

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
 Data File : BF094845.D
 Acq On : 3 May 2017 21:06
 Operator : SJ/MA
 Sample : I2914-09
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-11-1.0-2.0

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	5.042	523	528	544	rBV	279180	542634	18.91%	2.101%
2	5.678	631	636	665	rBV	1798494	2530652	88.20%	9.800%
3	6.242	729	732	746	rVB3	22969	41641	1.45%	0.161%
4	7.272	901	907	921	rBV	1875770	2749942	95.84%	10.650%
5	7.389	921	927	935	rVB	2237407	2869257	100.00%	11.112%
6	7.572	954	958	972	rBV5	8931	32471	1.13%	0.126%
7	7.725	980	984	995	rVB	494890	556121	19.38%	2.154%
8	7.966	1019	1025	1034	rBV	1619411	1940700	67.64%	7.516%
9	8.624	1131	1137	1146	rBV	1354165	1706014	59.46%	6.607%
10	9.742	1322	1327	1339	rBV	643510	751128	26.18%	2.909%
11	11.518	1623	1629	1641	rBV	2044412	2418960	84.31%	9.368%
12	12.207	1741	1746	1755	rBV	516018	608513	21.21%	2.357%
13	12.571	1803	1808	1818	rBV2	655116	865454	30.16%	3.352%
14	12.877	1856	1860	1869	rBV	22202	33194	1.16%	0.129%
15	13.418	1949	1952	1956	rVB2	34390	38012	1.32%	0.147%
16	13.865	2022	2028	2041	rBV	1192673	1596570	55.64%	6.183%
17	14.195	2079	2084	2086	rBV	36010	45966	1.60%	0.178%
18	14.924	2201	2208	2211	rBV2	26336	32631	1.14%	0.126%
19	14.971	2211	2216	2228	rVB	674309	830351	28.94%	3.216%
20	15.942	2376	2381	2395	rBV2	157694	205462	7.16%	0.796%
21	17.030	2563	2566	2569	rBV	34027	39986	1.39%	0.155%
22	17.300	2606	2612	2616	rBV	1535859	1811507	63.14%	7.015%
23	17.689	2671	2678	2682	rBV2	32160	55155	1.92%	0.214%
24	18.559	2819	2826	2835	rBV2	164361	384643	13.41%	1.490%
25	18.636	2835	2839	2847	rVB	610457	679984	23.70%	2.633%
26	19.336	2954	2958	2959	rBV2	73769	87624	3.05%	0.339%
27	19.365	2959	2963	2975	rVB3	161505	380881	13.27%	1.475%
28	19.706	3016	3021	3024	rBV4	21089	32239	1.12%	0.125%
29	19.753	3024	3029	3037	rVB10	17515	44528	1.55%	0.172%
30	20.059	3077	3081	3086	rBV	237057	266144	9.28%	1.031%
31	20.112	3086	3090	3102	rVV4	64637	142663	4.97%	0.552%
32	20.300	3116	3122	3126	rBV	458631	538969	18.78%	2.087%
33	20.418	3136	3142	3146	rBV7	34679	60582	2.11%	0.235%
34	20.483	3149	3153	3158	rBV7	22317	35553	1.24%	0.138%

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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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35	20.671	3182	3185	3189	rBV4	26510	41739	1.45%	0.162%
36	20.759	3196	3200	3201	rBV4	25799	29372	1.02%	0.114%
37	20.788	3201	3205	3211	rVB	74775	125157	4.36%	0.485%
38	20.877	3214	3220	3224	rBV4	51777	109106	3.80%	0.423%
39	21.818	3375	3380	3390	rVB9	36333	104706	3.65%	0.405%
40	22.112	3424	3430	3437	rVB7	61831	113391	3.95%	0.439%
41	22.365	3465	3473	3480	rBV7	16809	47792	1.67%	0.185%
42	22.512	3491	3498	3506	rVB6	93998	214847	7.49%	0.832%
43	22.800	3545	3547	3555	rVB8	16414	31708	1.11%	0.123%
44	23.753	3704	3709	3716	rVB8	19495	48034	1.67%	0.186%

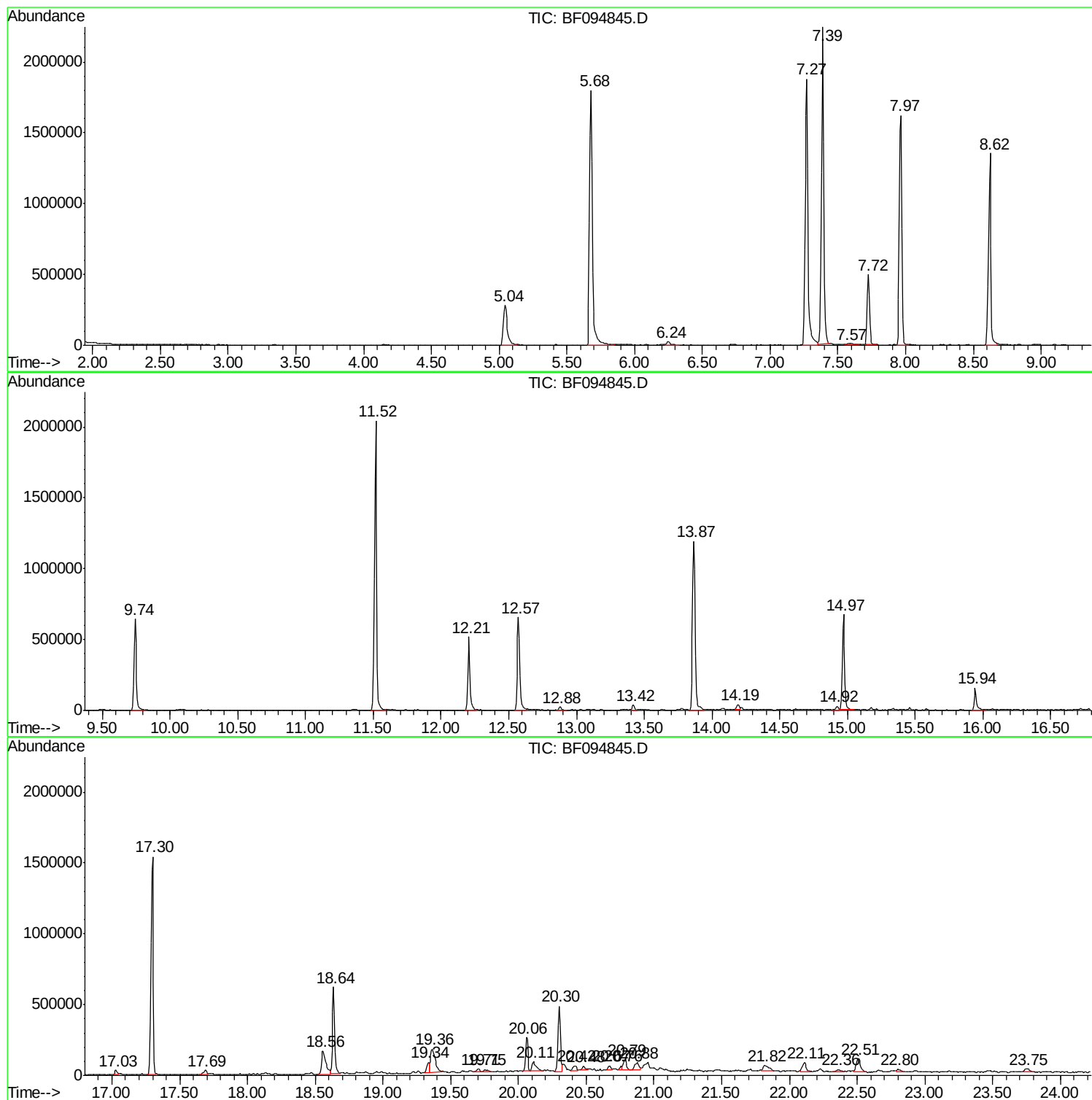
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
SB-11-1.0-2.0

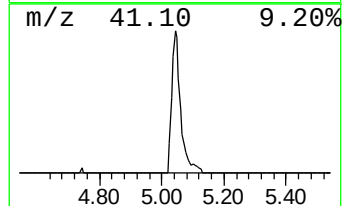
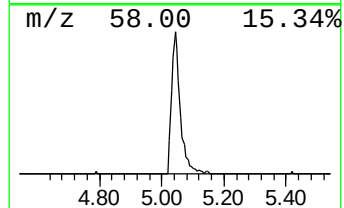
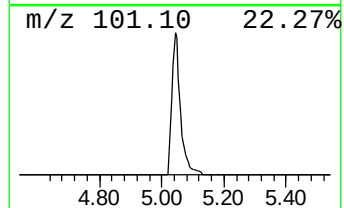
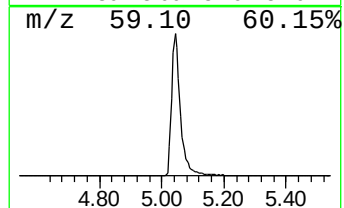
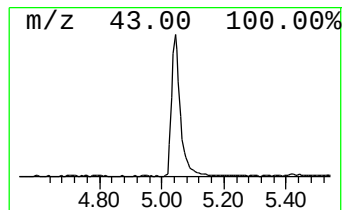
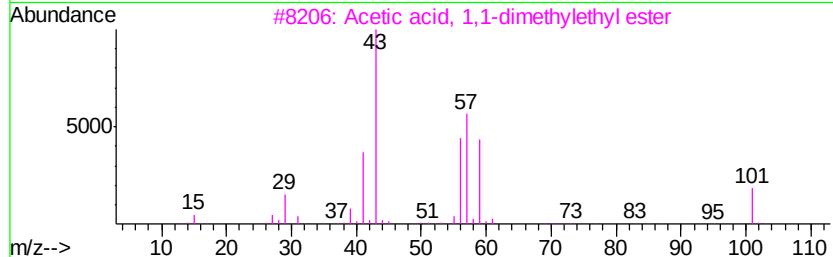
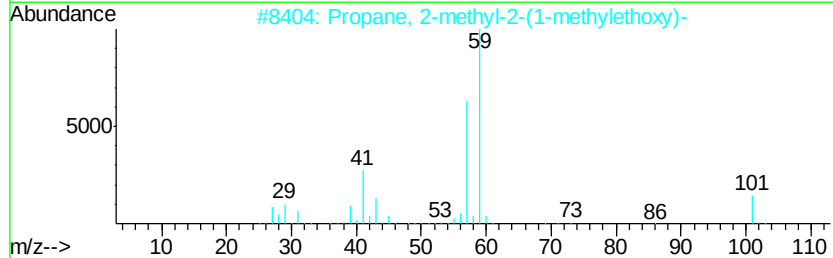
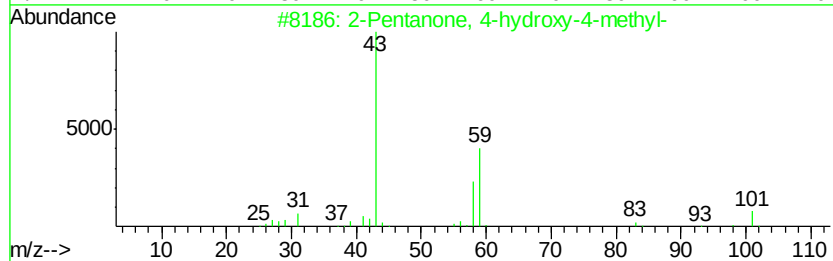
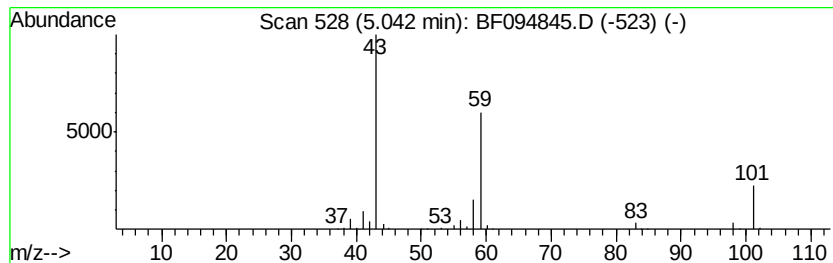
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	19.52 ng	542634	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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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Instrument :
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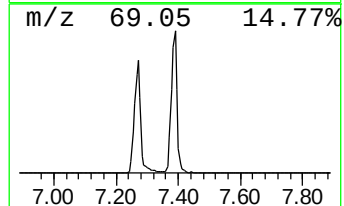
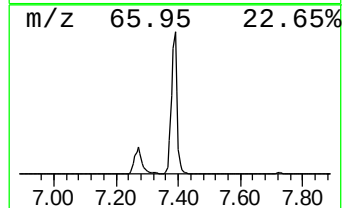
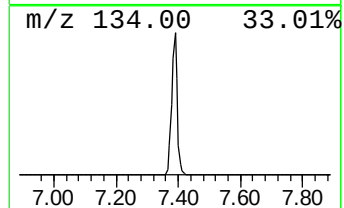
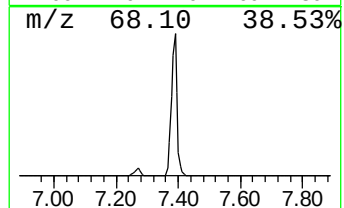
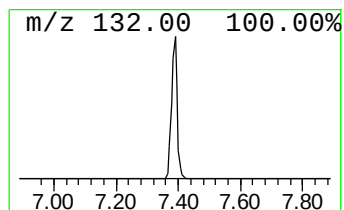
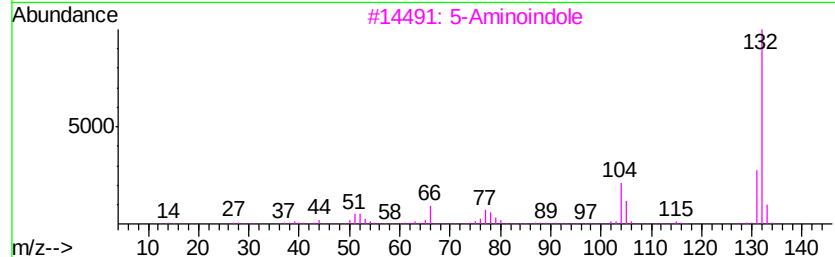
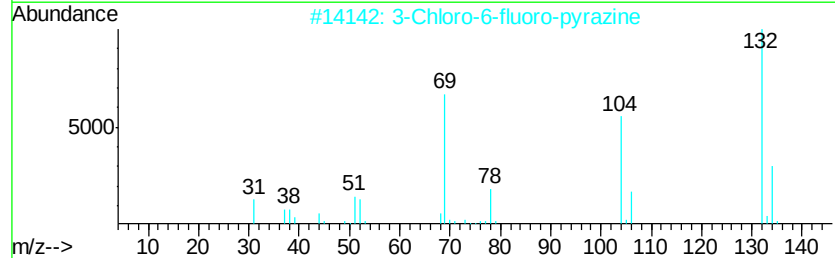
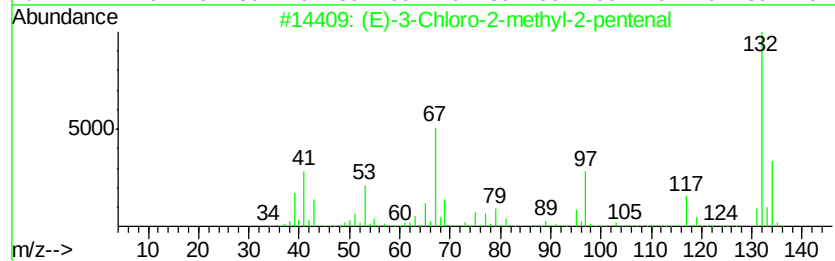
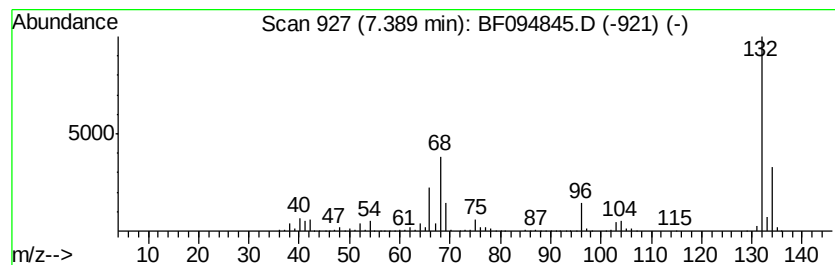
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Peak Number 2 unknown7.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.39	103.19 ng	2869260	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	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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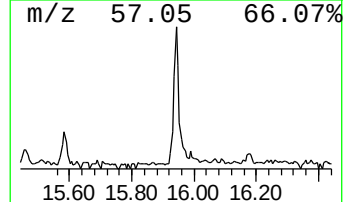
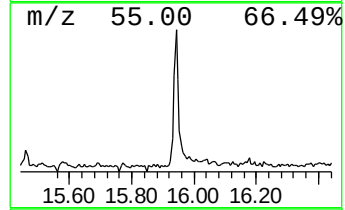
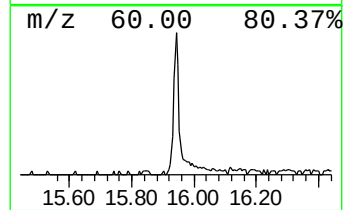
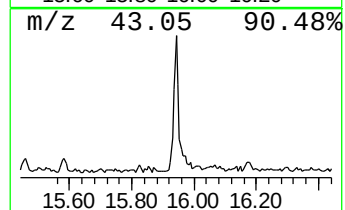
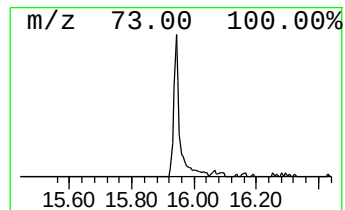
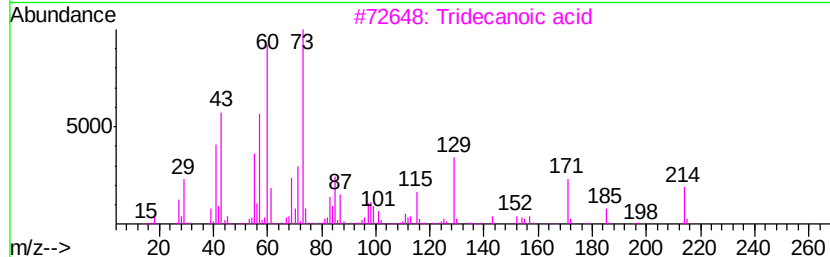
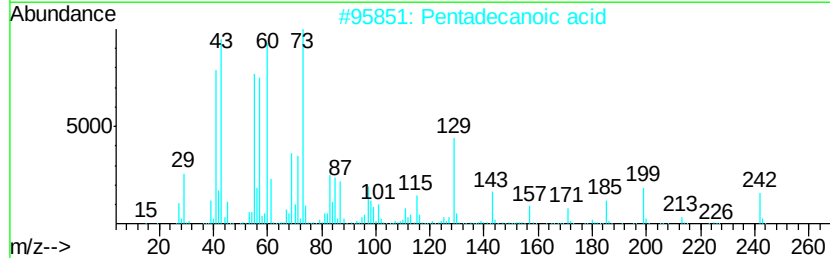
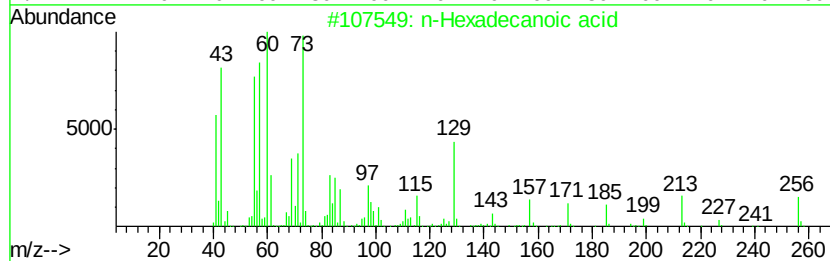
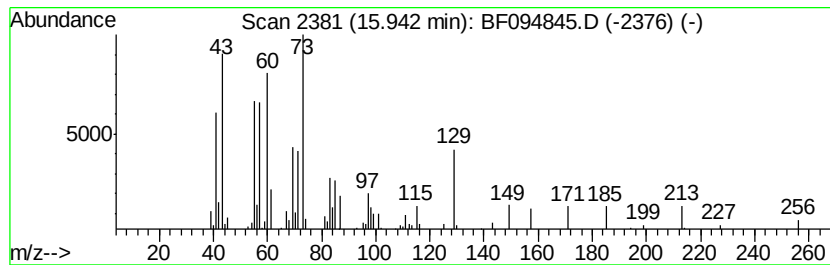
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.95 ng	205462	Phenanthrene-d10	14.97

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	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	18



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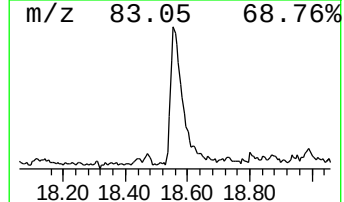
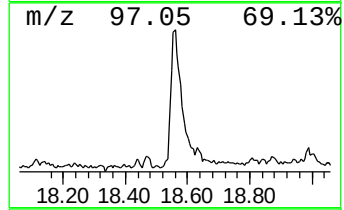
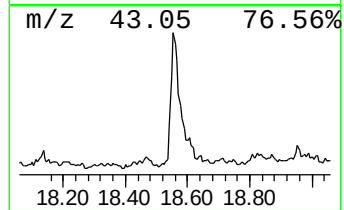
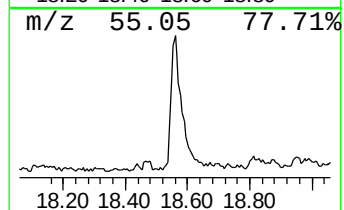
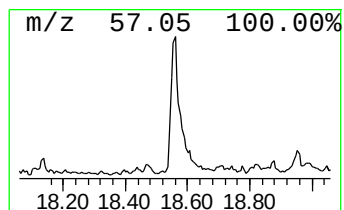
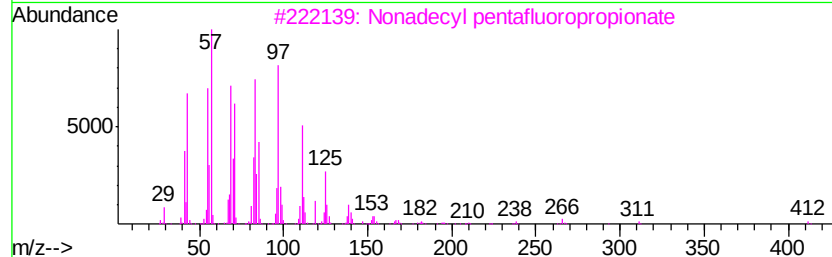
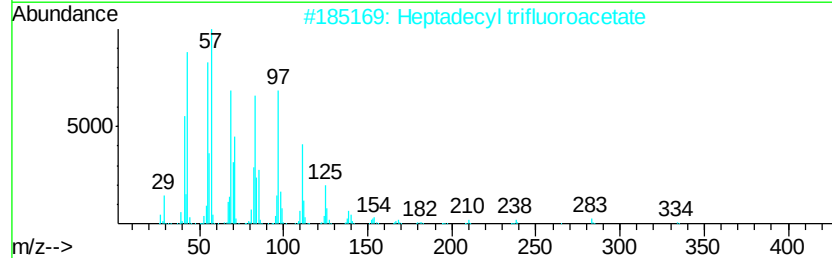
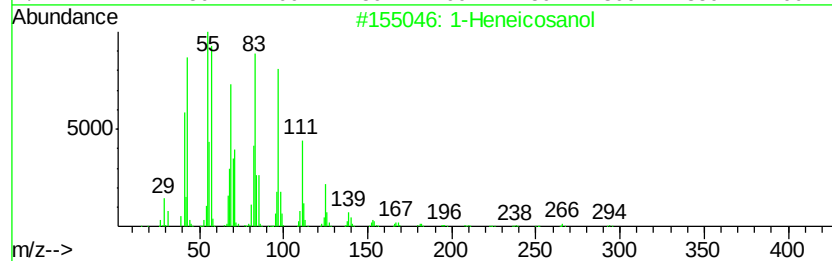
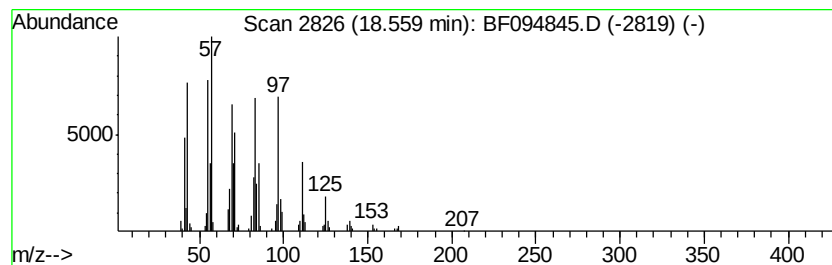
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	11.31 ng	384643	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	93
2	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	91
3	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	91
4	1-Docosene		308	C22H44	001599-67-3	91
5	17-Pentatriacontene		491	C35H70	006971-40-0	91



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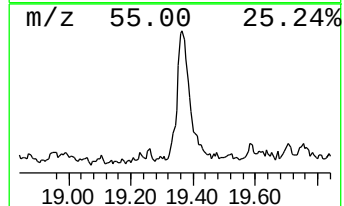
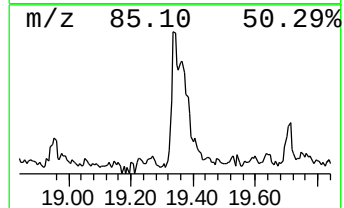
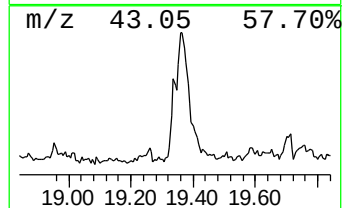
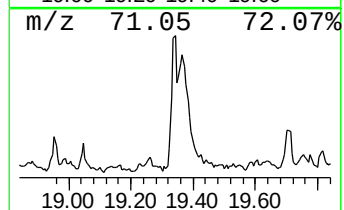
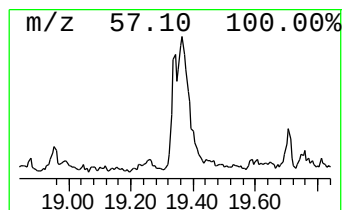
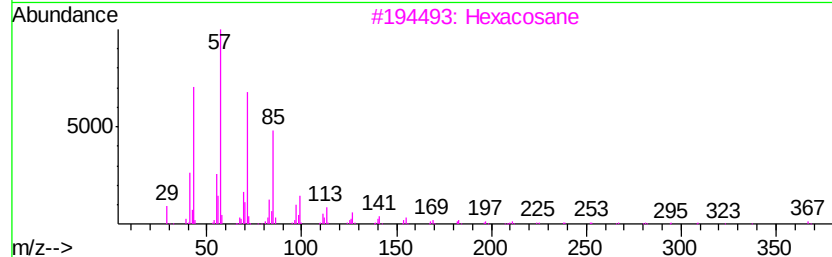
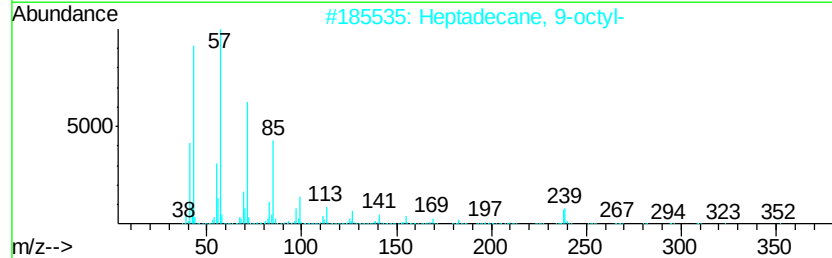
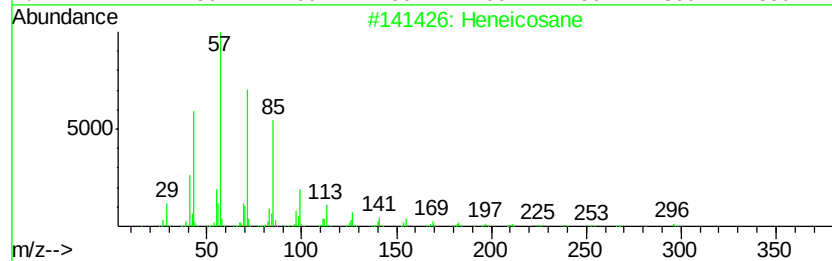
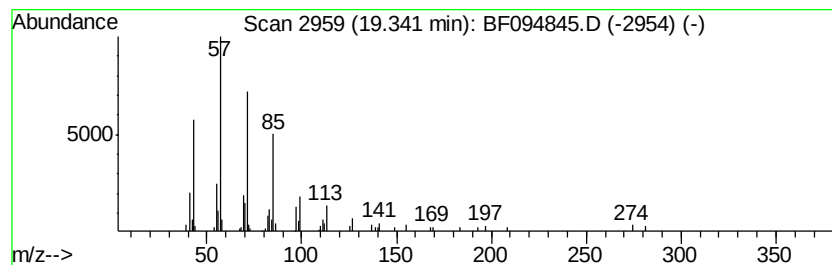
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	2.58 ng	87624	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	83
3	Hexacosane		366	C26H54	000630-01-3	83
4	Heptadecane		240	C17H36	000629-78-7	83
5	Triacontane		422	C30H62	000638-68-6	83



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Operator : SJ/MA
Sample : I2914-09
Misc :
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Instrument :
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ClientSampleId :
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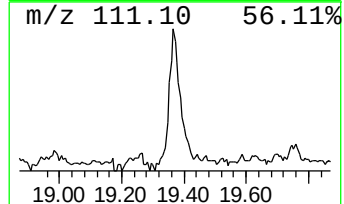
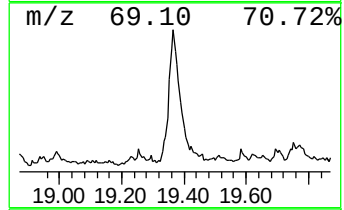
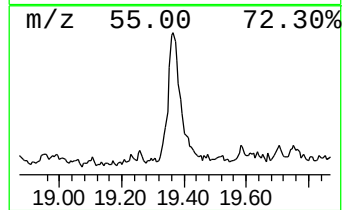
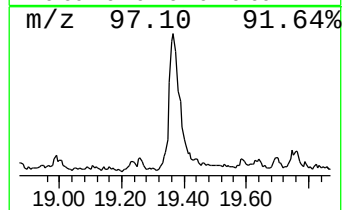
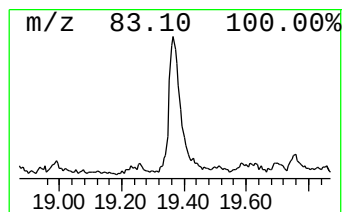
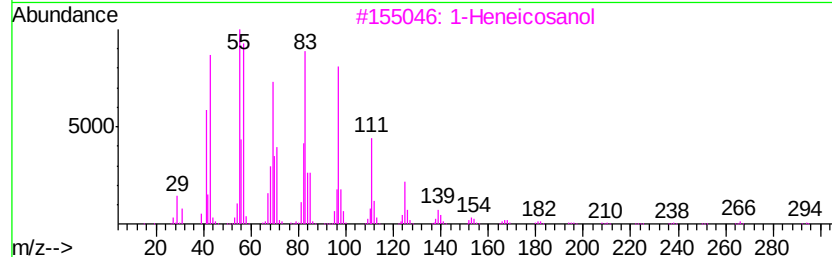
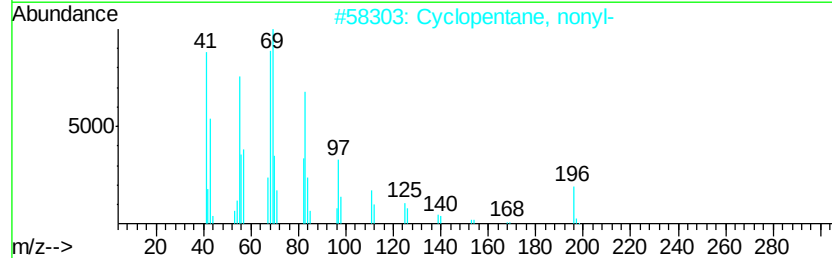
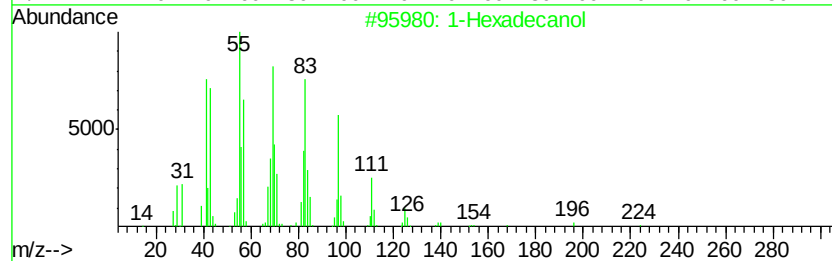
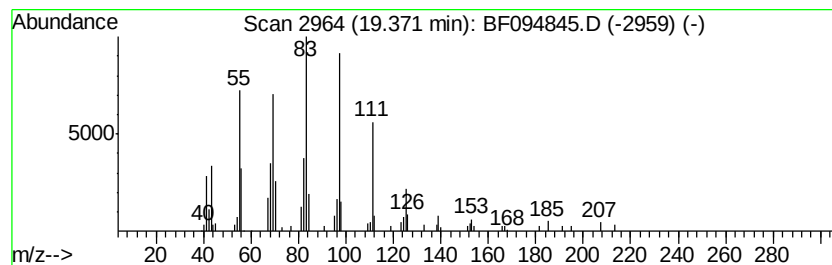
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown19.37 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	11.20 ng	380881	Chrysene-d12	18.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	46
2	Cyclopentane, nonyl-	196	C14H28	002882-98-6	38
3	1-Heneicosanol	312	C21H44O	015594-90-8	38
4	Behenic alcohol	326	C22H46O	000661-19-8	38
5	Cyclopentane, hexyl-	154	C11H22	004457-00-5	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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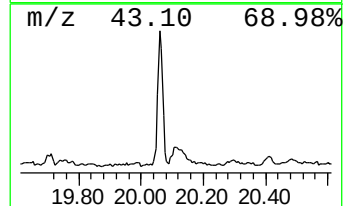
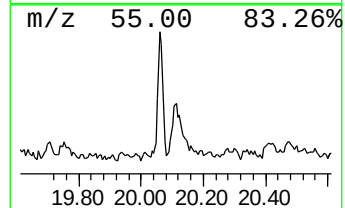
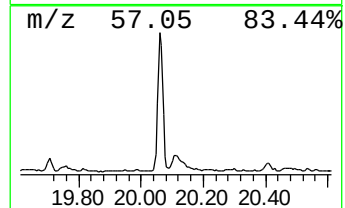
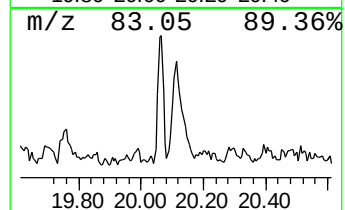
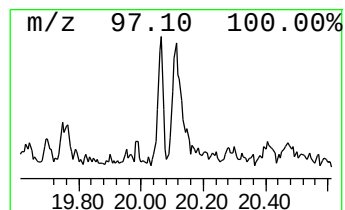
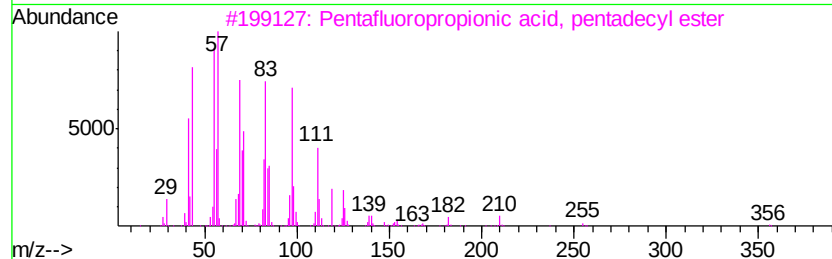
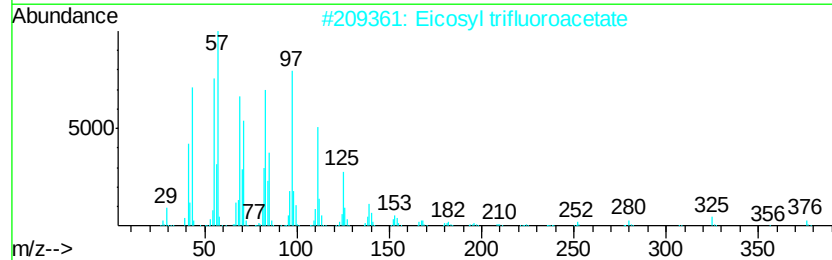
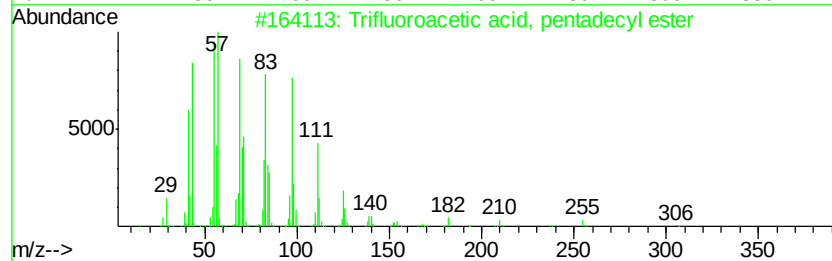
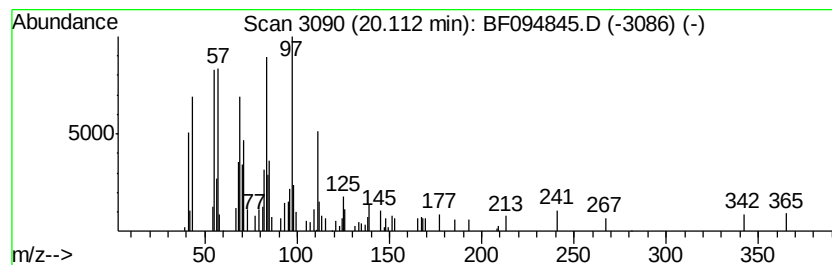
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trifluoroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.11	5.29 ng	142663	Perylene-d12	20.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90



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Acq On : 3 May 2017 21:06
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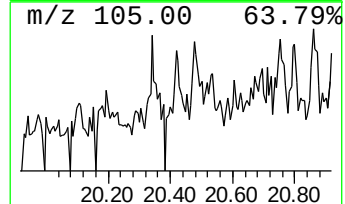
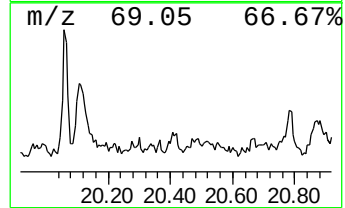
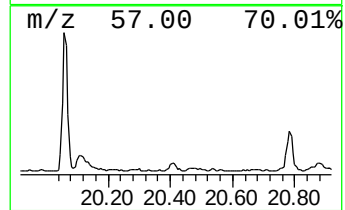
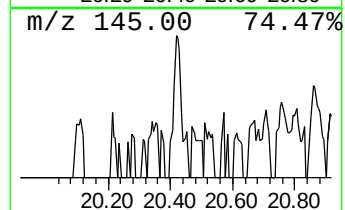
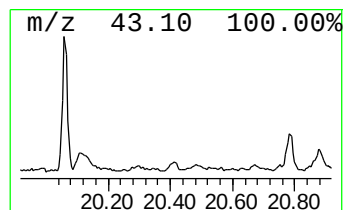
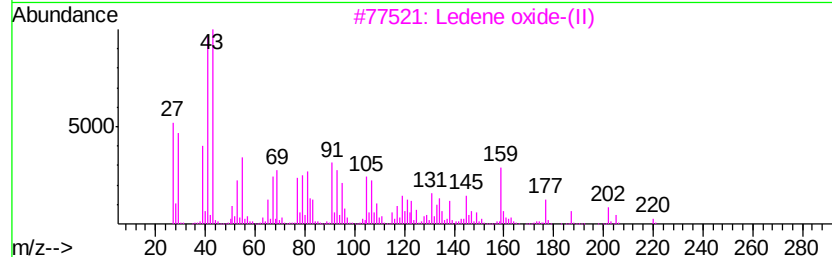
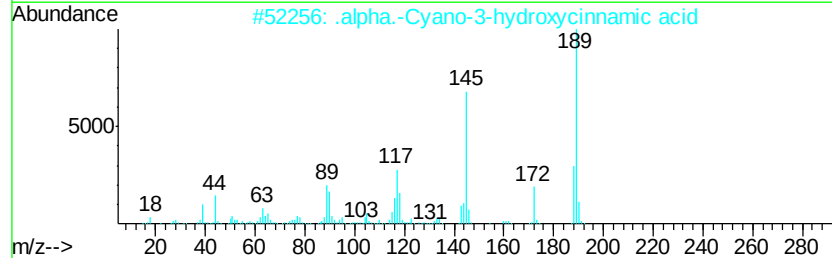
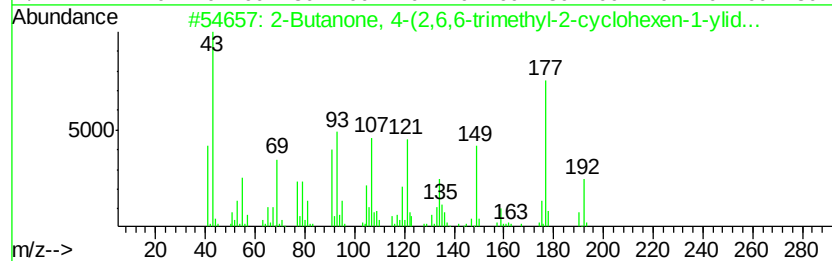
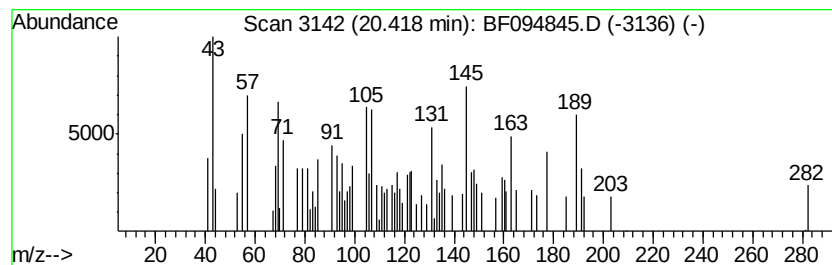
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.42 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.42	2.25 ng	60582	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanone, 4-(2,6,6-trimethyl-2...	192	C13H20O	056052-61-0	25
2		.alpha.-Cyano-3-hydroxycinnamic ...	189	C10H7NO3	054673-07-3	22
3		Ledene oxide-(II)	220	C15H24O	1000159-36-7	12
4		Benzeneethanol, .alpha.-methyl-3...	178	C12H18O	054518-11-5	12
5		4(1H)-Quinolinone, 3-methoxy-1-m...	189	C11H11NO2	052381-20-1	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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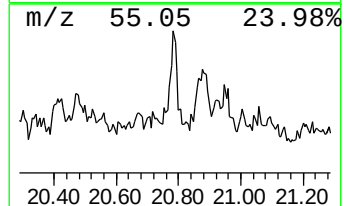
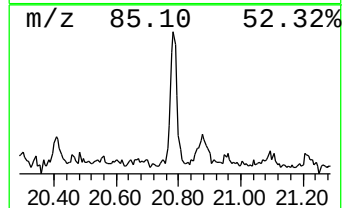
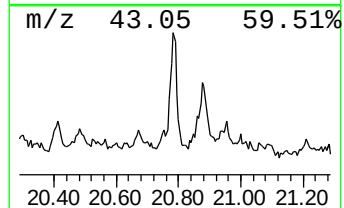
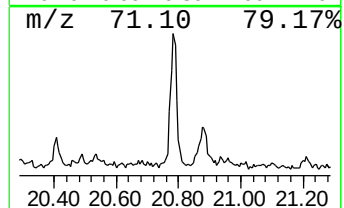
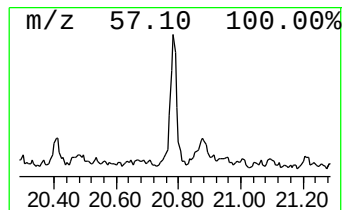
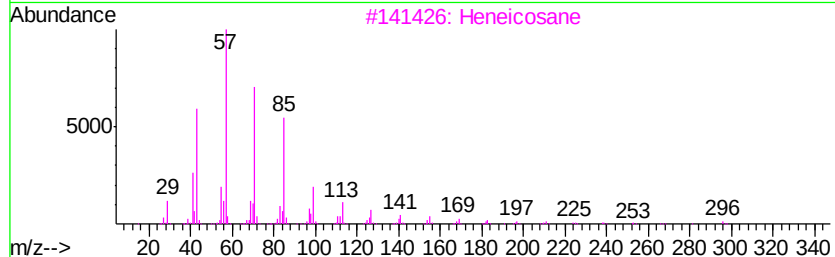
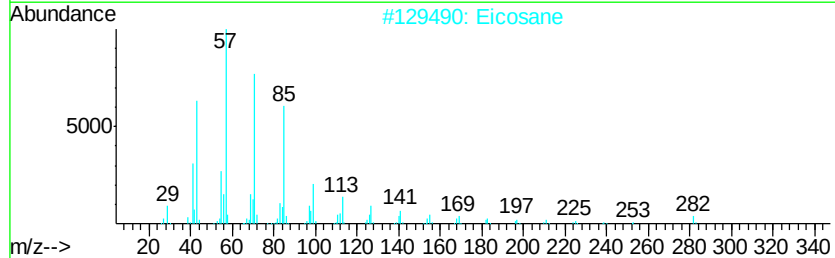
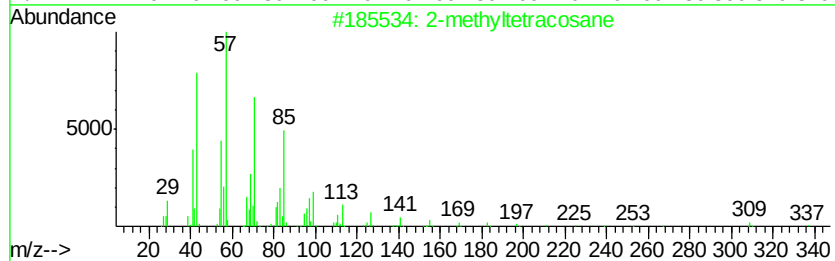
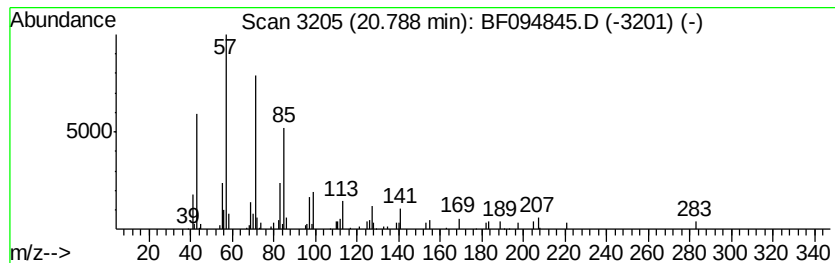
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2-methyltetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	4.64 ng	125157	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyltetracosane	352	C25H52	1000376-72-6	83
2			Eicosane	282	C20H42	000112-95-8	80
3			Heneicosane	296	C21H44	000629-94-7	80
4			Hexacosane	366	C26H54	000630-01-3	72
5			Triacontane	422	C30H62	000638-68-6	72



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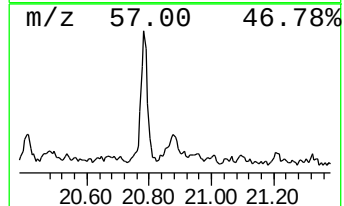
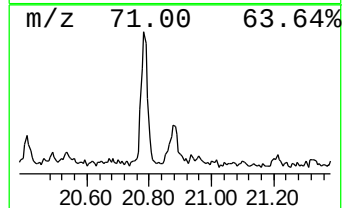
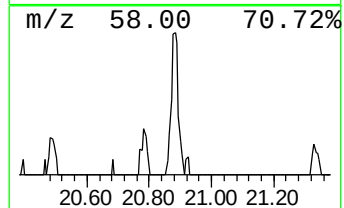
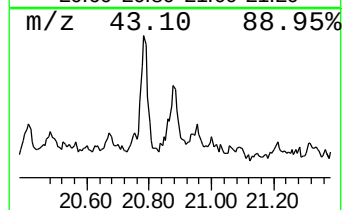
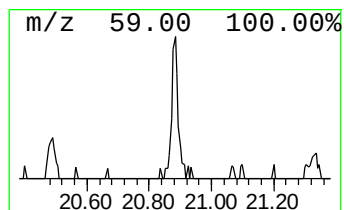
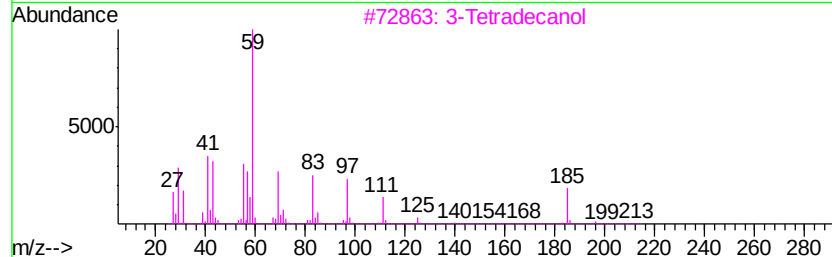
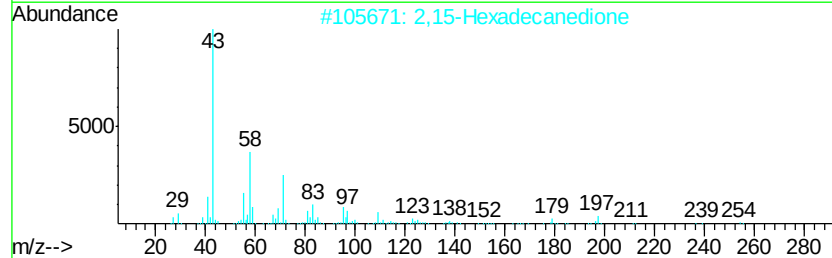
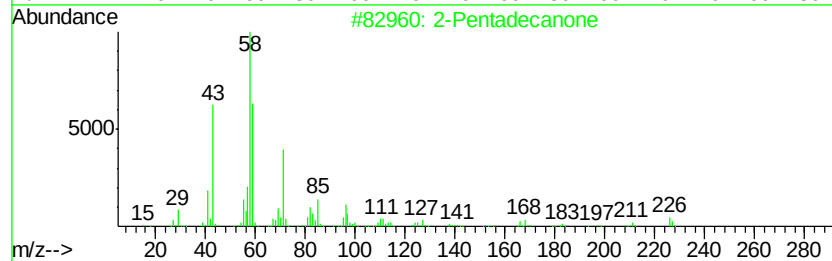
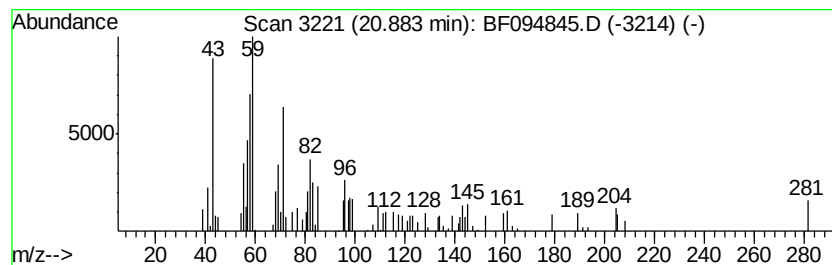
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 2-Pentadecanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.88	4.05 ng	109106	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentadecanone	226	C15H30O	002345-28-0	50
2			2,15-Hexadecanedione	254	C16H30O2	018650-13-0	38
3			3-Tetradecanol	214	C14H30O	001653-32-3	35
4			2-Decanone	156	C10H20O	000693-54-9	27
5			Diazene, [1-[2,2-bis(1-methyleth...	200	C10H24N4	059856-63-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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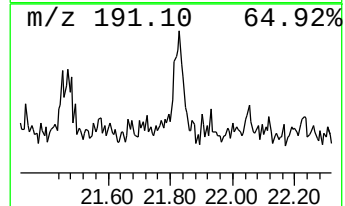
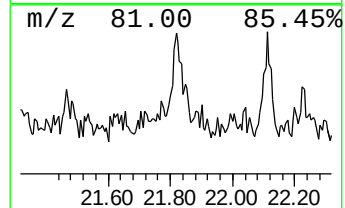
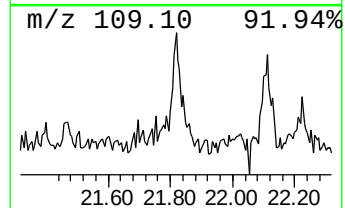
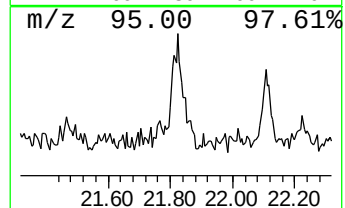
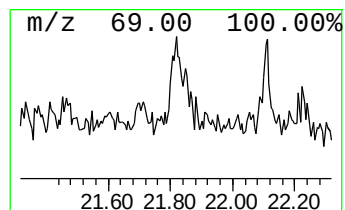
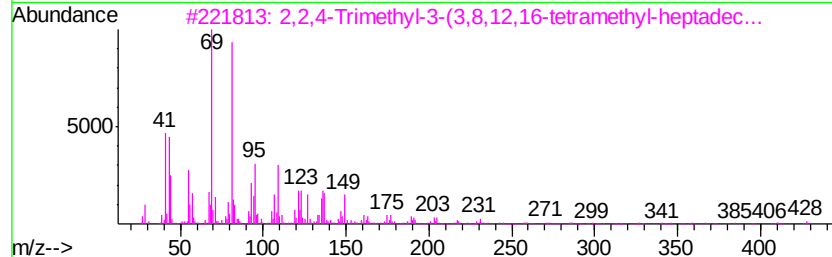
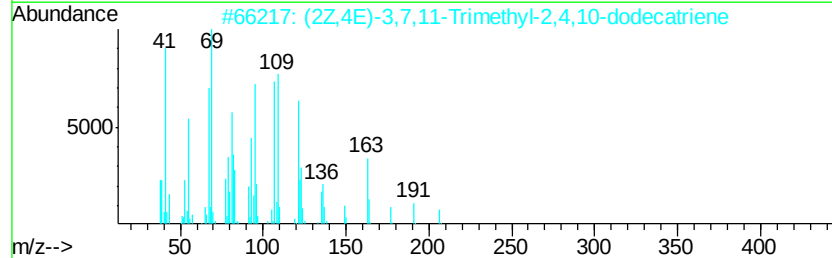
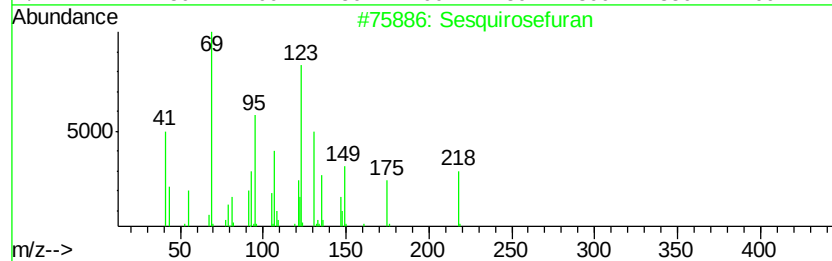
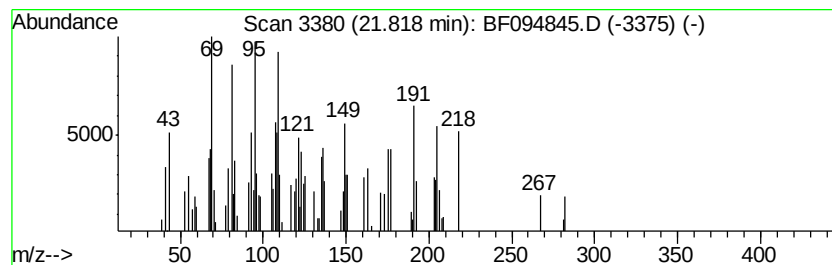
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown21.82 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.82	3.89 ng	104706	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sesquirosefuran	218	C15H22O	039007-93-7	46
2		(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	38
3		2,2,4-Trimethyl-3-(3,8,12,16-tet...	428	C30H52O	1000194-01-4	35
4		2-Butanone, 4-(2,6,6-trimethyl-2...	194	C13H22O	039721-65-8	22
5		1,8-Nonadiene, 2,7-dimethyl-5-(1...	192	C14H24	068702-20-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
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Sample : I2914-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

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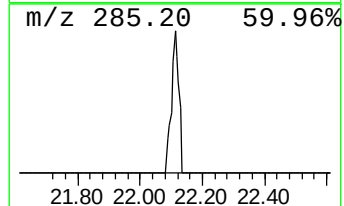
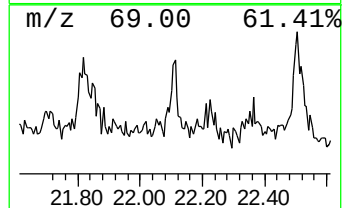
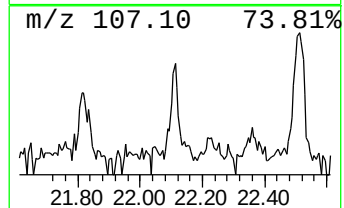
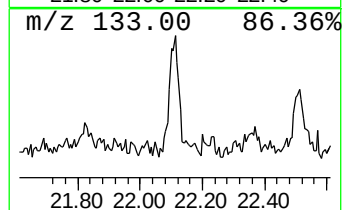
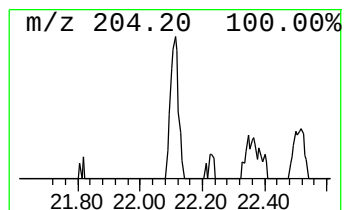
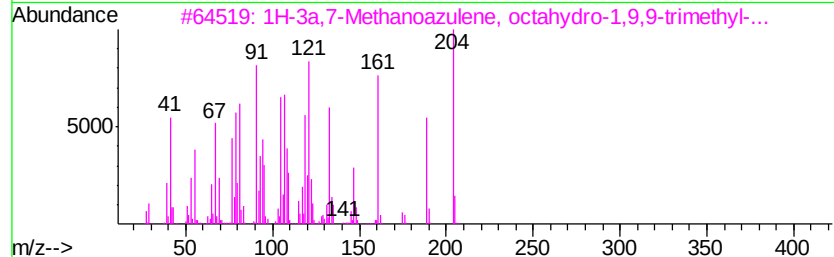
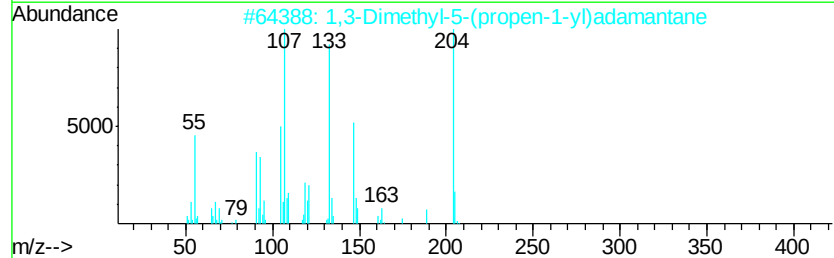
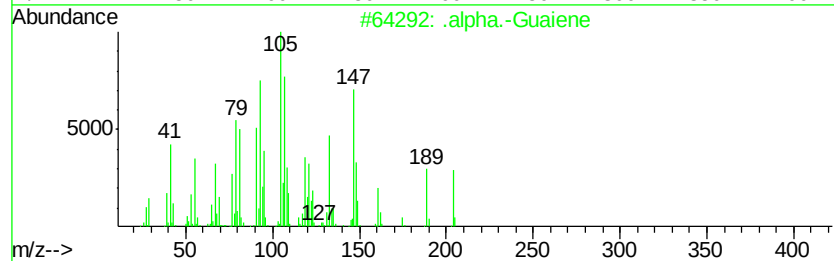
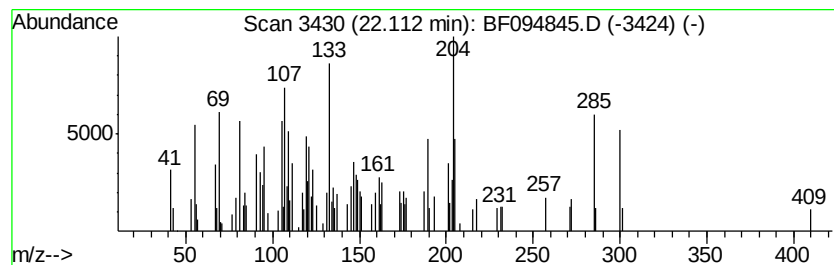
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown22.11 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	4.21 ng	113391	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Guaiene	204	C15H24	003691-12-1	49
2		1,3-Dimethyl-5-(propen-1-yl)adam...	204	C15H24	057040-48-9	49
3		1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	47
4		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	43
5		2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
Data File : BF094845.D
Acq On : 3 May 2017 21:06
Operator : SJ/MA
Sample : I2914-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11-1.0-2.0

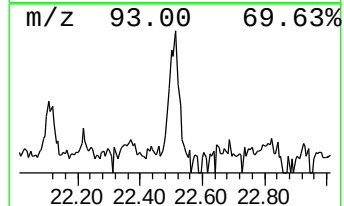
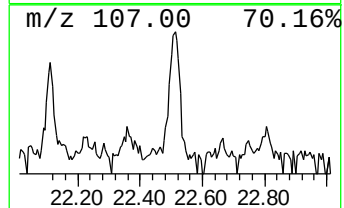
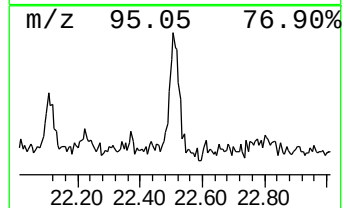
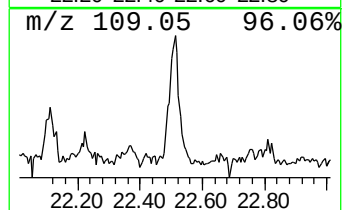
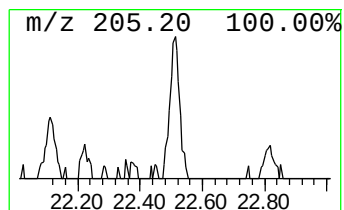
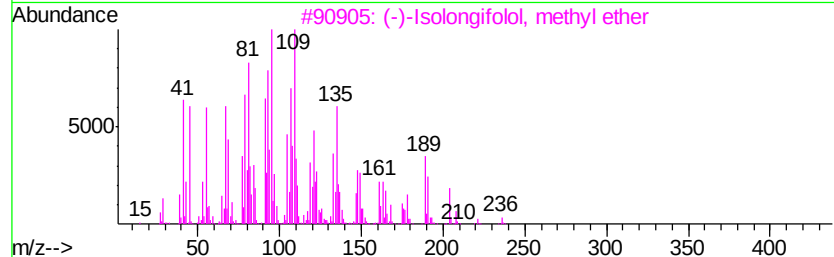
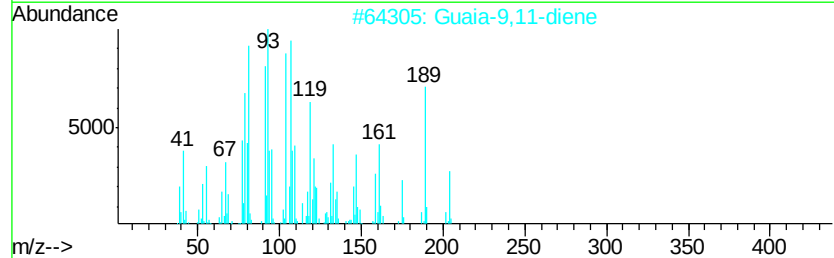
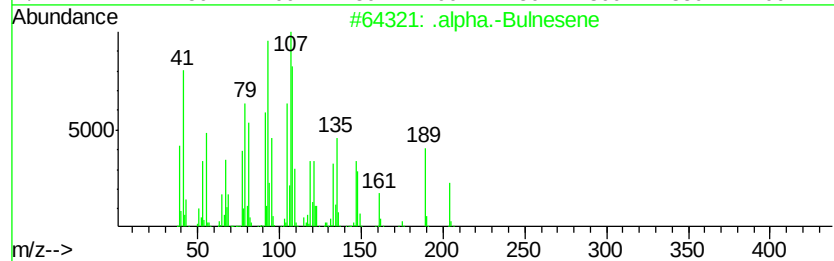
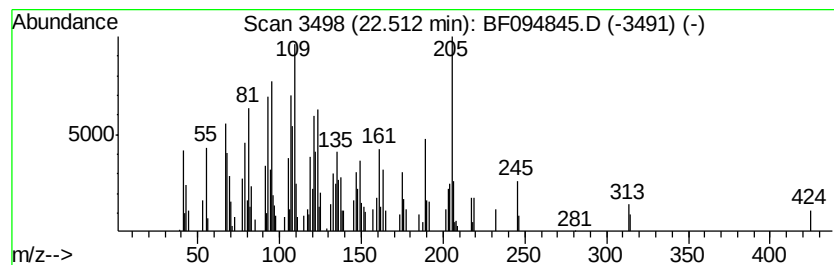
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .alpha.-Bulnesene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	7.97 ng	214847	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Bulnesene	204	C15H24	1000374-19-9	59
2		Guaia-9,11-diene	204	C15H24	1000374-19-8	55
3		(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	45
4		But-3-enal, 2-methyl-4-(2,6,6-tr...	206	C14H22O	104900-59-6	41
5		(1As-(1a.alpha.,4b.beta.,8as)-4a...	206	C14H22O	082262-79-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
 Data File : BF094845.D
 Acq On : 3 May 2017 21:06
 Operator : SJ/MA
 Sample : I2914-09
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-11-1.0-2.0

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	19.5	ng	542634	1	7.72	556121	20.0
unknown7.39	7.39	103.2	ng	2869260	1	7.72	556121	20.0
n-Hexadecanoic acid	15.94	5.0	ng	205462	4	14.97	830351	20.0
1-Heneicosanol	18.56	11.3	ng	384643	5	18.64	679984	20.0
Heneicosane	19.34	2.6	ng	87624	5	18.64	679984	20.0
unknown19.37	19.37	11.2	ng	380881	5	18.64	679984	20.0
Trifluoroacetic a...	20.11	5.3	ng	142663	6	20.30	538969	20.0
unknown20.42	20.42	2.3	ng	60582	6	20.30	538969	20.0
2-methyltetracosane	20.79	4.6	ng	125157	6	20.30	538969	20.0
2-Pentadecanone	20.88	4.0	ng	109106	6	20.30	538969	20.0
unknown21.82	21.82	3.9	ng	104706	6	20.30	538969	20.0
unknown22.11	22.11	4.2	ng	113391	6	20.30	538969	20.0
.alpha.-Bulnesene	22.51	8.0	ng	214847	6	20.30	538969	20.0