

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043018\
 Data File : BF104937.D
 Acq On : 30 Apr 2018 17:14
 Operator : JU/SJ
 Sample : J2609-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01B

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	4.998	490	495	505	rBV	99887	136384	5.27%	0.588%
2	5.410	561	565	583	rBV	2222104	2212874	85.57%	9.534%
3	6.434	734	739	753	rBV	1949077	2257395	87.29%	9.726%
4	6.563	757	761	764	rBV	2576832	2285285	88.37%	9.846%
5	6.787	796	799	803	rBV	854499	707703	27.37%	3.049%
6	6.945	822	826	829	rBV	2114800	1843025	71.27%	7.941%
7	7.357	891	896	899	rBV	1465700	1390121	53.75%	5.989%
8	8.075	1014	1018	1026	rBV	1050694	919396	35.55%	3.961%
9	9.151	1196	1201	1204	rBV	2980686	2586082	100.00%	11.142%
10	9.545	1264	1268	1274	rVB	232750	225006	8.70%	0.969%
11	9.751	1300	1303	1307	rVB	88352	64093	2.48%	0.276%
12	9.828	1312	1316	1325	rVB2	1122084	1038613	40.16%	4.475%
13	10.251	1385	1388	1391	rVB2	112800	87884	3.40%	0.379%
14	10.469	1419	1425	1428	rBV	31152	40078	1.55%	0.173%
15	10.622	1447	1451	1461	rBV	1595426	1507063	58.28%	6.493%
16	10.722	1466	1468	1476	rVB	87402	115890	4.48%	0.499%
17	11.175	1541	1545	1547	rBV2	54860	51002	1.97%	0.220%
18	11.198	1547	1549	1557	rVB4	22127	32147	1.24%	0.139%
19	11.322	1566	1570	1572	rBV	1095076	946744	36.61%	4.079%
20	11.339	1572	1573	1580	rVB	99555	89098	3.45%	0.384%
21	11.839	1649	1658	1666	rBV3	119772	201790	7.80%	0.869%
22	11.933	1671	1674	1676	rBV	40102	34417	1.33%	0.148%
23	12.533	1773	1776	1781	rVB	135552	123285	4.77%	0.531%
24	12.763	1810	1815	1818	rBV2	92671	111875	4.33%	0.482%
25	12.910	1835	1840	1843	rBV	2197937	2069960	80.04%	8.918%
26	13.086	1865	1870	1873	rBV4	24074	41909	1.62%	0.181%
27	13.792	1987	1990	1998	rVB2	236712	245928	9.51%	1.060%
28	13.933	2011	2014	2016	rBV	215824	182986	7.08%	0.788%
29	13.969	2016	2020	2023	rVV	715675	691255	26.73%	2.978%
30	14.427	2095	2098	2103	rVB5	18275	31160	1.20%	0.134%
31	15.010	2194	2197	2201	rBV2	34182	43841	1.70%	0.189%
32	15.310	2245	2248	2254	rVB	25880	33626	1.30%	0.145%
33	15.433	2264	2269	2285	rVB	514150	709623	27.44%	3.057%
34	15.915	2347	2351	2355	rBV7	23208	37682	1.46%	0.162%

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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	17.815	2667	2674	2682	rVB2	47588	114957	4.45%	0.495%
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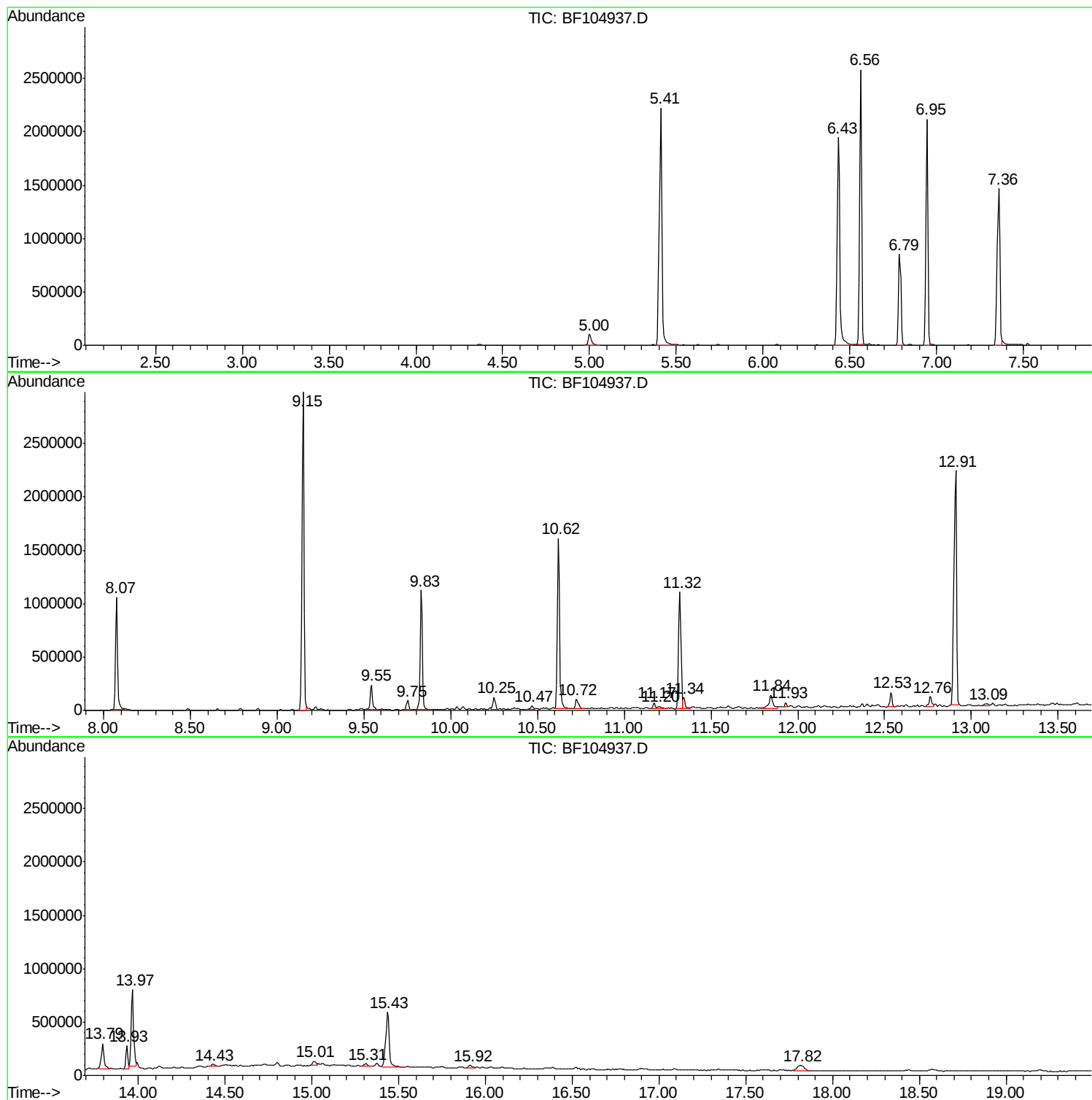
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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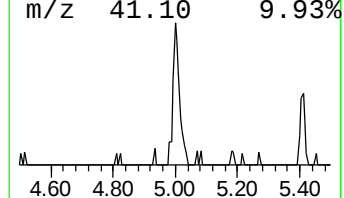
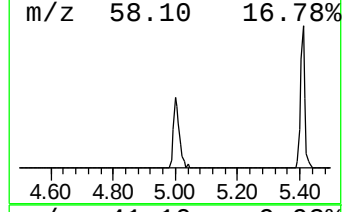
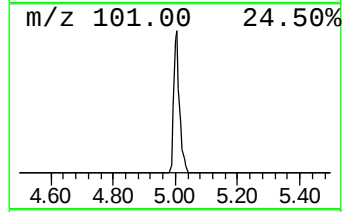
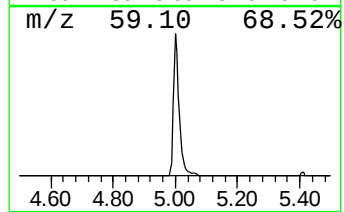
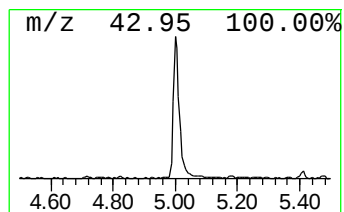
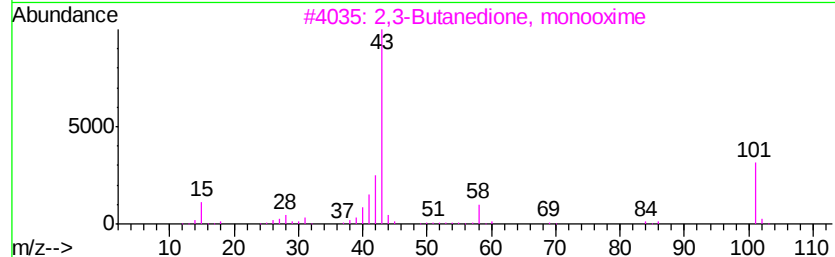
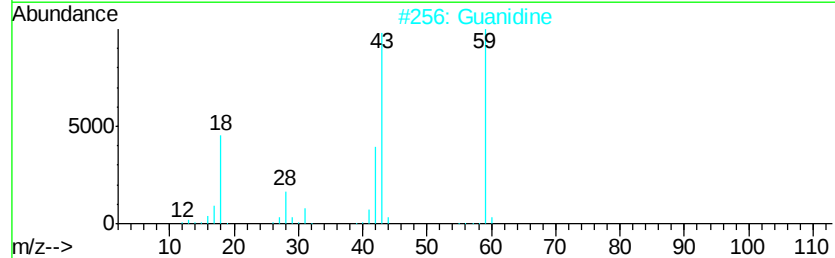
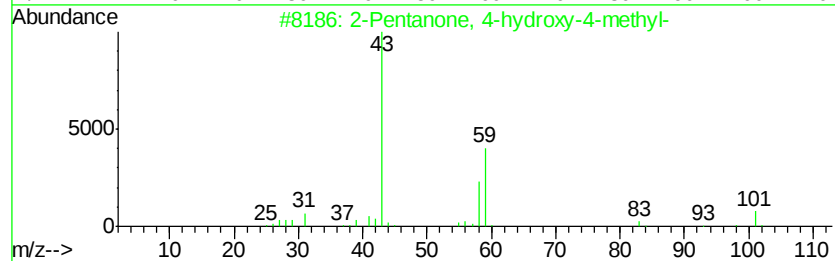
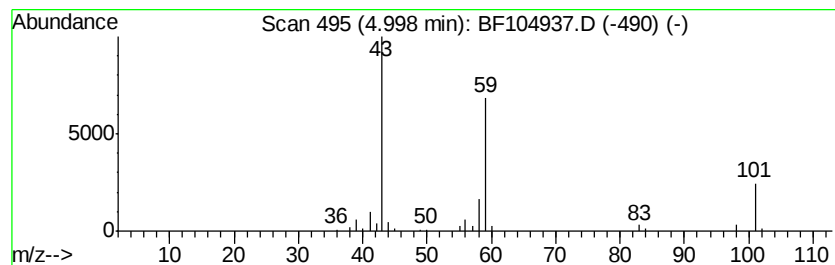
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.85 ng	136384	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	43
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4		3-Hexanol	102	C6H14O	000623-37-0	25
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25



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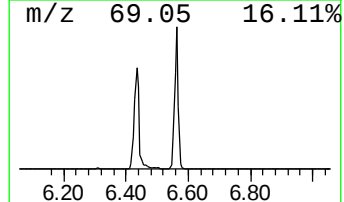
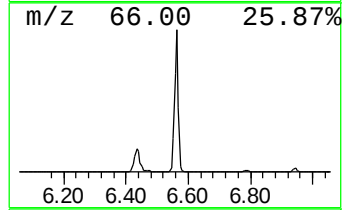
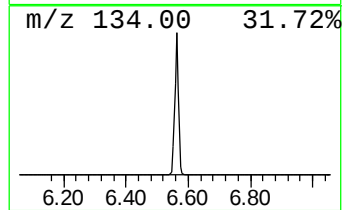
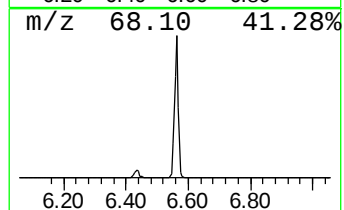
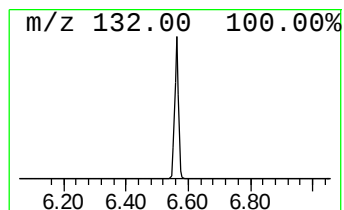
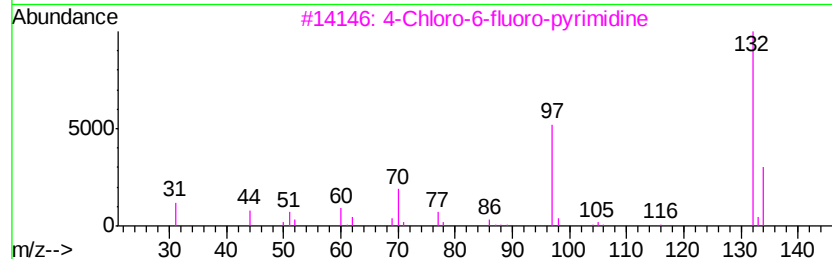
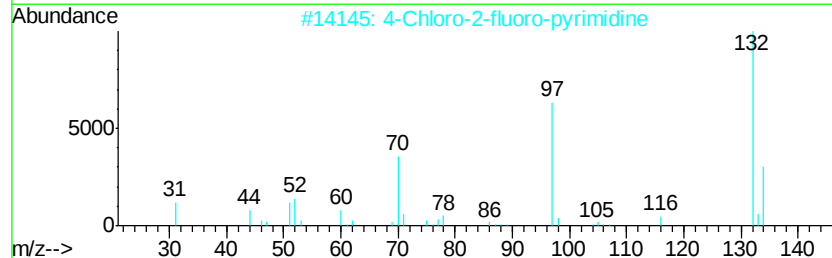
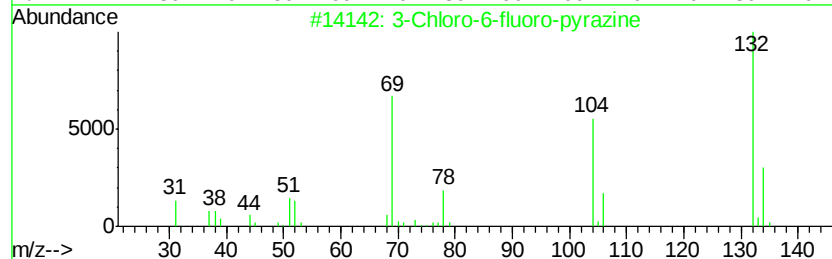
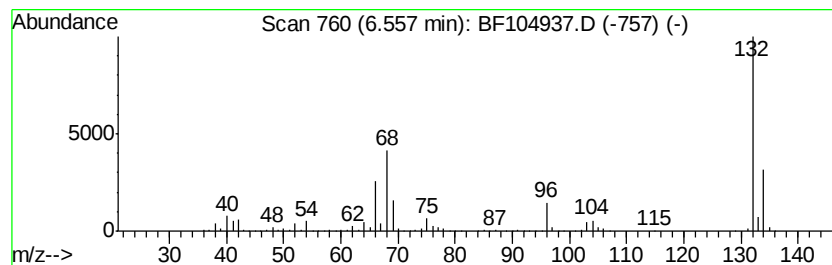
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	64.58 ng	2285290	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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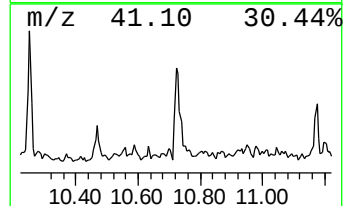
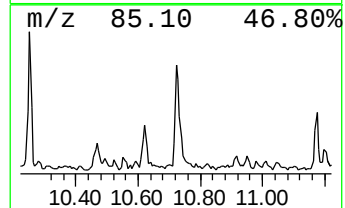
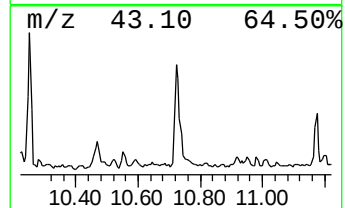
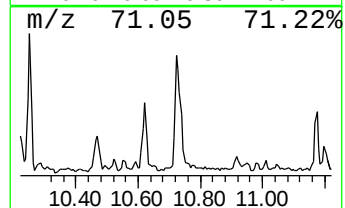
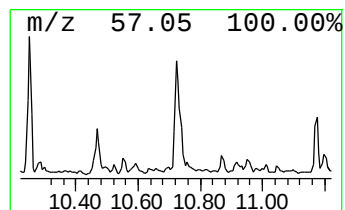
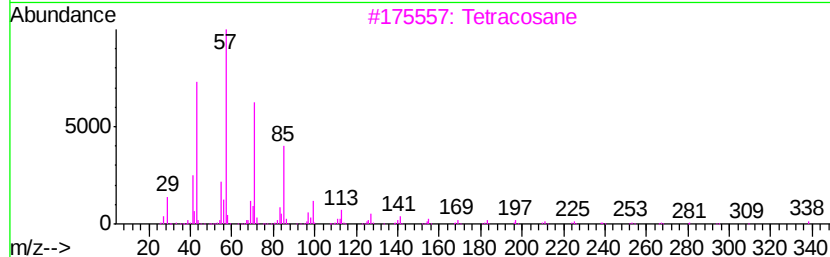
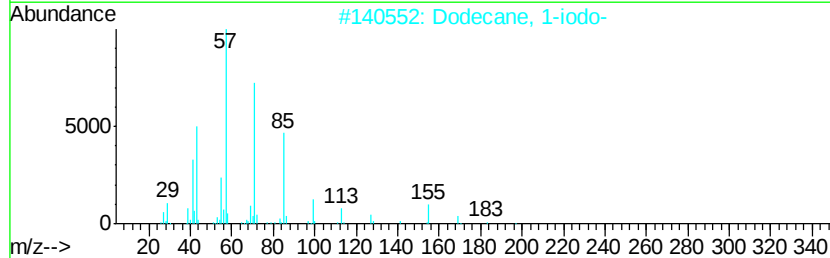
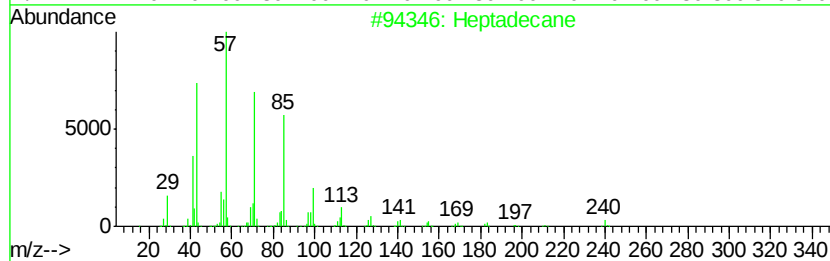
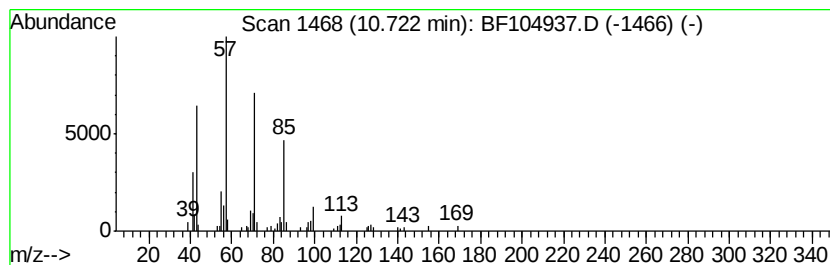
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.45 ng	115890	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
3	Tetracosane		338	C24H50	000646-31-1	86
4	Octadecane		254	C18H38	000593-45-3	86
5	9-methylheptadecane		254	C18H38	026741-18-4	80



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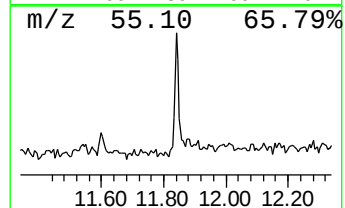
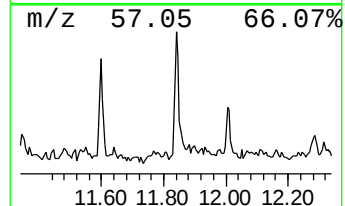
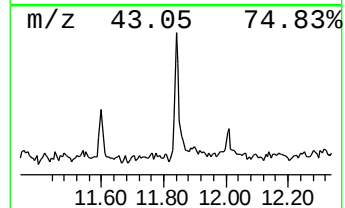
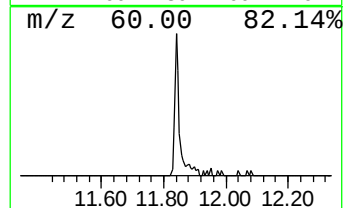
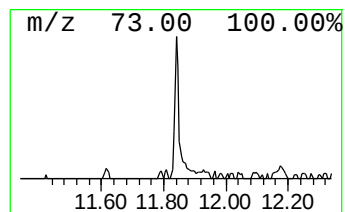
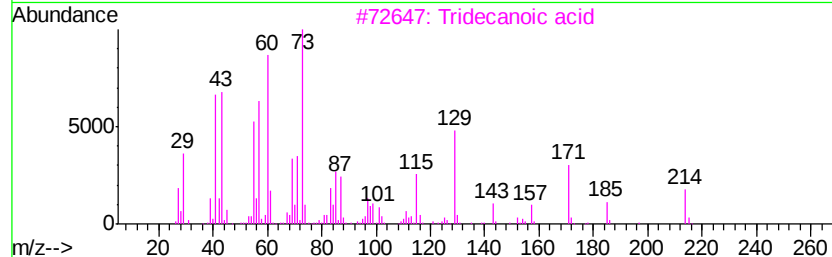
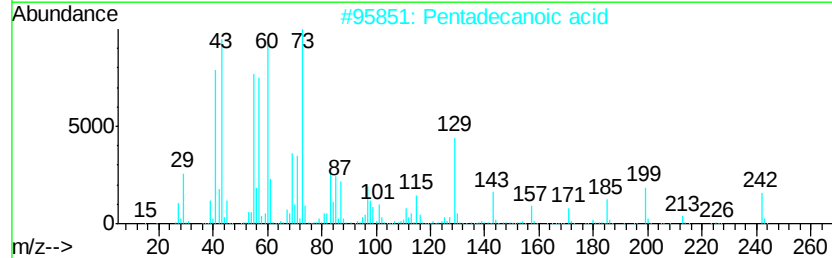
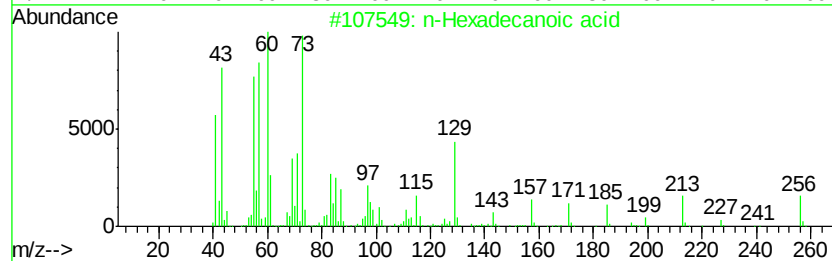
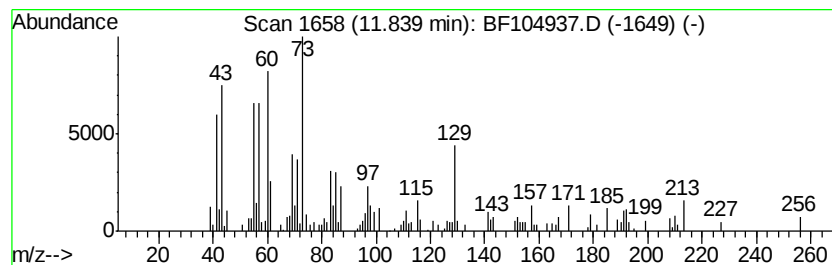
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.84	4.26 ng	201790	Phenanthrene-d10		11.32
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	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



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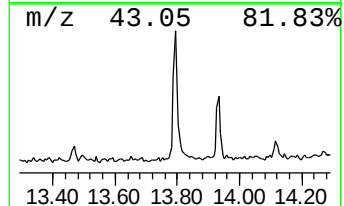
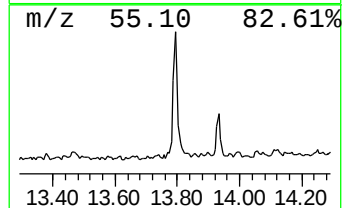
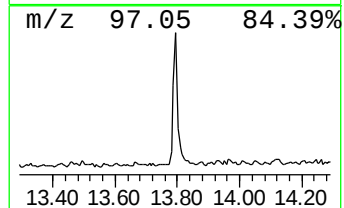
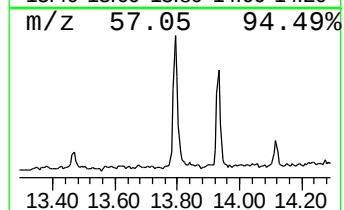
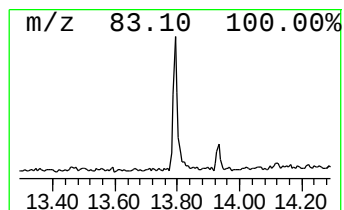
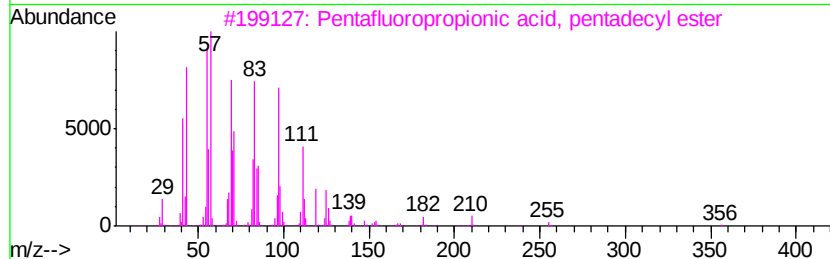
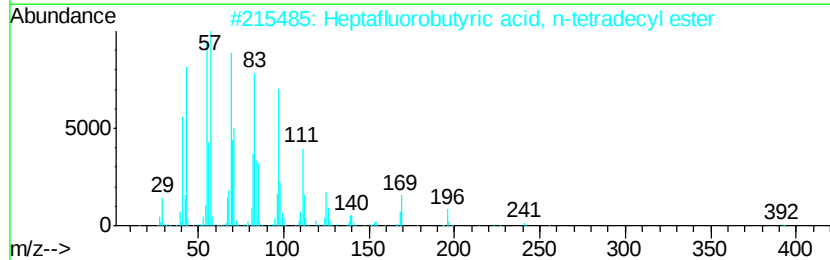
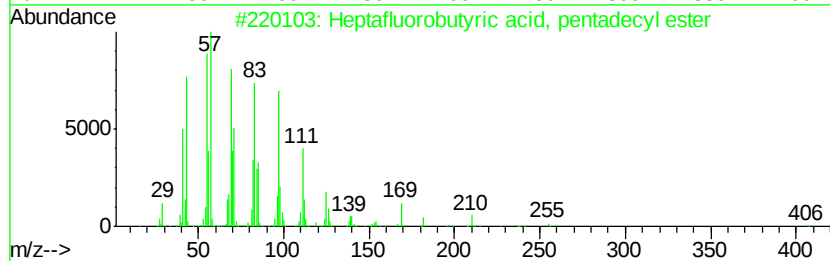
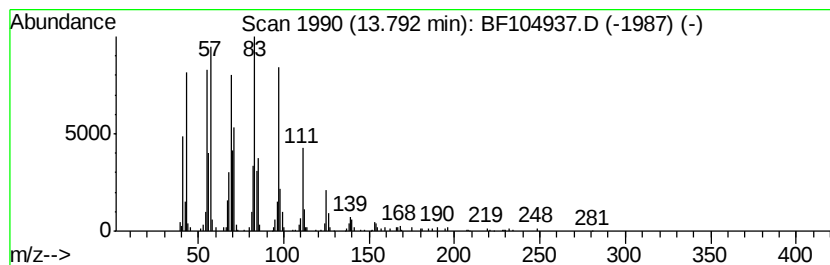
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.12 ng	245928	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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Sample : J2609-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01B

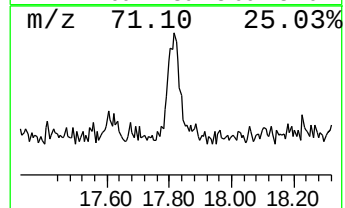
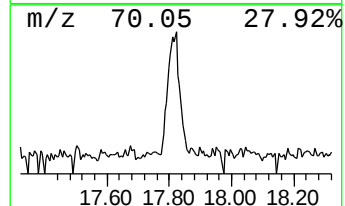
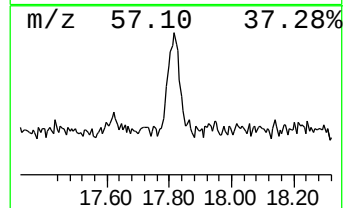
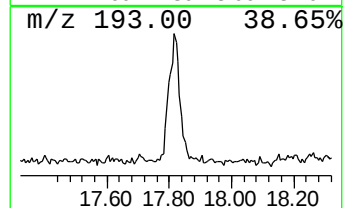
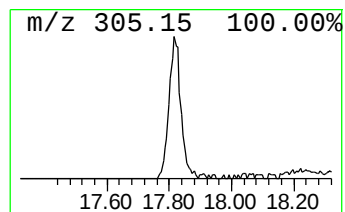
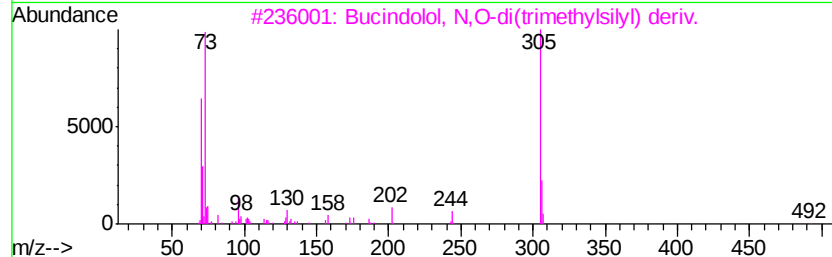
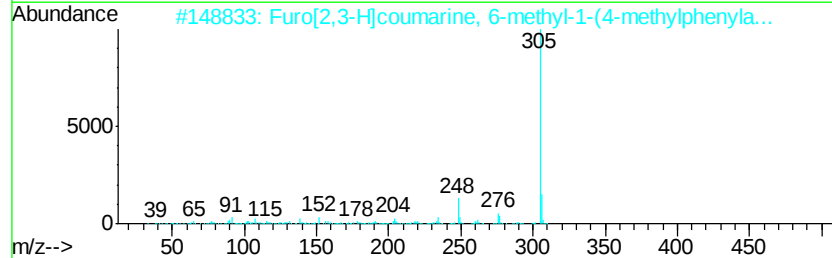
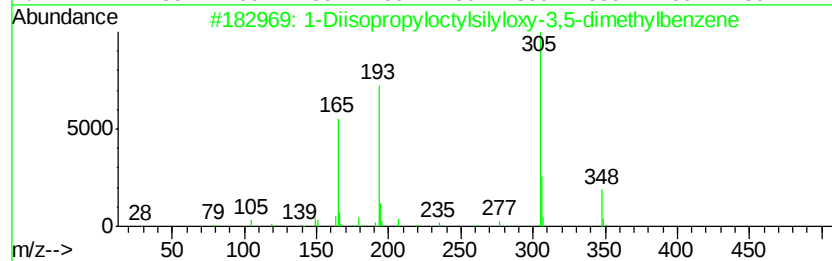
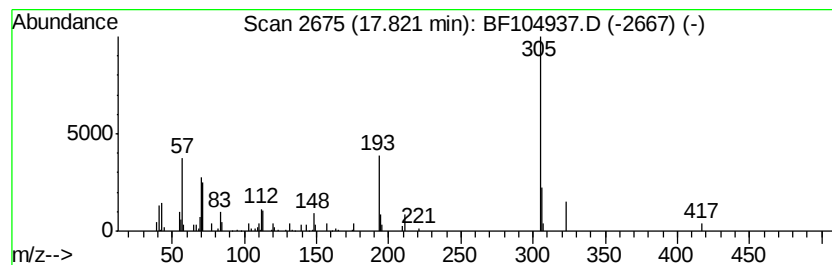
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Diisopropyloctylsilyloxy-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	3.24 ng	114957	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Diisopropylsilyloxy-3,5-d...	348	C22H40OSi	1000307-85-1	59
2		Furo[2,3-H]coumarine, 6-methyl-1...	305	C19H15N03	298684-60-3	32
3		Bucindolol, N,O-di(trimethylsilyl)...	507	C28H41N3O2Si2	1000292-78-4	32
4		N-[4,6-Dimethoxynaphthylmethyl]en...	305	C20H19N02	1000257-03-0	23
5		4-(2,4-Diphenyl-2H-pyrazol-3-yl)...	305	C19H19N3O	088743-50-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043018\
Data File : BF104937.D
Acq On : 30 Apr 2018 17:14
Operator : JU/SJ
Sample : J2609-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01B

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...	5.00	3.9	ng	136384	1	6.79	707703	20.0
unknown6.56	6.56	64.6	ng	2285290	1	6.79	707703	20.0
Heptadecane	10.72	2.5	ng	115890	4	11.32	946744	20.0
n-Hexadecanoic acid	11.84	4.3	ng	201790	4	11.32	946744	20.0
Heptafluorobutyri...	13.79	7.1	ng	245928	5	13.97	691255	20.0
1-Diisopropylocty...	17.82	3.2	ng	114957	6	15.43	709623	20.0