

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
 Data File : BF094847.D
 Acq On : 3 May 2017 22:10
 Operator : SJ/MA
 Sample : I2914-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10-COMP(0-6.5)

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	5.054	524	530	547	rBV	339098	694020	22.29%	2.539%
2	5.684	631	637	665	rBV	2109728	3093119	99.35%	11.316%
3	6.248	729	733	741	rVB	28266	41184	1.32%	0.151%
4	7.272	901	907	922	rBV	1877494	2969223	95.37%	10.862%
5	7.389	922	927	943	rVB	2392599	3113496	100.00%	11.390%
6	7.725	980	984	995	rVB	503404	572994	18.40%	2.096%
7	7.966	1019	1025	1036	rVB	1991322	2306349	74.08%	8.437%
8	8.625	1131	1137	1146	rBV	1384907	1836964	59.00%	6.720%
9	9.742	1322	1327	1339	rBV	646080	757197	24.32%	2.770%
10	11.518	1623	1629	1633	rBV	2485042	2908364	93.41%	10.640%
11	12.207	1741	1746	1753	rBV	555540	646341	20.76%	2.365%
12	12.571	1803	1808	1817	rBV2	726531	887614	28.51%	3.247%
13	13.418	1948	1952	1957	rVB2	28752	32915	1.06%	0.120%
14	13.865	2023	2028	2043	rBV	1335307	1870229	60.07%	6.842%
15	14.189	2079	2083	2086	rBV	35929	42588	1.37%	0.156%
16	14.971	2211	2216	2229	rVB	651116	825432	26.51%	3.020%
17	15.942	2377	2381	2391	rVB2	131684	143954	4.62%	0.527%
18	17.030	2562	2566	2569	rBV3	29160	34562	1.11%	0.126%
19	17.300	2606	2612	2616	rBV	2127304	2363076	75.90%	8.645%
20	18.530	2818	2821	2823	rBV	56412	54627	1.75%	0.200%
21	18.565	2823	2827	2835	rVV4	55925	157058	5.04%	0.575%
22	18.636	2835	2839	2849	rVB	610840	702112	22.55%	2.569%
23	19.336	2953	2958	2961	rBV2	35570	46755	1.50%	0.171%
24	19.377	2961	2965	2976	rVB5	30477	85565	2.75%	0.313%
25	20.059	3076	3081	3086	rBV	163677	181277	5.82%	0.663%
26	20.300	3118	3122	3131	rBV	476338	581069	18.66%	2.126%
27	20.783	3199	3204	3210	rVB	97412	142007	4.56%	0.520%
28	20.871	3213	3219	3227	rBV8	32313	86799	2.79%	0.318%
29	22.106	3423	3429	3436	rBV8	13481	33240	1.07%	0.122%
30	22.224	3445	3449	3455	rVB4	24657	36397	1.17%	0.133%
31	22.506	3492	3497	3506	rVB9	35136	88572	2.84%	0.324%

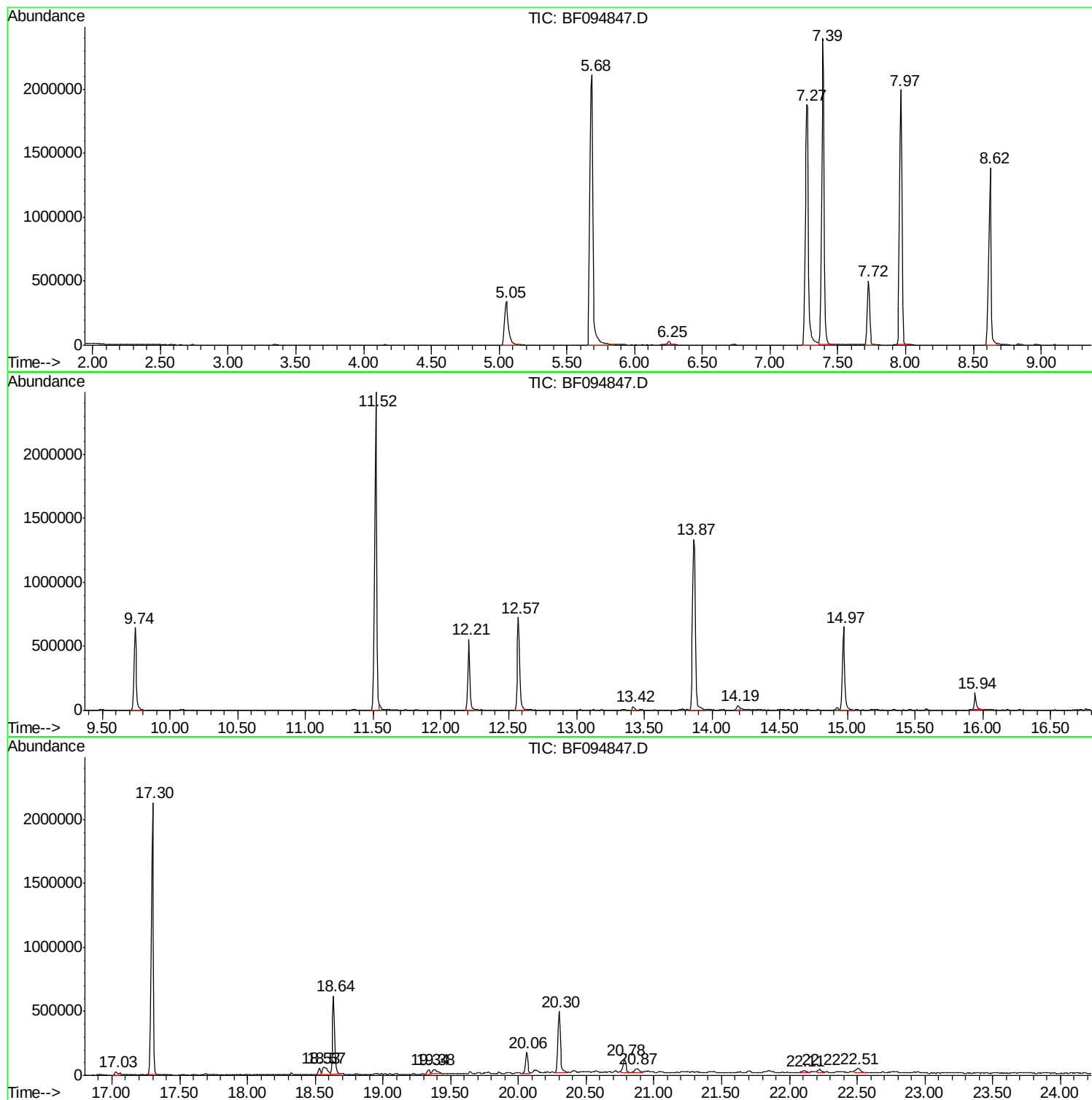
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Instrument :
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ClientSampleId :
SB-10-COMP(0-6.5)

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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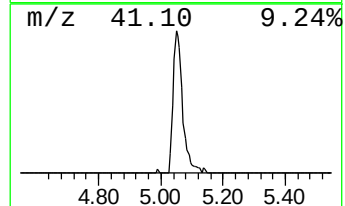
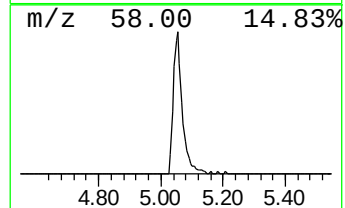
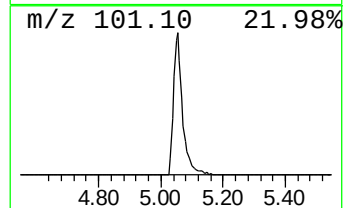
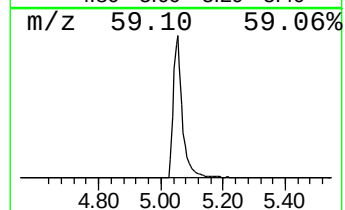
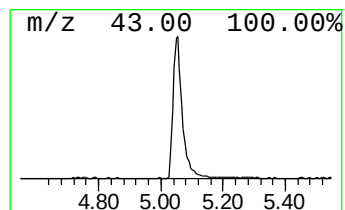
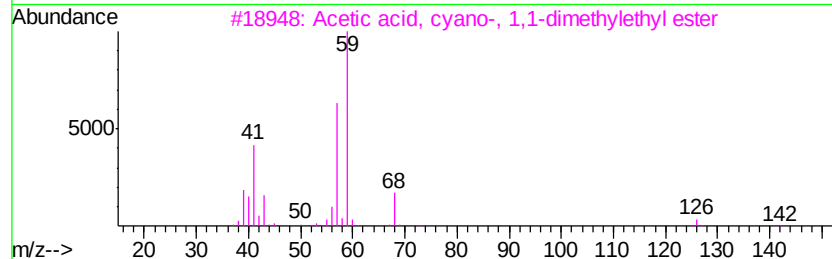
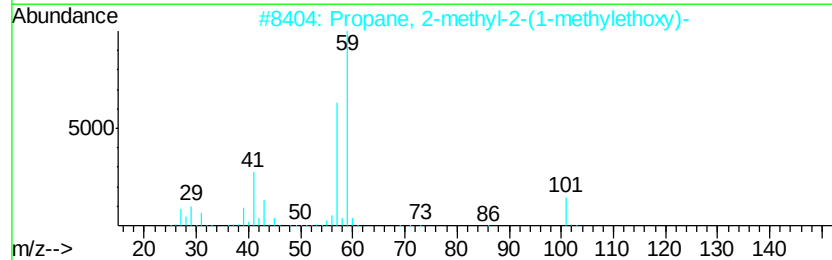
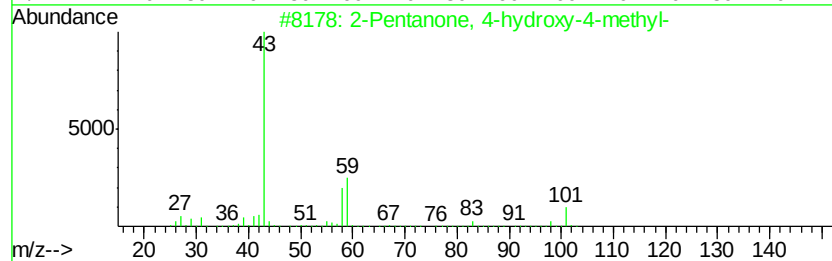
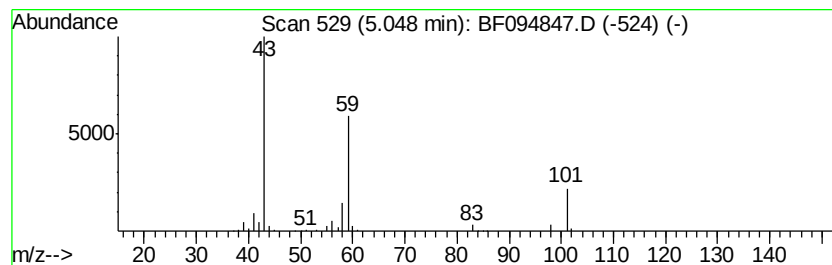
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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	24.22 ng	694020	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	64	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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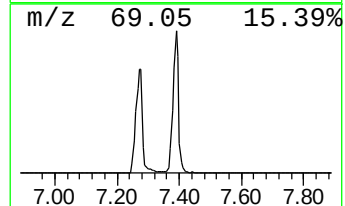
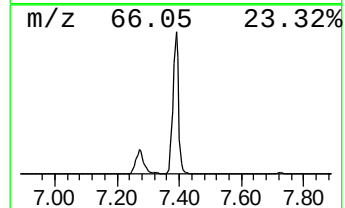
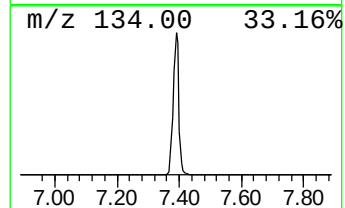
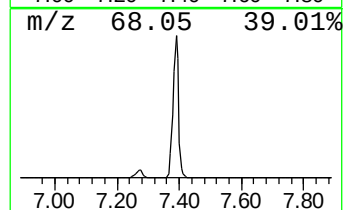
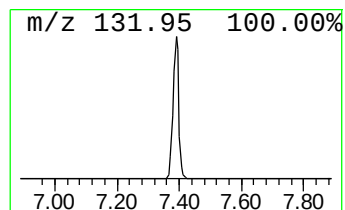
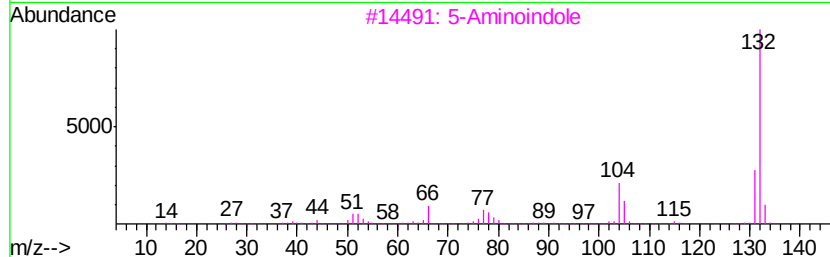
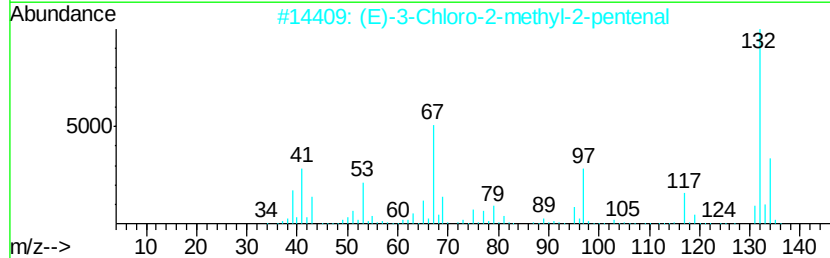
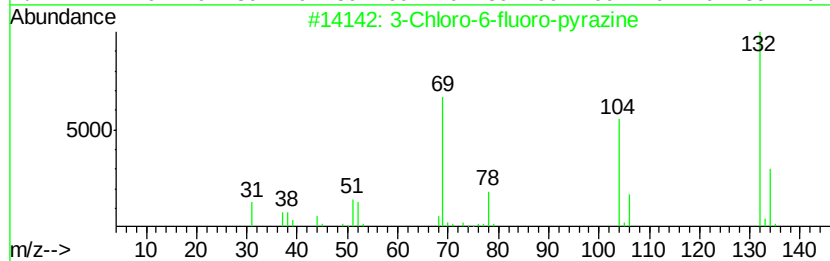
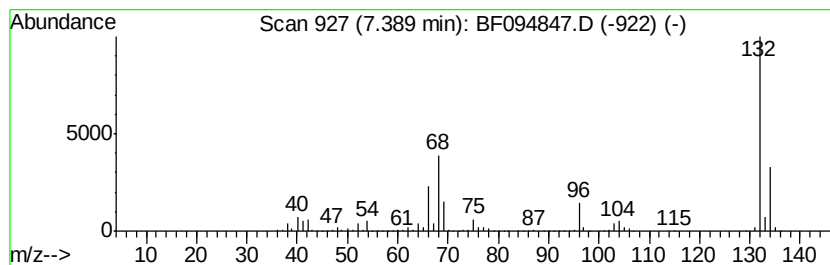
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Peak Number 2 unknown7.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.39	108.68 ng	3113500	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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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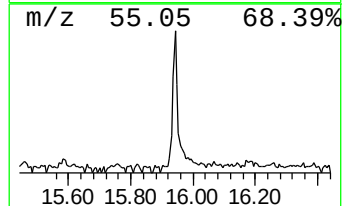
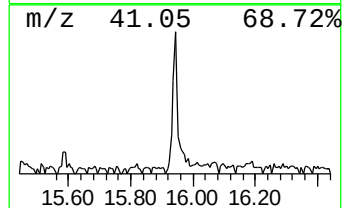
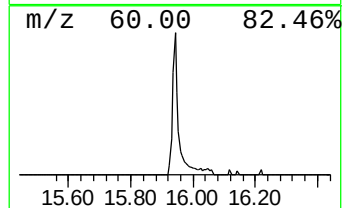
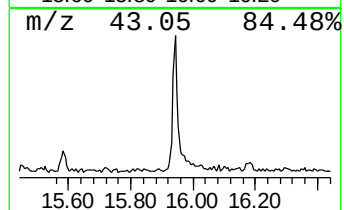
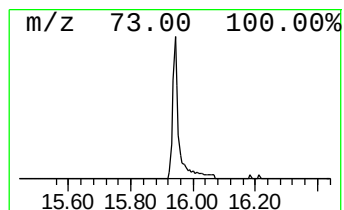
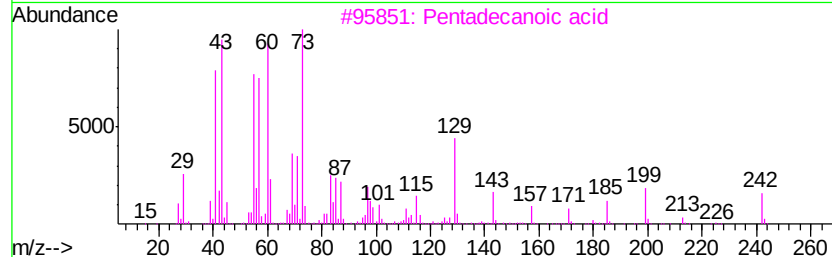
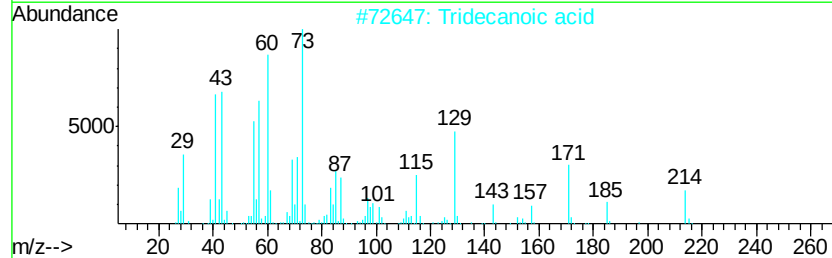
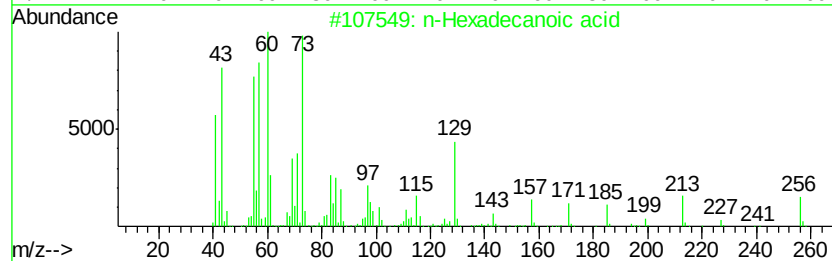
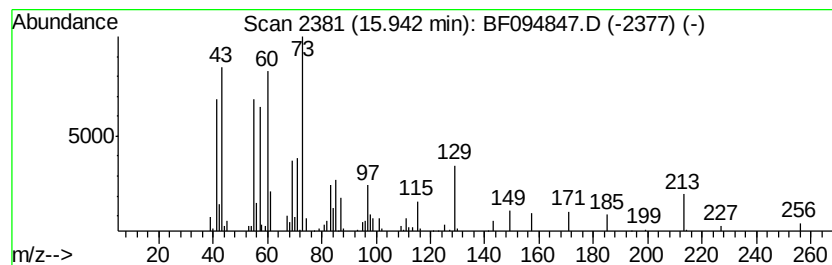
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.49 ng	143954	Phenanthrene-d10	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
5		Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	18



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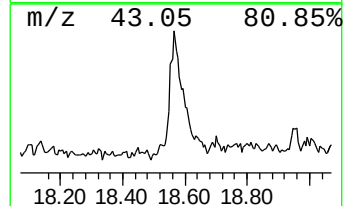
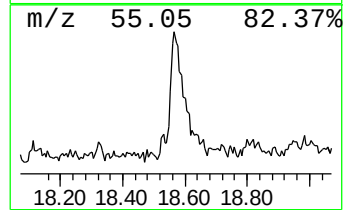
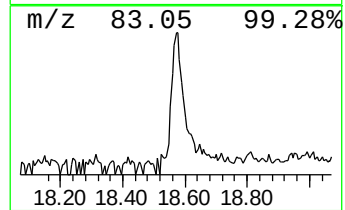
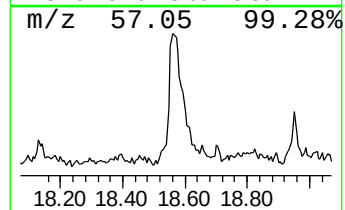
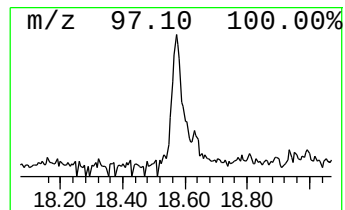
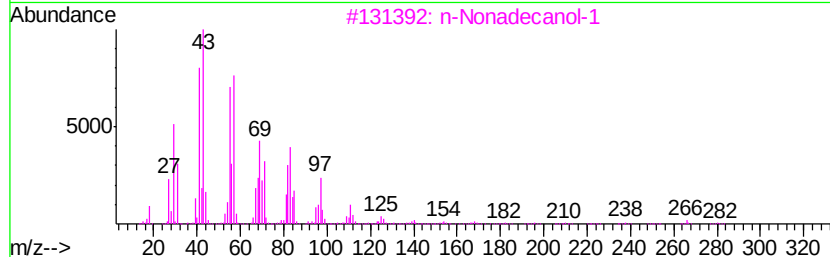
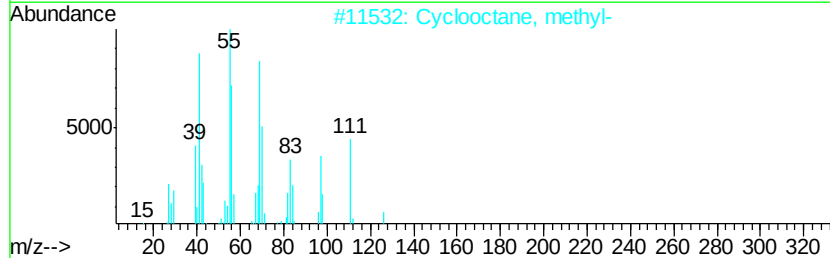
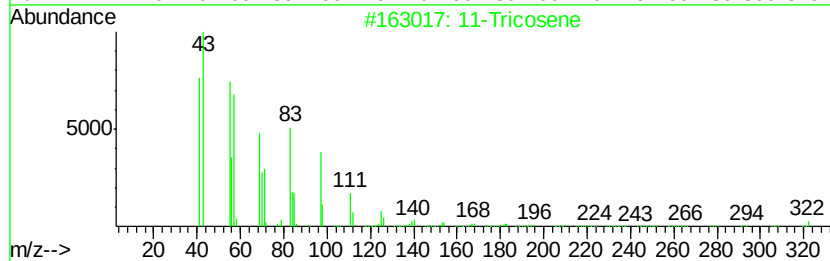
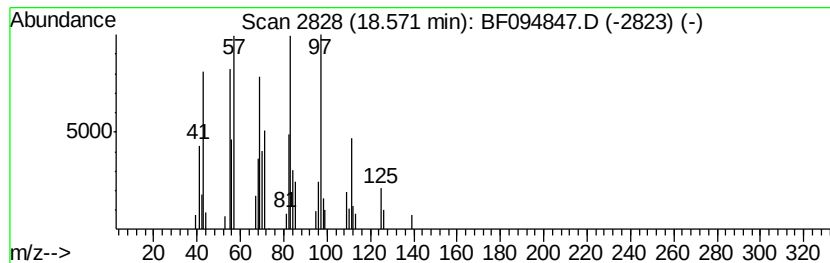
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Peak Number 5 11-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.57	4.47 ng	157058	Chrysene-d12	18.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	72
2	Cyclooctane, methyl-	126	C9H18	001502-38-1	46
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	35
4	1-Eicosanol	298	C20H42O	000629-96-9	35
5	4,4-Dimethylpent-2-enal	112	C7H12O	1000195-01-6	27



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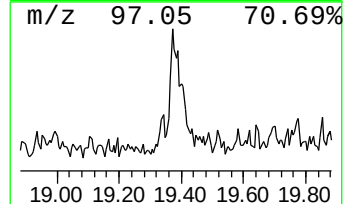
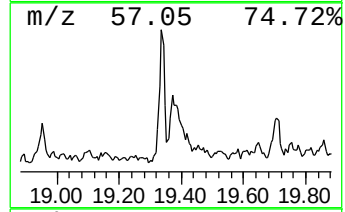
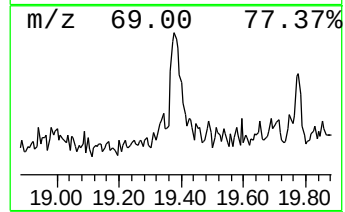
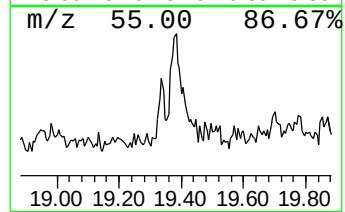
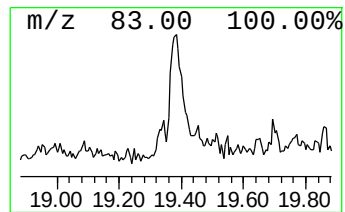
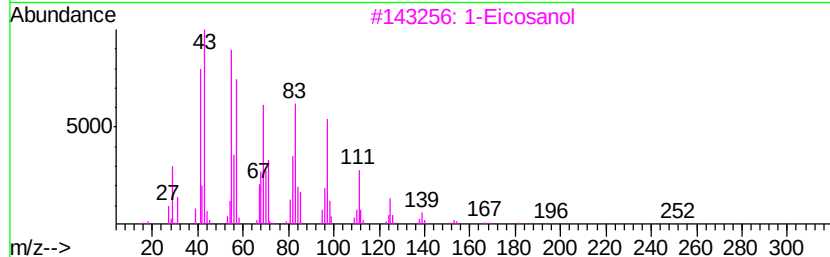
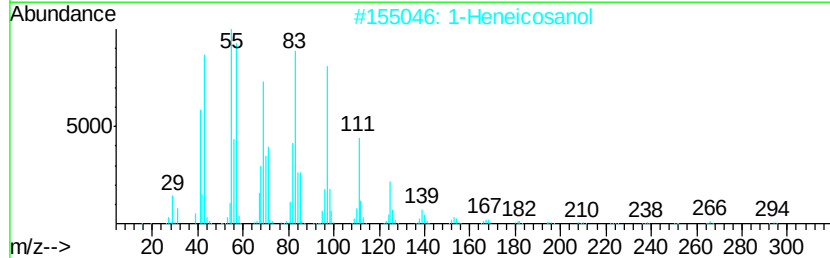
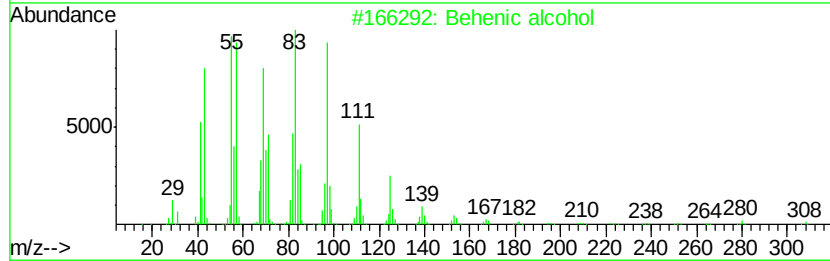
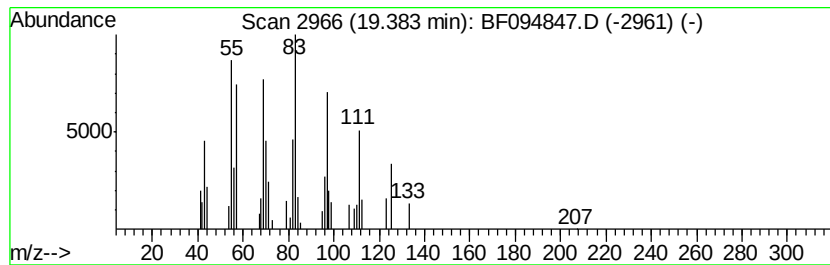
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Peak Number 6 Behenic alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.38	2.44 ng	85565	Chrysene-d12	18.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	72
2		1-Heneicosanol	312	C21H44O	015594-90-8	72
3		1-Eicosanol	298	C20H42O	000629-96-9	58
4		4-Undecene, 6-methyl-	168	C12H24	1000061-85-4	46
5		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	27



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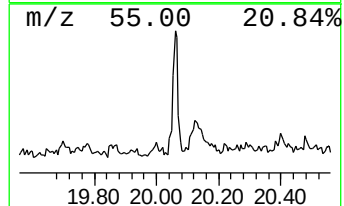
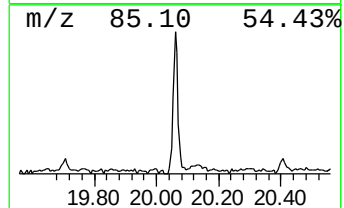
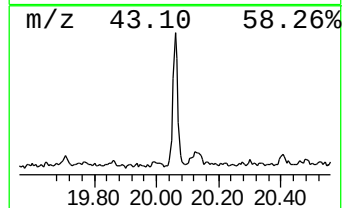
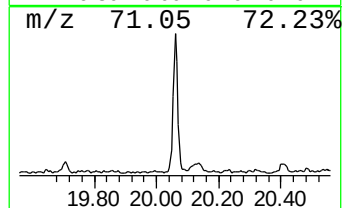
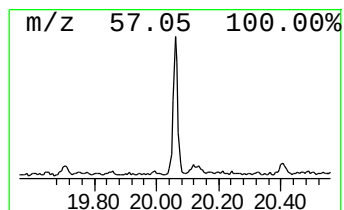
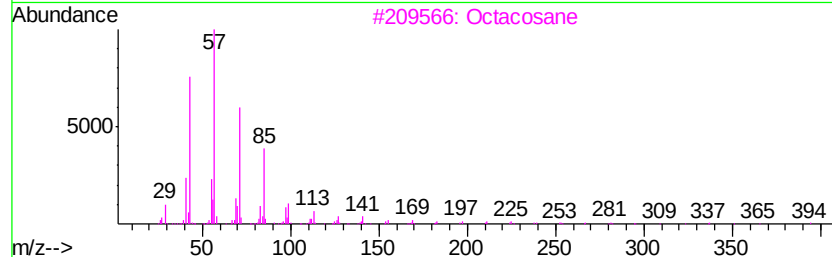
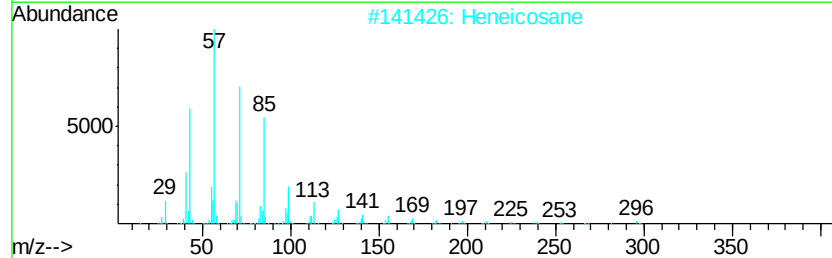
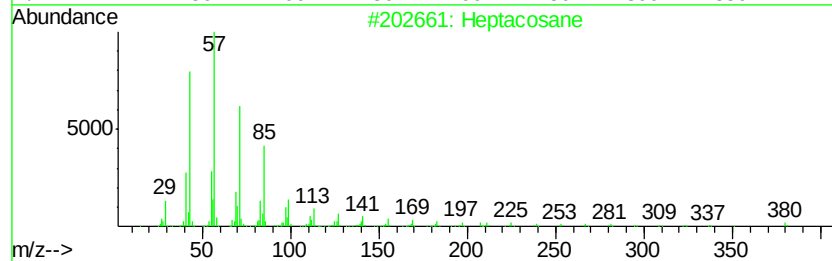
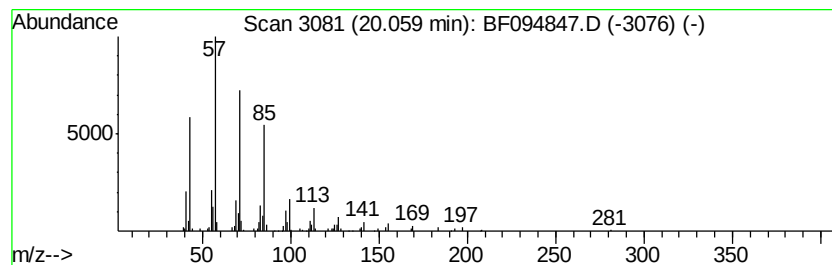
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.06	6.24 ng	181277	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094847.D
Acq On : 3 May 2017 22:10
Operator : SJ/MA
Sample : I2914-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP(0-6.5)

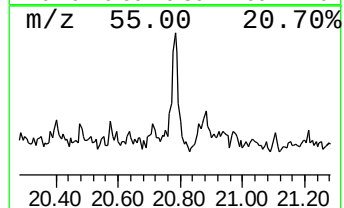
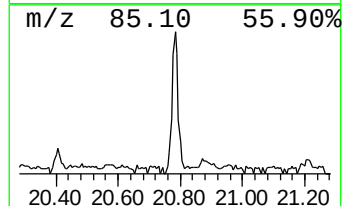
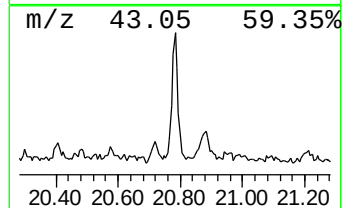
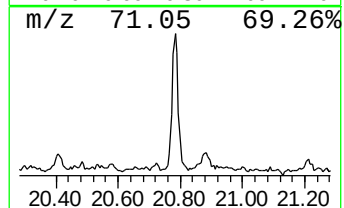
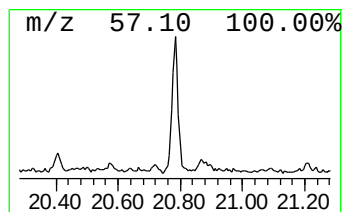
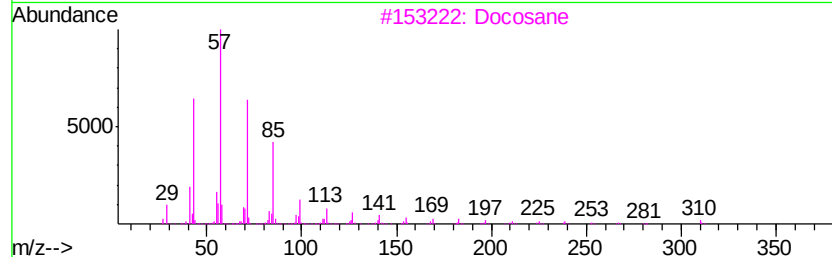
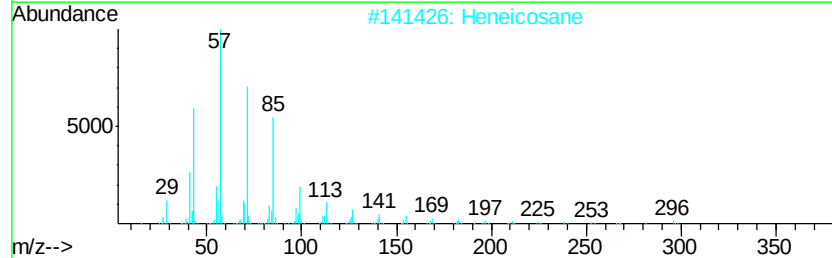
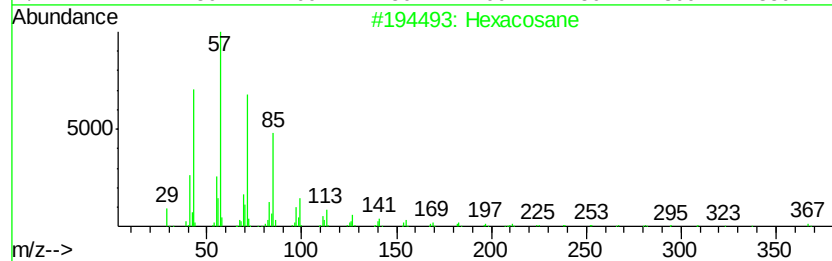
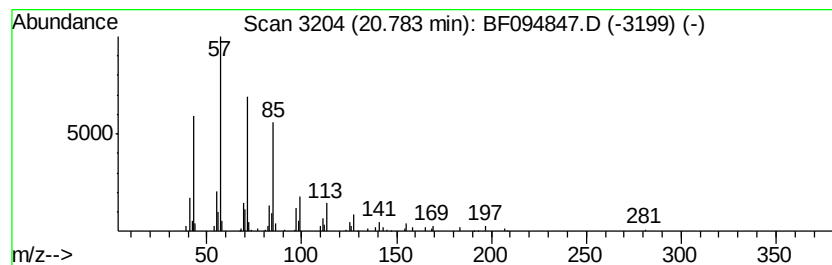
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	4.89 ng	142007	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Docosane	310	C22H46	000629-97-0	91
4		Octacosane	394	C28H58	000630-02-4	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094847.D
Acq On : 3 May 2017 22:10
Operator : SJ/MA
Sample : I2914-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP(0-6.5)

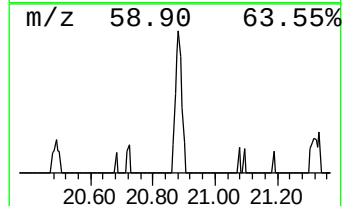
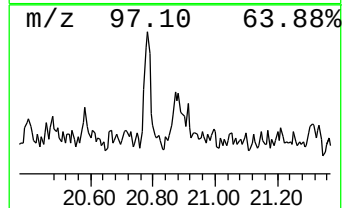
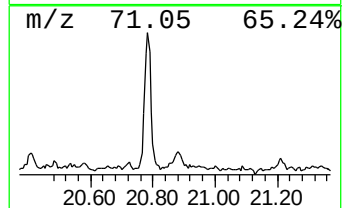
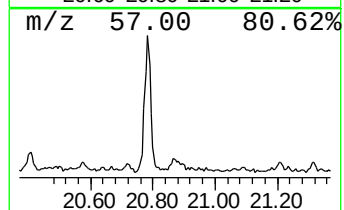
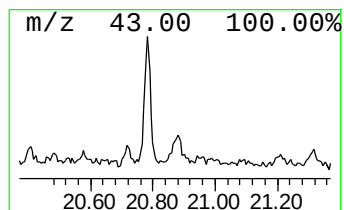
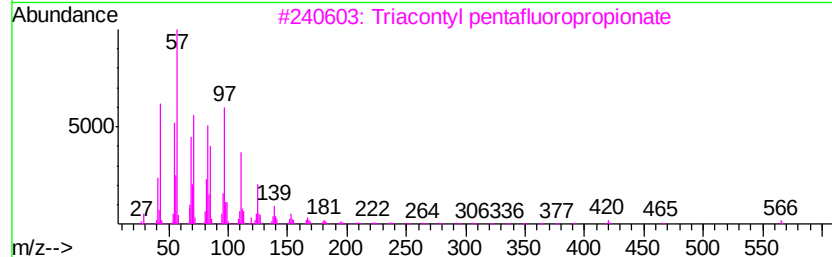
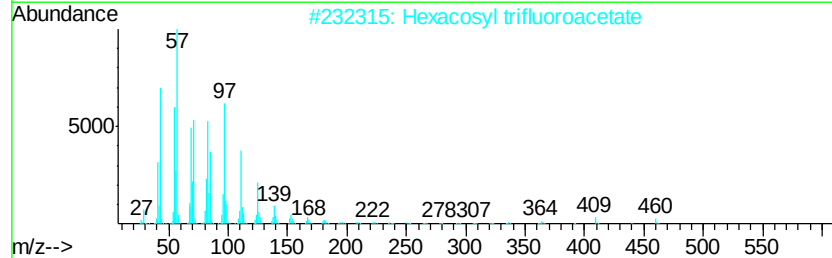
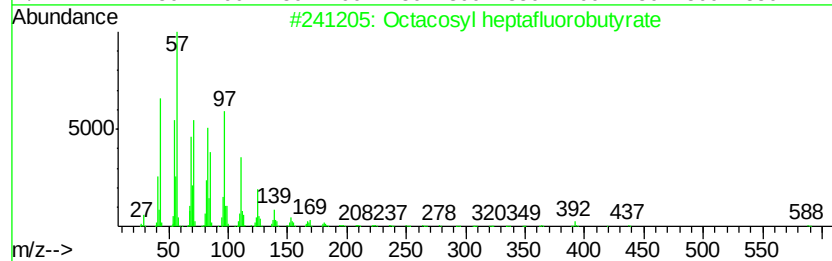
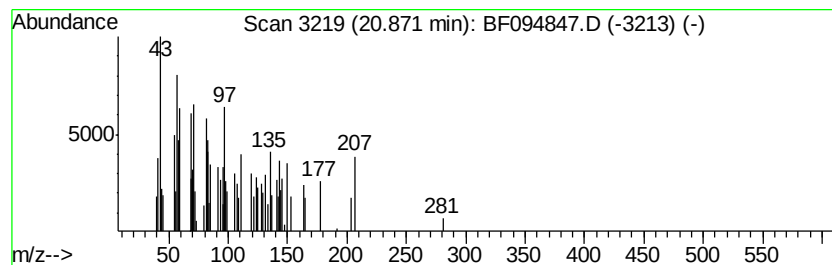
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown20.87 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	2.99 ng	86799	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	11
2		Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	11
3		Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	11
4		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	11
5		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094847.D
Acq On : 3 May 2017 22:10
Operator : SJ/MA
Sample : I2914-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP(0-6.5)

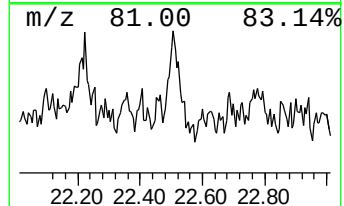
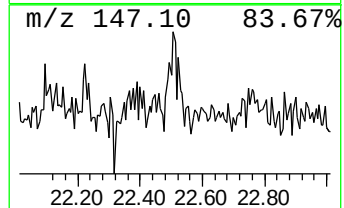
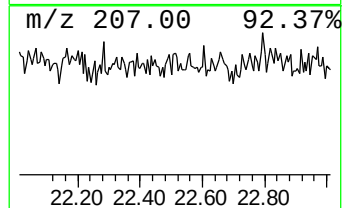
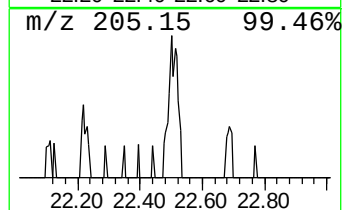
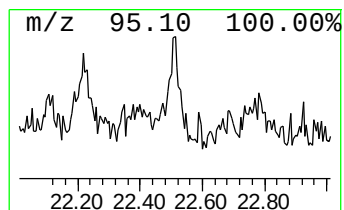
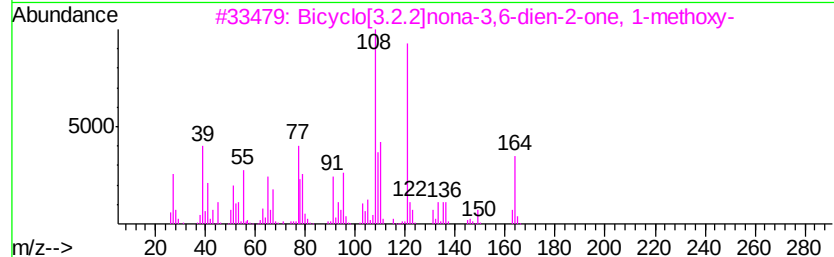
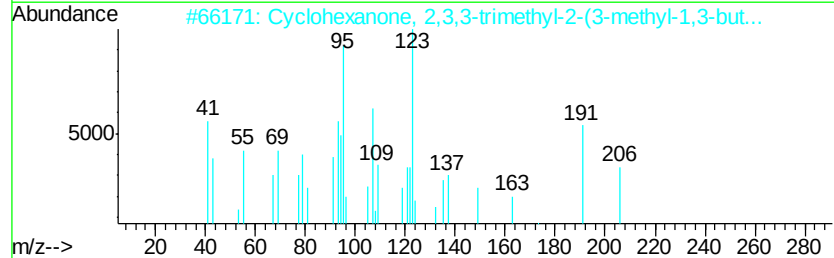
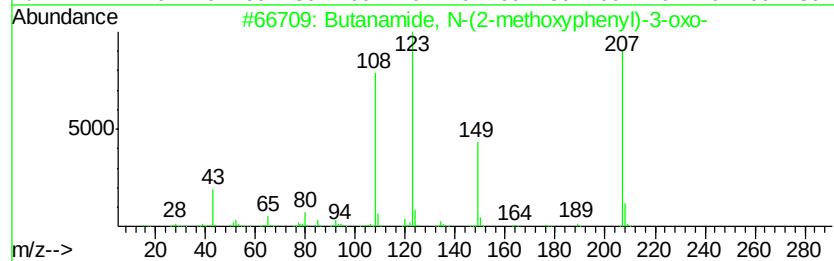
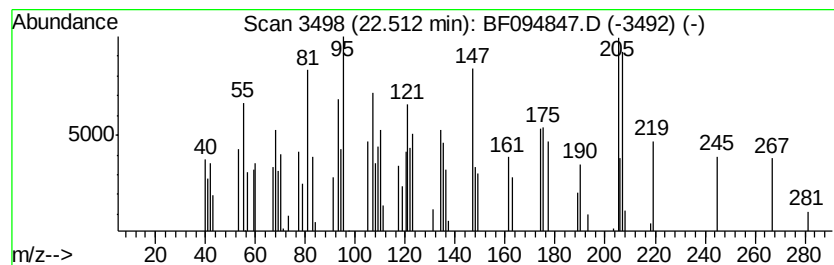
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.51 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	3.05 ng	88572	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanamide, N-(2-methoxyphenyl)-...	207	C11H13NO3	000092-15-9	22
2		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	18
3		Bicyclo[3.2.2]nona-3,6-dien-2-on...	164	C10H12O2	073830-82-7	14
4		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	10
5		2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094847.D
Acq On : 3 May 2017 22:10
Operator : SJ/MA
Sample : I2914-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP(0-6.5)

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	24.2	ng	694020	1	7.72	572994	20.0
unknown7.39	7.39	108.7	ng	3113500	1	7.72	572994	20.0
n-Hexadecanoic acid	15.94	3.5	ng	143954	4	14.97	825432	20.0
11-Tricosene	18.57	4.5	ng	157058	5	18.64	702112	20.0
Behenic alcohol	19.38	2.4	ng	85565	5	18.64	702112	20.0
Heptacosane	20.06	6.2	ng	181277	6	20.30	581069	20.0
Hexacosane	20.78	4.9	ng	142007	6	20.30	581069	20.0
unknown20.87	20.87	3.0	ng	86799	6	20.30	581069	20.0
unknown22.51	22.51	3.0	ng	88572	6	20.30	581069	20.0