

Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
 Data File : BF104316.D
 Acq On : 6 Apr 2018 20:10
 Operator : JU/SJ
 Sample : J2214-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HH-STONE

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-BF040618.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	5.028	496	500	508	rVB	136716	190743	4.41%	0.546%
2	5.416	560	566	569	rBV	3330330	3760422	86.99%	10.758%
3	6.081	675	679	681	rBV	71209	57299	1.33%	0.164%
4	6.434	732	739	743	rBV	3306414	3923150	90.76%	11.224%
5	6.575	757	763	766	rBV	3571534	3832001	88.65%	10.963%
6	6.804	798	802	805	rBV	1011165	844508	19.54%	2.416%
7	6.963	824	829	832	rVB	3081149	3011580	69.67%	8.616%
8	7.369	892	898	901	rBV	2365379	2410149	55.76%	6.895%
9	8.086	1015	1020	1023	rBV	1307567	1149167	26.58%	3.288%
10	9.163	1198	1203	1206	rBV	4166950	4322646	100.00%	12.367%
11	9.557	1266	1270	1273	rBV	319462	284069	6.57%	0.813%
12	9.769	1303	1306	1310	rVB	79069	65178	1.51%	0.186%
13	9.839	1314	1318	1322	rVB2	1408042	1216447	28.14%	3.480%
14	10.269	1389	1391	1395	rVB	109243	91294	2.11%	0.261%
15	10.492	1423	1429	1431	rBV	38471	47015	1.09%	0.135%
16	10.627	1447	1452	1456	rBV	2249124	2386122	55.20%	6.827%
17	10.745	1469	1472	1481	rVB	120694	124515	2.88%	0.356%
18	11.192	1545	1548	1551	rBV2	50001	46785	1.08%	0.134%
19	11.327	1567	1571	1573	rBV	1256775	1049387	24.28%	3.002%
20	11.351	1573	1575	1577	rVB	74168	57035	1.32%	0.163%
21	11.857	1657	1661	1665	rBV	133315	136034	3.15%	0.389%
22	12.539	1773	1777	1780	rBV	118984	108539	2.51%	0.311%
23	12.763	1808	1815	1819	rBV	97902	112131	2.59%	0.321%
24	12.921	1837	1842	1845	rBV	3209168	3143459	72.72%	8.993%
25	13.810	1990	1993	1997	rBV	154779	148116	3.43%	0.424%
26	13.968	2015	2020	2023	rBV	966789	958572	22.18%	2.742%
27	13.992	2023	2024	2031	rVB	64497	48219	1.12%	0.138%
28	14.451	2099	2102	2105	rBV	72845	79879	1.85%	0.229%
29	15.004	2193	2196	2199	rBV2	39189	51609	1.19%	0.148%
30	15.092	2207	2211	2218	rBV	159504	201134	4.65%	0.575%
31	15.298	2243	2246	2252	rVB2	35399	49213	1.14%	0.141%
32	15.357	2253	2256	2261	rBV	42200	55938	1.29%	0.160%
33	15.427	2263	2268	2272	rBV	681304	808742	18.71%	2.314%
34	15.898	2344	2348	2353	rBV	68985	98752	2.28%	0.283%

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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	17.445	2607	2611	2617	rVB9	43736	83302	1.93%	0.238%
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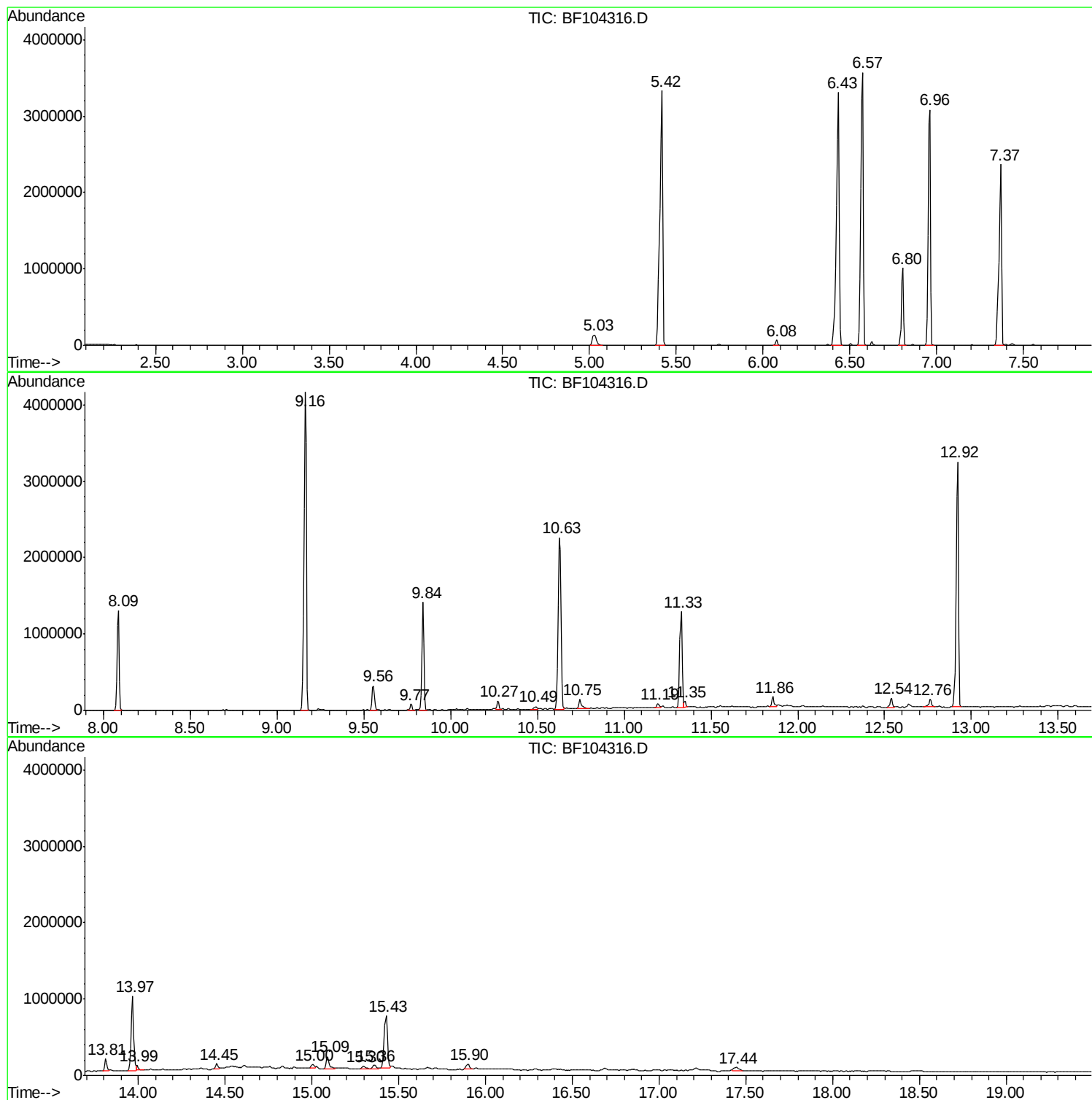
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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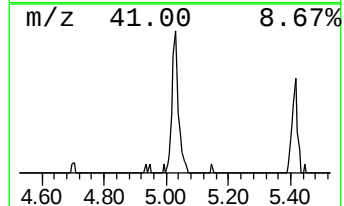
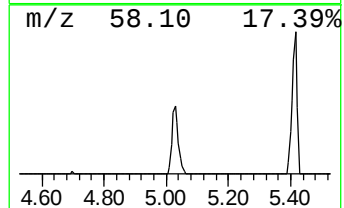
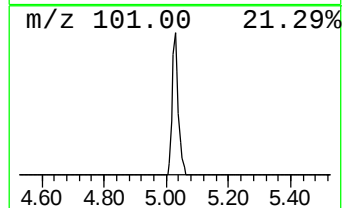
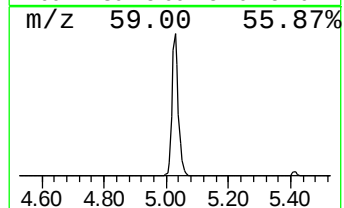
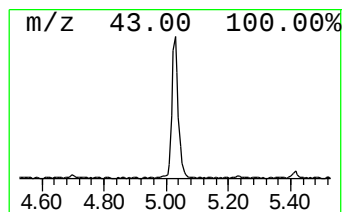
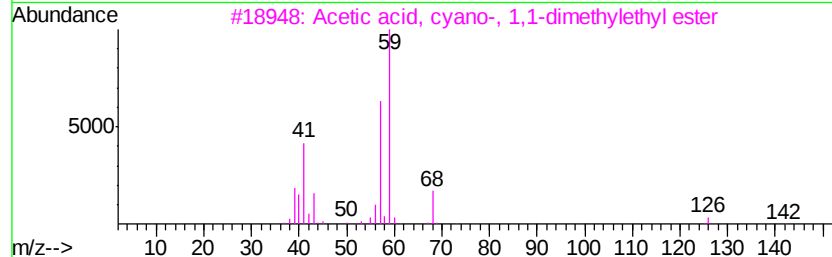
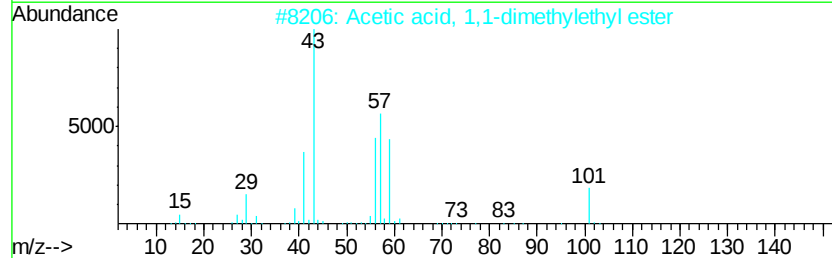
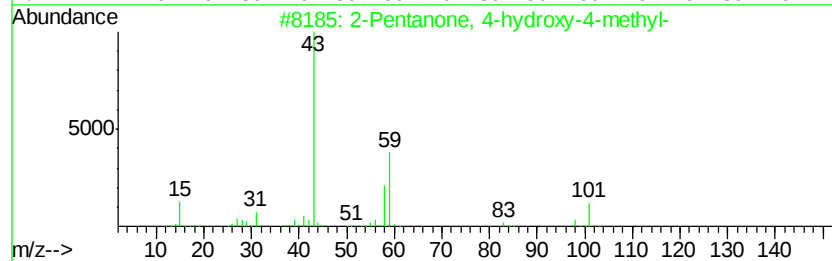
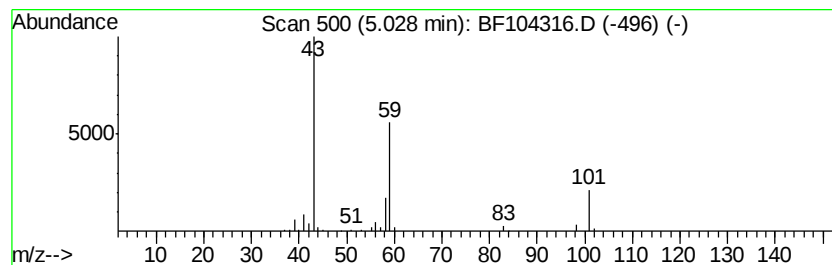
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.03	4.52 ng	190743	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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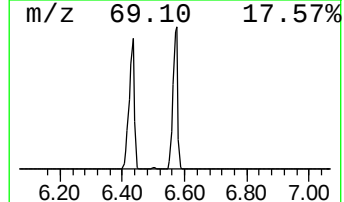
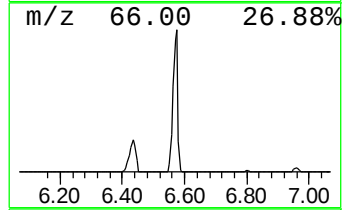
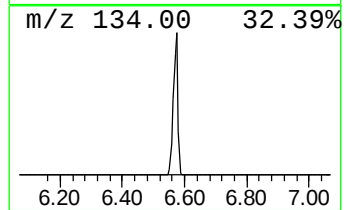
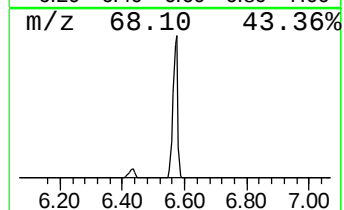
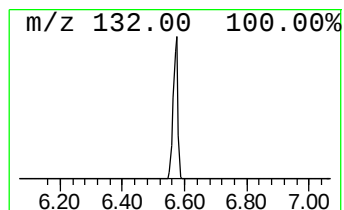
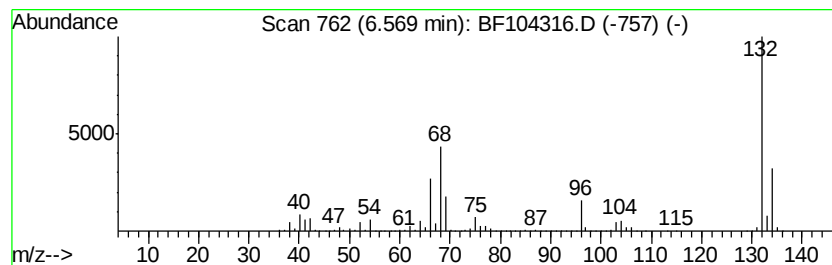
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	90.75 ng	3832000	1,4-Dichlorobenzene-d4	6.80

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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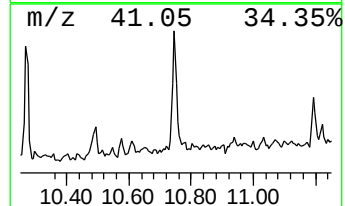
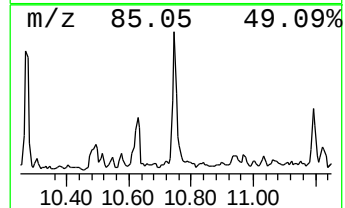
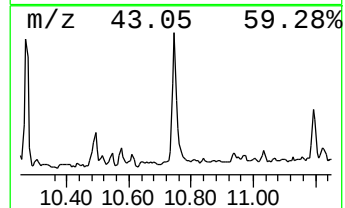
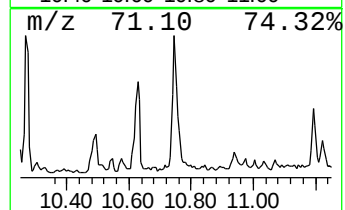
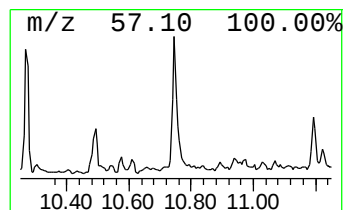
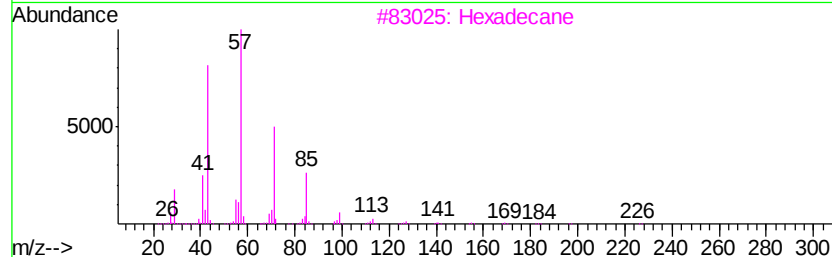
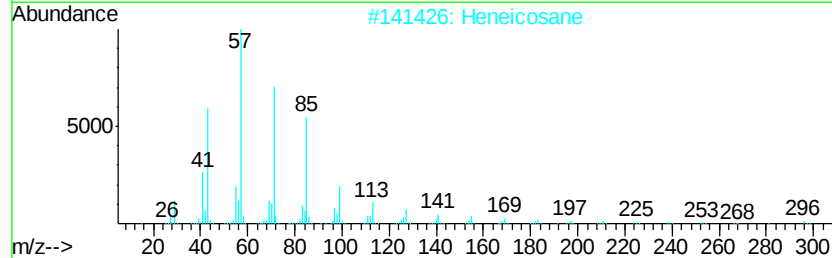
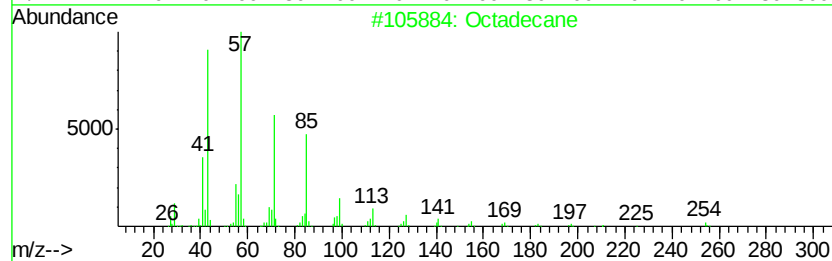
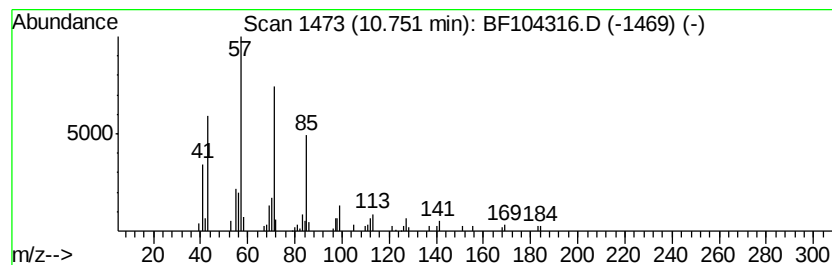
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.37 ng	124515	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Octacosane		394	C28H58	000630-02-4	87
5	Heptadecane		240	C17H36	000629-78-7	87



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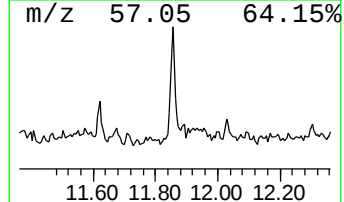
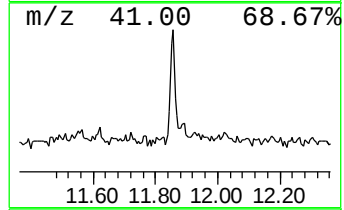
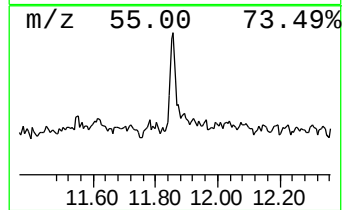
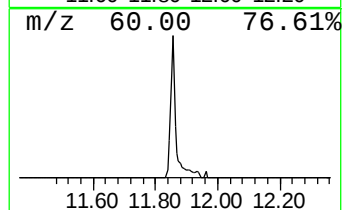
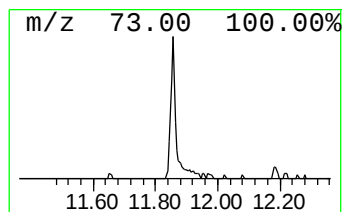
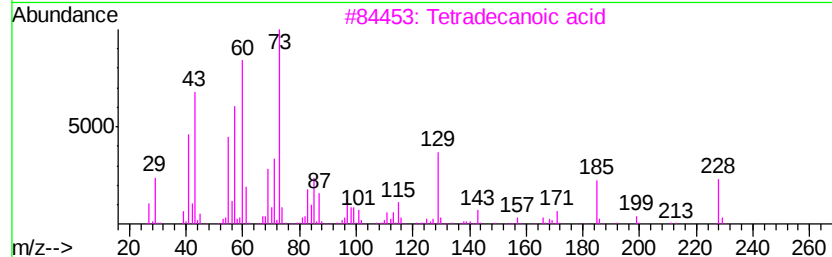
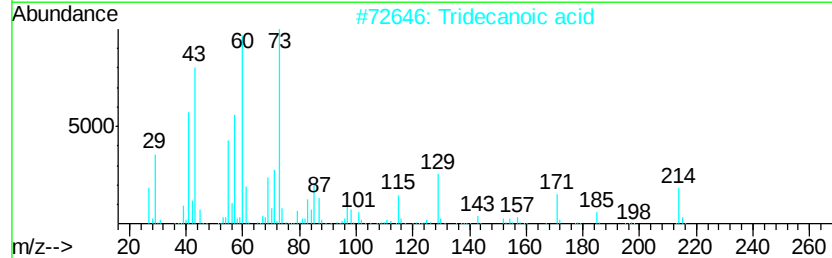
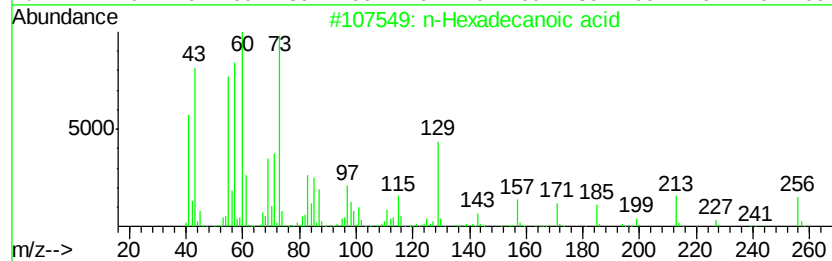
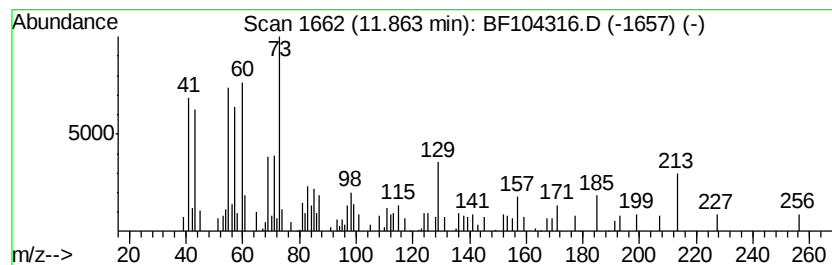
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.59 ng	136034	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	43



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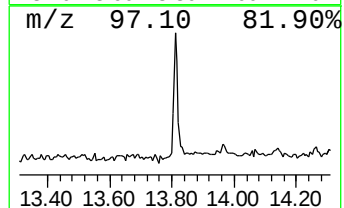
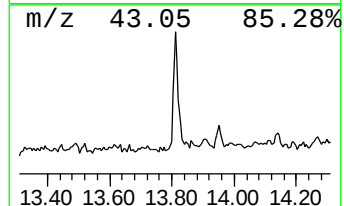
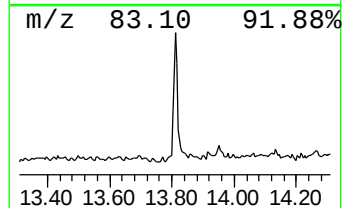
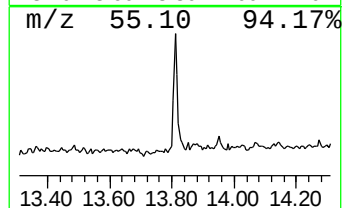
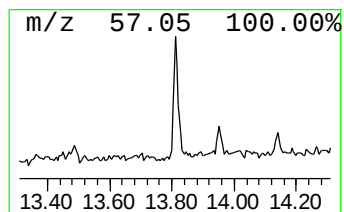
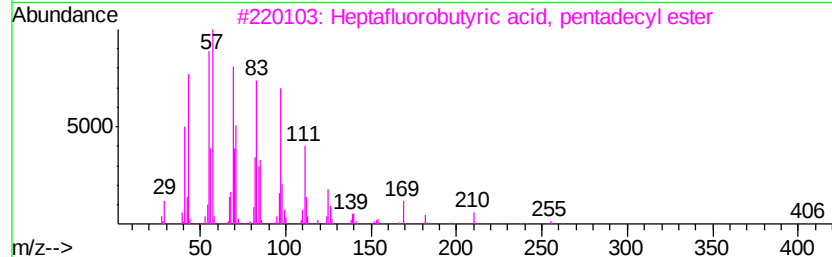
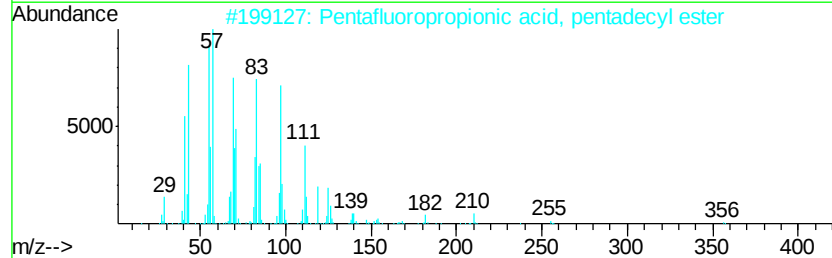
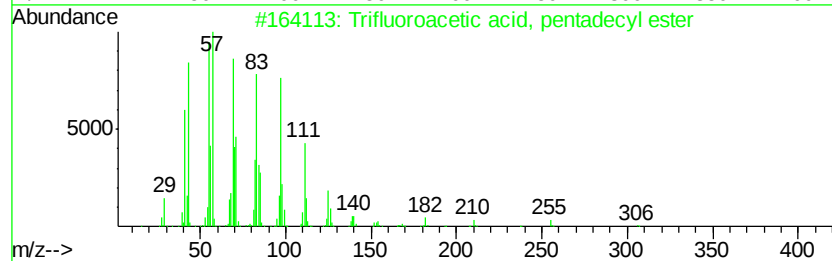
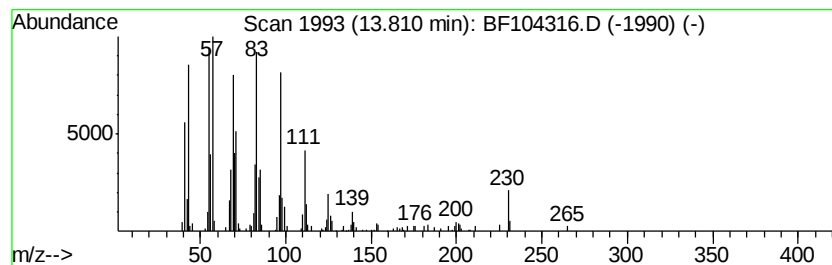
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.09 ng	148116	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



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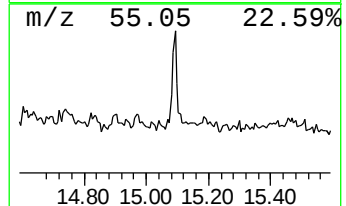
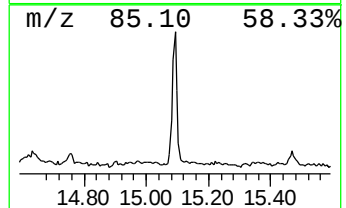
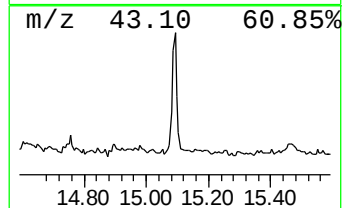
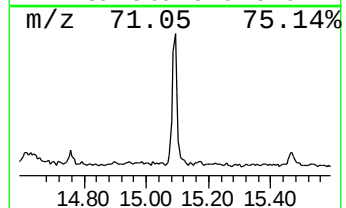
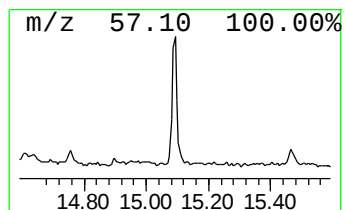
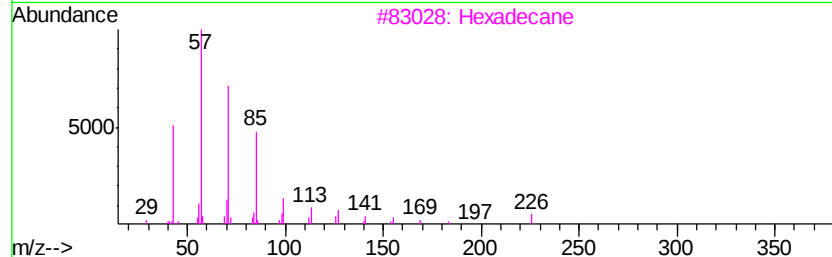
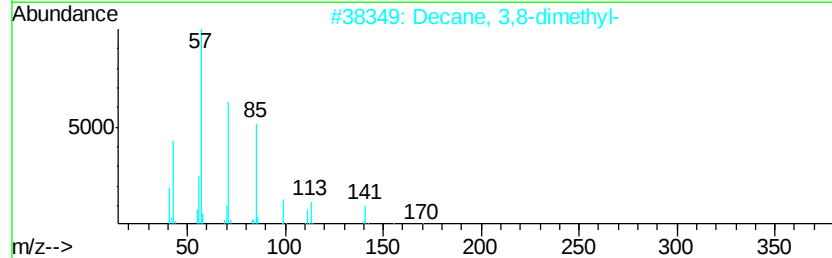
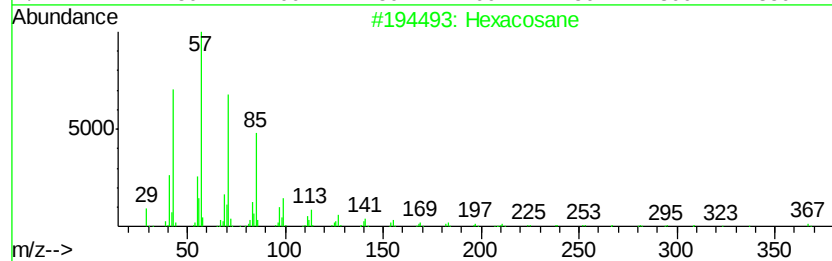
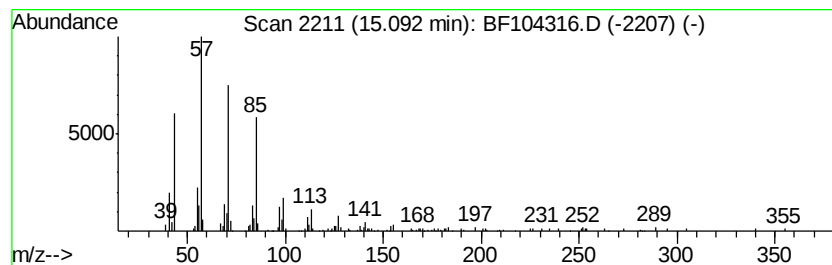
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	4.97 ng	201134	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	91
3	Hexadecane		226	C16H34	000544-76-3	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104316.D
Acq On : 6 Apr 2018 20:10
Operator : JU/SJ
Sample : J2214-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HH-STONE

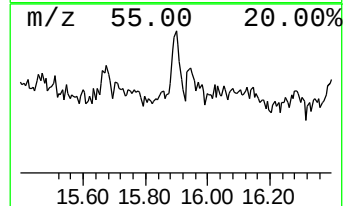
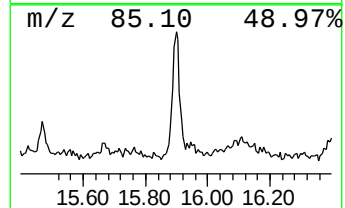
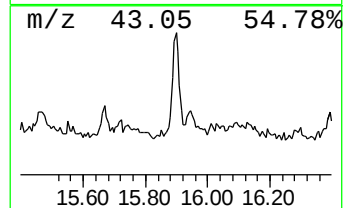
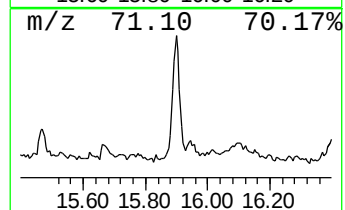
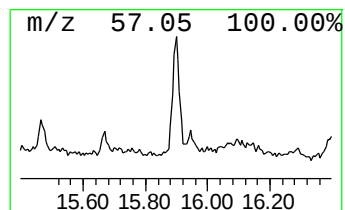
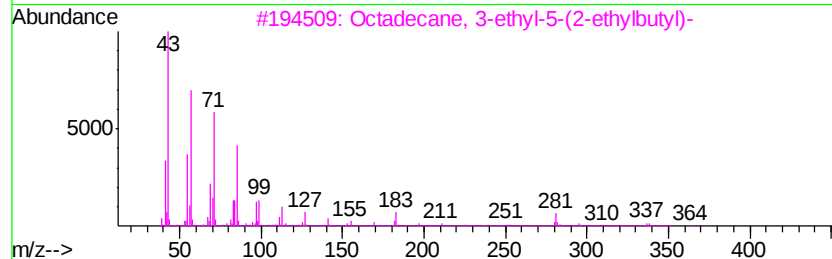
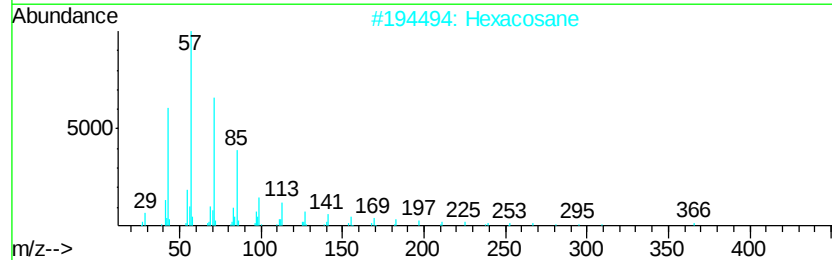
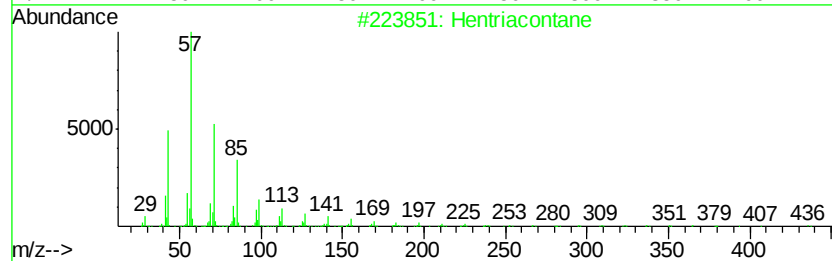
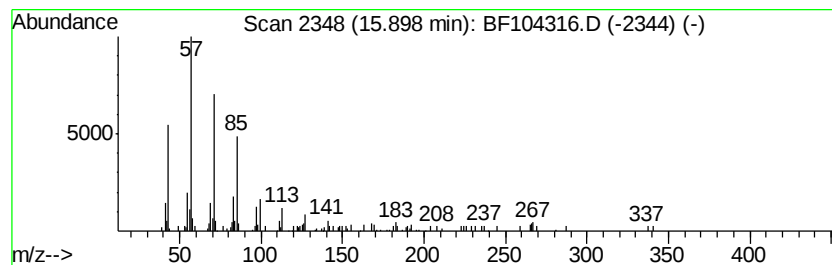
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	2.44 ng	98752	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	87
2	Hexacosane		366	C26H54	000630-01-3	86
3	Octadecane, 3-ethyl-5-(2-ethylbu...		366	C26H54	055282-12-7	86
4	Triacontane		422	C30H62	000638-68-6	86
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	86



Data Path : Z:\HPCHEM1\BNA_F\Data\BF040618\
Data File : BF104316.D
Acq On : 6 Apr 2018 20:10
Operator : JU/SJ
Sample : J2214-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HH-STONE

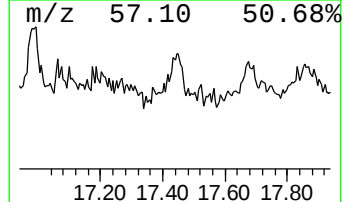
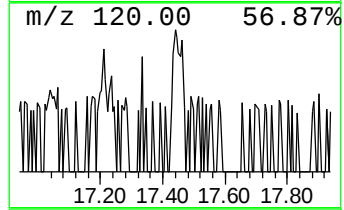
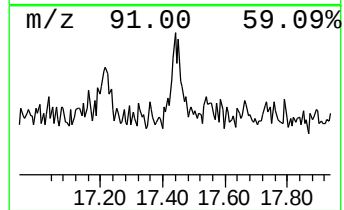
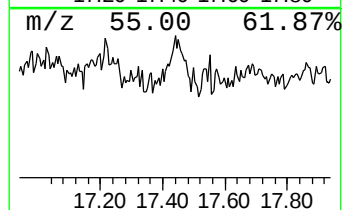
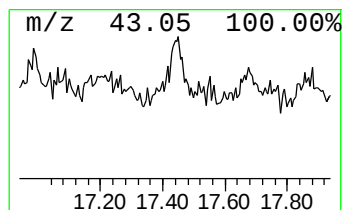
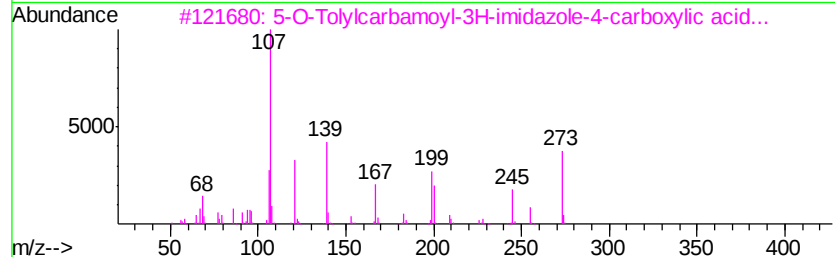
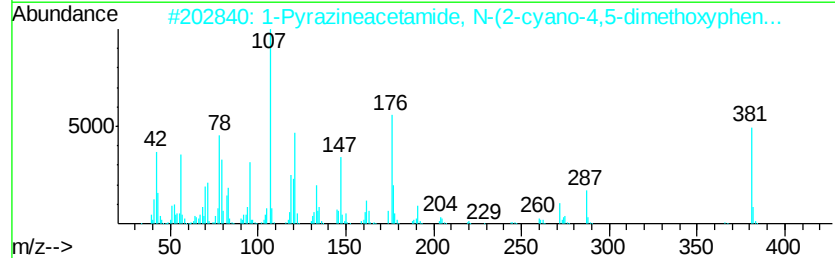
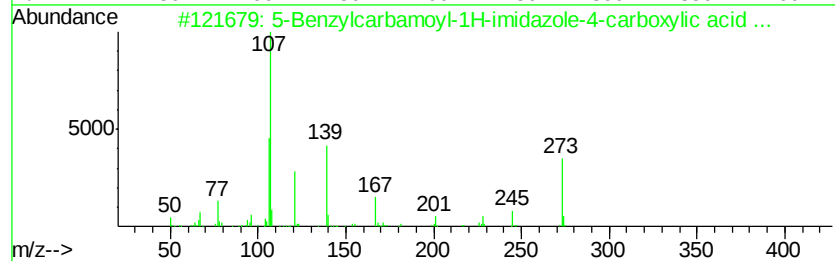
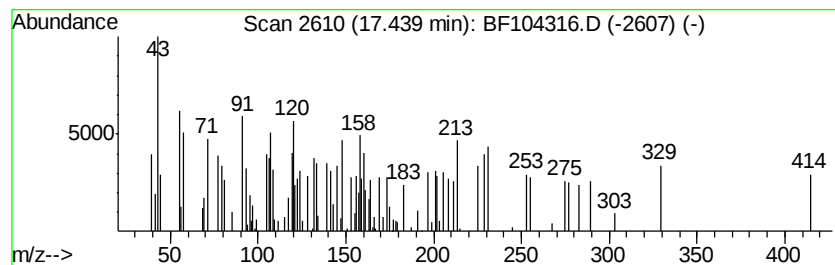
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.44 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	2.06 ng	83302	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Benzylcarbamoyl-1H-imidazole-4...	273	C14H15N3O3	312758-83-1	14
2		1-Pyrazineacetamide, N-(2-cyano-...	381	C20H23N5O3	1000319-00-2	12
3		5-O-Tolylcarbamoyl-3H-imidazole-...	273	C14H15N3O3	313251-31-9	12
4		5,16-Pregnenolone oxime	329	C21H31NO2	001045-71-2	11
5		Ethanone, 1-(2-furyl)-, 4-(3-met...	273	C14H15N3OS	324055-34-7	10



Data Path : Z:\HPCHEM1\BNA_F\Data\BF040618\
Data File : BF104316.D
Acq On : 6 Apr 2018 20:10
Operator : JU/SJ
Sample : J2214-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HH-STONE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	4.5	ng	190743	1	6.80	844508	20.0
unknown6.57	6.57	90.8	ng	3832000	1	6.80	844508	20.0
Octadecane	10.75	2.4	ng	124515	4	11.33	1049390	20.0
n-Hexadecanoic acid	11.86	2.6	ng	136034	4	11.33	1049390	20.0
Trifluoroacetic a...	13.81	3.1	ng	148116	5	13.97	958572	20.0
Hexacosane	15.09	5.0	ng	201134	6	15.43	808742	20.0
Hentriacontane	15.90	2.4	ng	98752	6	15.43	808742	20.0
unknown17.44	17.44	2.1	ng	83302	6	15.43	808742	20.0