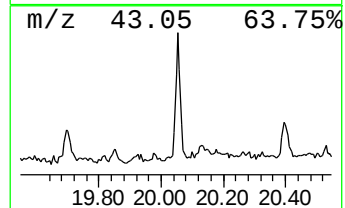
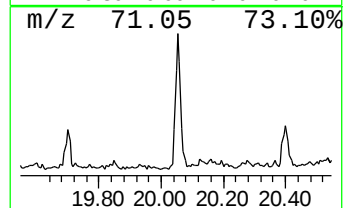
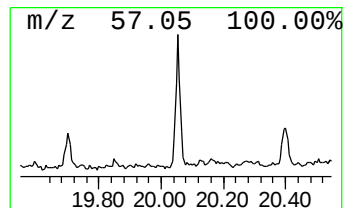
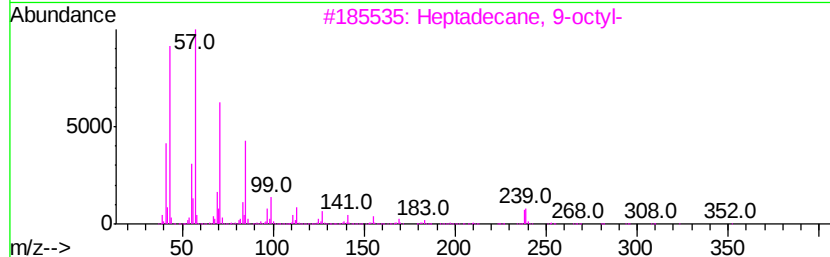
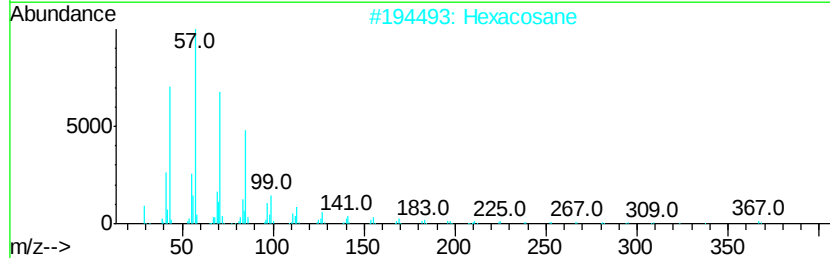
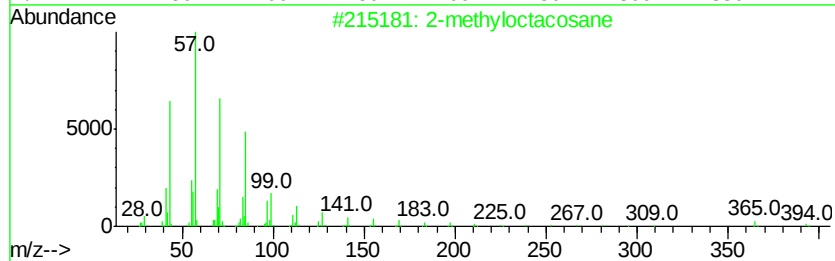
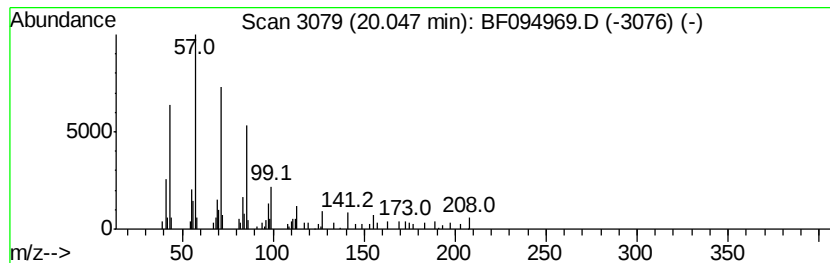
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.05	3.85 ng	110631	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094969.D
Acq On : 8 May 2017 5:10
Operator : SJ/MA
Sample : I2947-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

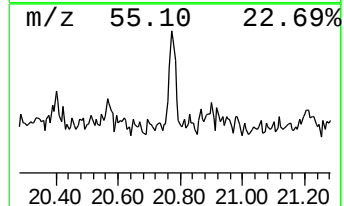
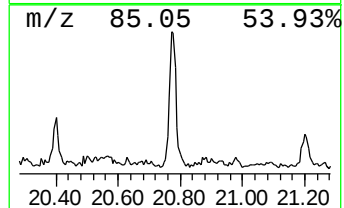
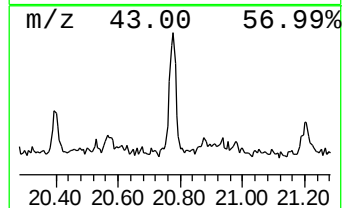
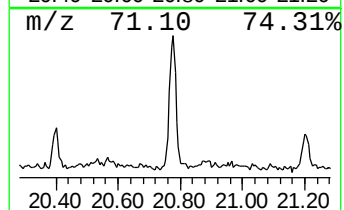
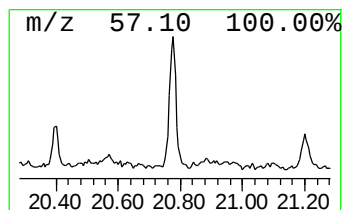
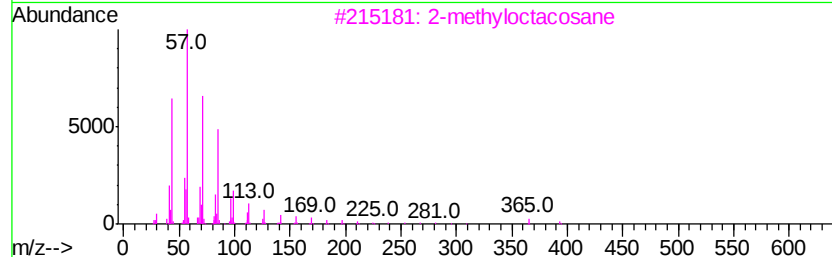
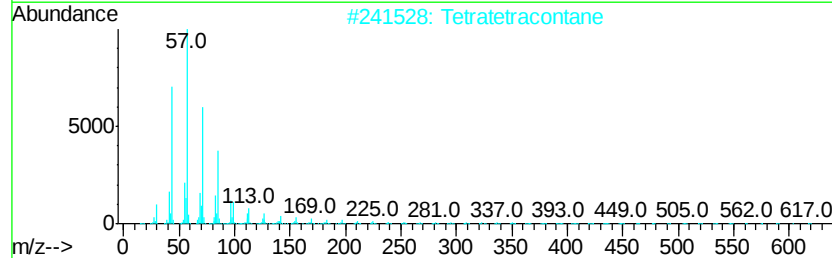
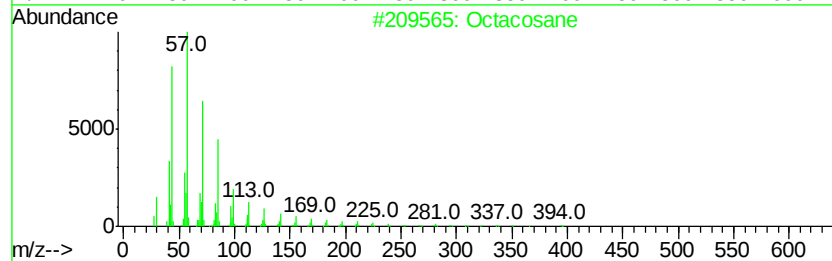
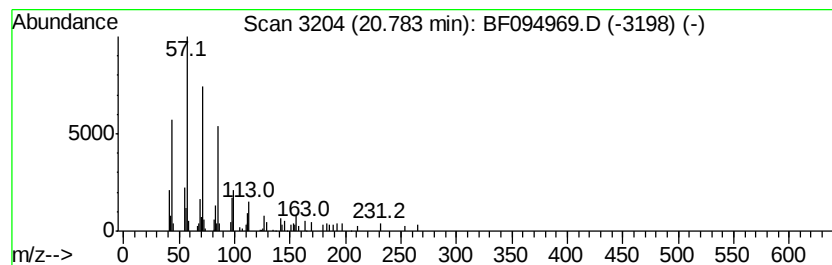
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	4.34 ng	124810	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094969.D
Acq On : 8 May 2017 5:10
Operator : SJ/MA
Sample : I2947-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

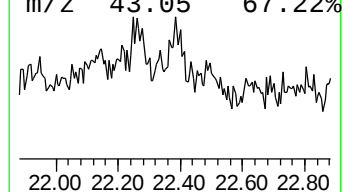
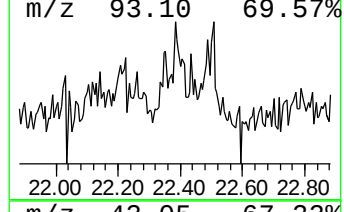
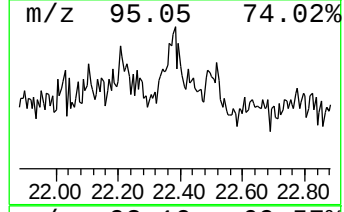
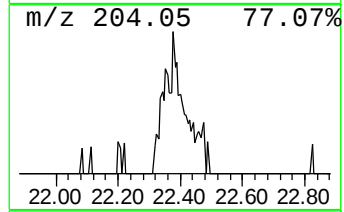
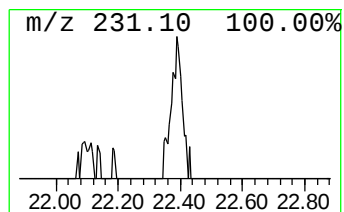
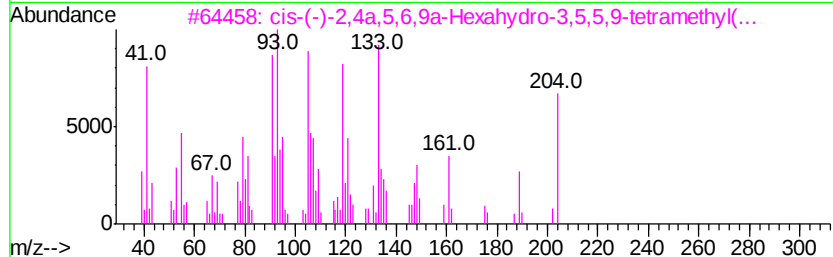
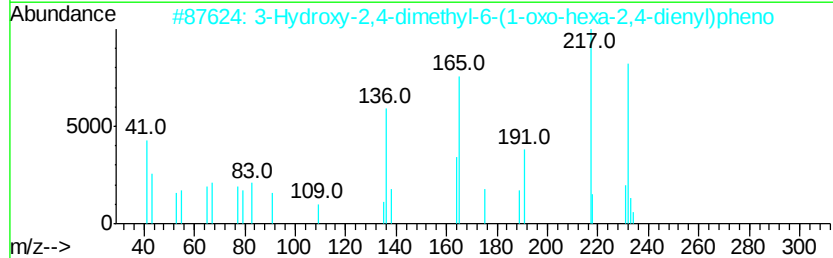
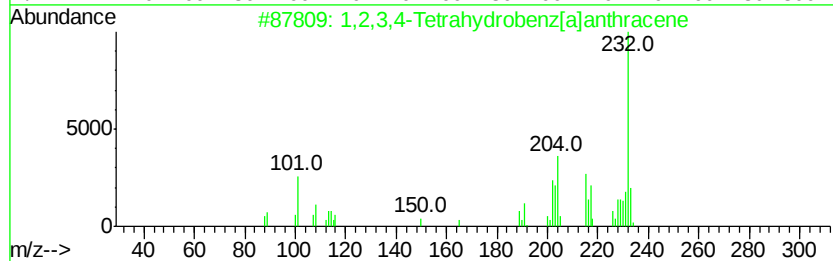
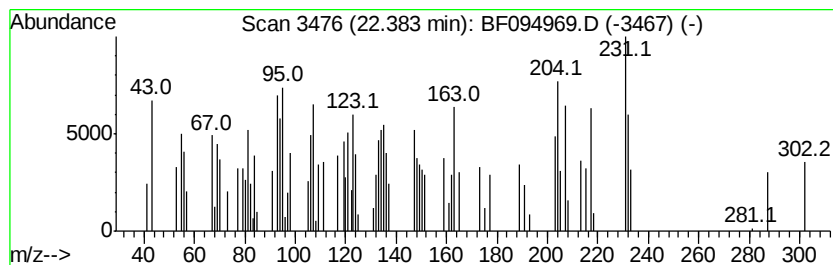
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.38 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.38	3.13 ng	89997	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,3,4-Tetrahydrobenz[a]anthracene	232	C18H16	004483-98-1	27
2		3-Hydroxy-2,4-dimethyl-6-(1-oxo-...	232	C14H16O3	079950-85-9	25
3		cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	25
4		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	25
5		3-Fluorobenzoic acid, 2,7-dimeth...	274	C17H19FO2	1000292-60-6	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094969.D
Acq On : 8 May 2017 5:10
Operator : SJ/MA
Sample : I2947-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

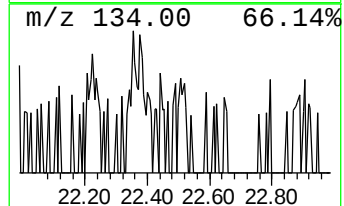
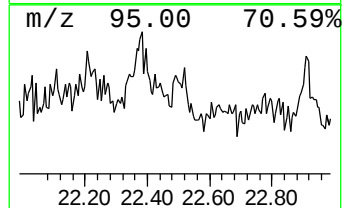
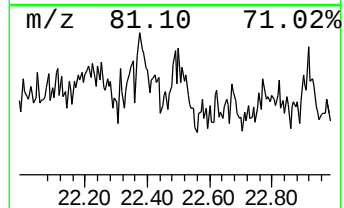
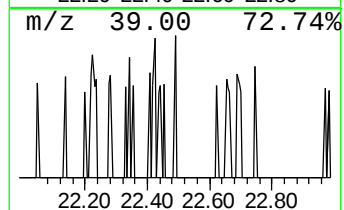
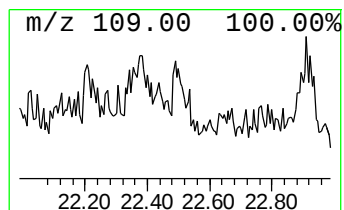
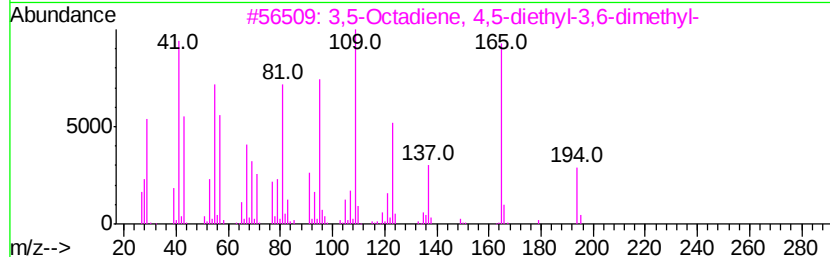
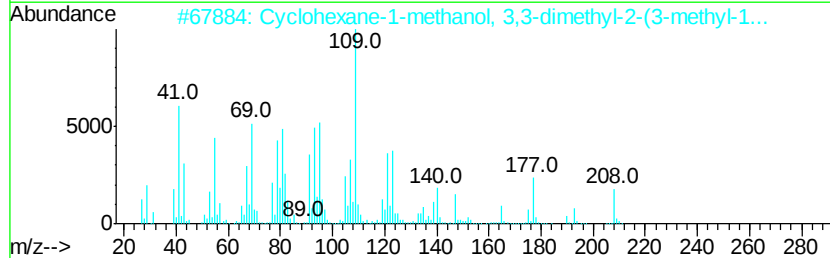
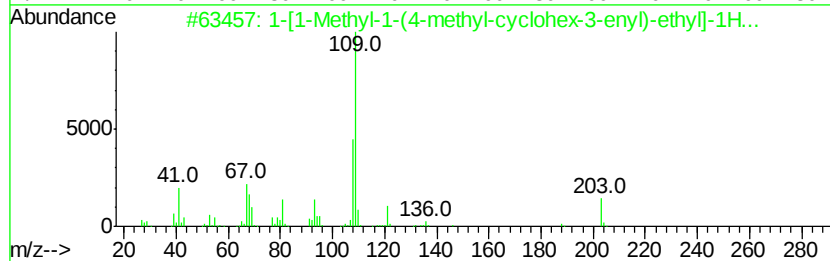
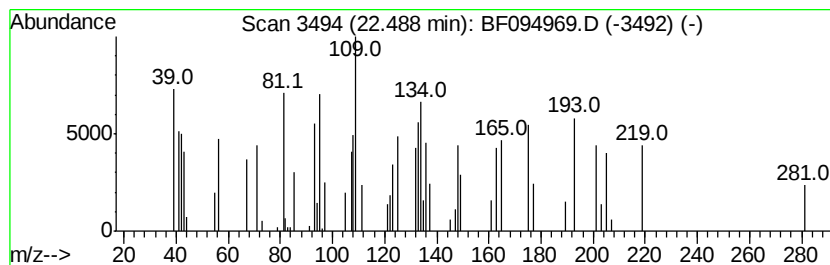
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown22.49 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.75 ng	79141	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-[1-Methyl-1-(4-methyl-cyclohex...	203	C14H21N	1000192-41-8	10
2			Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	10
3			3,5-Octadiene, 4,5-diethyl-3,6-d...	194	C14H26	061233-79-2	10
4			4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	10
5			4-(2-Propyn-1-yloxy)phenol	148	C9H8O2	034596-27-5	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094969.D
Acq On : 8 May 2017 5:10
Operator : SJ/MA
Sample : I2947-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

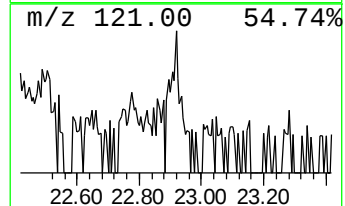
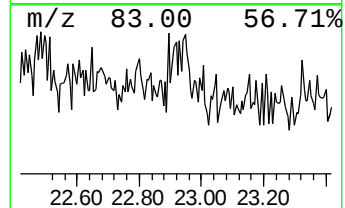
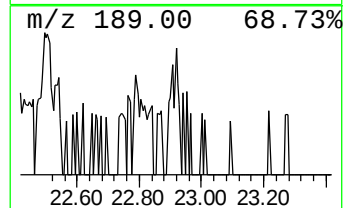
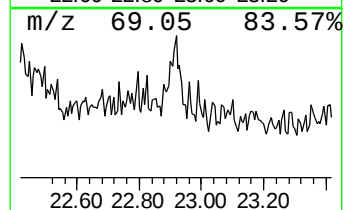
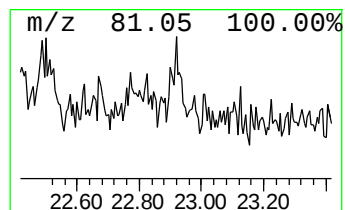
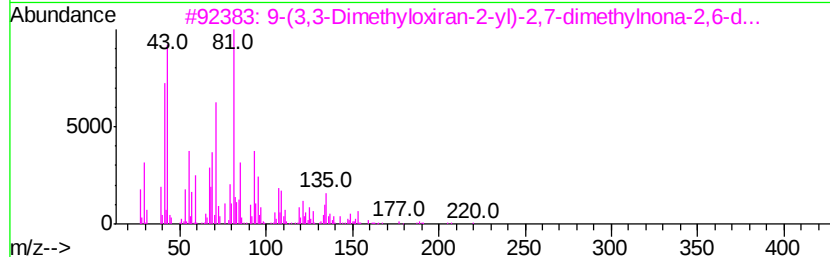
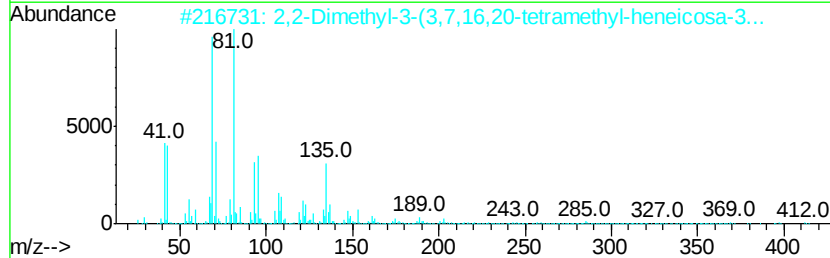
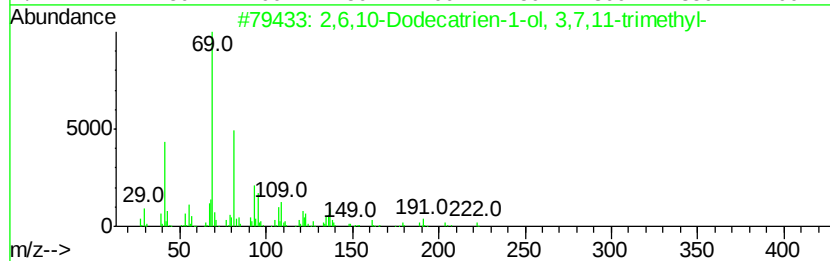
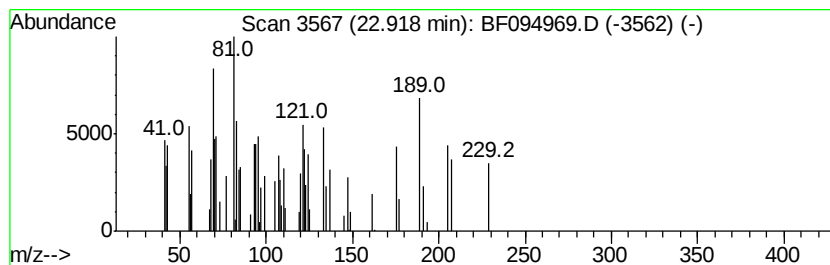
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown22.92 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.92	2.13 ng	61335	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	16		
2	2,2-Dimethyl-3-(3,7,16,20-tetram...	412	C29H48O	1000194-78-6	12		
3	9-(3,3-Dimethyloxiran-2-yl)-2,7-...	238	C15H26O2	1000192-15-6	12		
4	3-(Trifluoromethoxy)benzamide	205	C8H6F3N2O2	000658-91-3	11		
5	p-Trifluoromethoxybenzamide	205	C8H6F3N2O2	000456-71-3	11		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094969.D
Acq On : 8 May 2017 5:10
Operator : SJ/MA
Sample : I2947-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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	10.7	ng	302342	1	7.72	566732	20.0
unknown7.38	7.38	98.8	ng	2800010	1	7.72	566732	20.0
n-Hexadecanoic acid	15.94	4.2	ng	145432	4	14.97	699394	20.0
Hexadecanoic acid...	17.14	4.5	ng	137138	5	18.64	611718	20.0
Octadecanoic acid...	18.07	3.1	ng	93993	5	18.64	611718	20.0
2-methyloctacosane	20.05	3.9	ng	110631	6	20.30	574991	20.0
Octacosane	20.78	4.3	ng	124810	6	20.30	574991	20.0
unknown22.38	22.38	3.1	ng	89997	6	20.30	574991	20.0
unknown22.49	22.49	2.8	ng	79141	6	20.30	574991	20.0
unknown22.92	22.92	2.1	ng	61335	6	20.30	574991	20.0