

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041017\
 Data File : BF094326.D
 Acq On : 10 Apr 2017 22:06
 Operator : SJ/MA
 Sample : I2595-04
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-4

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-BF032217.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	2.652	125	130	140	rVB	732771	868271	17.43%	1.749%
2	3.981	351	356	367	rBV	699980	1000204	20.08%	2.015%
3	4.334	412	416	423	rBV	50885	60042	1.21%	0.121%
4	4.404	423	428	435	rBV	4029294	4367712	87.68%	8.798%
5	4.593	457	460	468	rVB	53558	55601	1.12%	0.112%
6	4.757	485	488	496	rBV	67386	71340	1.43%	0.144%
7	5.481	605	611	621	rVB2	3406061	4934108	99.05%	9.939%
8	5.598	626	631	634	rBV	4141915	4615989	92.67%	9.299%
9	5.840	667	672	675	rBV	1018369	942075	18.91%	1.898%
10	6.022	695	703	706	rBV	3221660	3656615	73.41%	7.366%
11	6.169	719	728	733	rBV3	33785	59079	1.19%	0.119%
12	6.298	745	750	753	rBV4	41837	51051	1.02%	0.103%
13	6.493	776	783	786	rBV	2562334	3011791	60.46%	6.067%
14	7.075	878	882	883	rBV2	50691	64408	1.29%	0.130%
15	7.087	883	884	889	rVB	58520	51080	1.03%	0.103%
16	7.340	922	927	934	rVB	1358115	1271808	25.53%	2.562%
17	7.828	1006	1010	1015	rVB3	71600	88515	1.78%	0.178%
18	8.275	1082	1086	1092	rBV	51667	65903	1.32%	0.133%
19	8.669	1144	1153	1156	rBV	4359758	4981224	100.00%	10.034%
20	9.163	1231	1237	1240	rBV	925044	886736	17.80%	1.786%
21	9.481	1284	1291	1295	rVB2	1235077	1338264	26.87%	2.696%
22	10.069	1387	1391	1395	rBV	59469	60839	1.22%	0.123%
23	10.457	1451	1457	1461	rBV	2182483	2668132	53.56%	5.375%
24	10.651	1487	1490	1493	rBV	75923	96795	1.94%	0.195%
25	11.210	1581	1585	1588	rBV	83527	80071	1.61%	0.161%
26	11.304	1596	1601	1604	rBV	1149261	1171263	23.51%	2.359%
27	11.739	1672	1675	1680	rVB	79901	75841	1.52%	0.153%
28	11.927	1703	1707	1710	rBV4	30342	51092	1.03%	0.103%
29	12.033	1721	1725	1732	rBV2	341400	416372	8.36%	0.839%
30	12.239	1758	1760	1764	rVB	53576	54006	1.08%	0.109%
31	12.722	1839	1842	1847	rVB3	52365	61576	1.24%	0.124%
32	12.792	1850	1854	1859	rVB	81406	100718	2.02%	0.203%
33	13.063	1897	1900	1904	rBV2	62837	66507	1.34%	0.134%
34	13.286	1932	1938	1941	rBV	3072277	3657332	73.42%	7.367%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.898	2036	2042	2046	rBV	3469412	4202652	84.37%	8.466%
36	14.051	2065	2068	2071	rVB2	84840	76248	1.53%	0.154%
37	14.457	2134	2137	2143	rVB2	141054	184622	3.71%	0.372%
38	14.551	2149	2153	2157	rBV	775822	877265	17.61%	1.767%
39	14.604	2160	2162	2165	rVB	105724	91486	1.84%	0.184%
40	14.727	2179	2183	2186	rVB	510193	531590	10.67%	1.071%
41	15.086	2241	2244	2249	rVB	348715	399628	8.02%	0.805%
42	15.210	2261	2265	2273	rVB3	550661	837868	16.82%	1.688%
43	15.333	2282	2286	2288	rBV3	334363	451638	9.07%	0.910%
44	15.592	2328	2330	2335	rBV3	127595	201040	4.04%	0.405%
45	16.180	2427	2430	2437	rVB	617299	785629	15.77%	1.583%

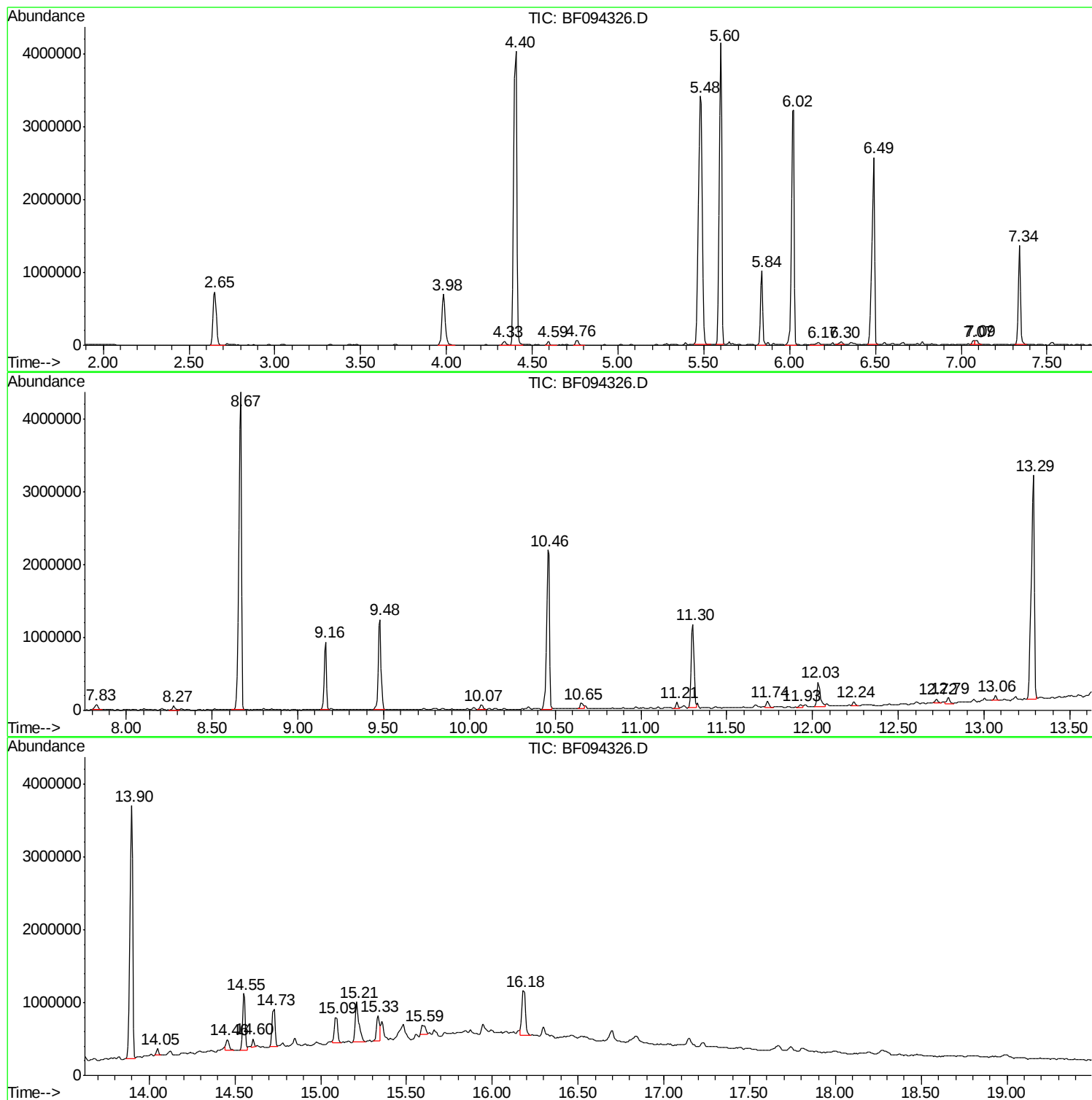
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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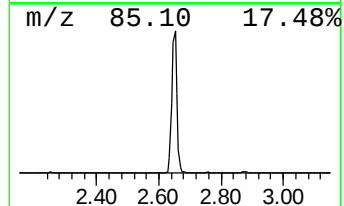
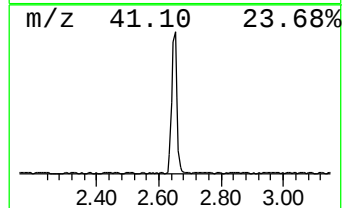
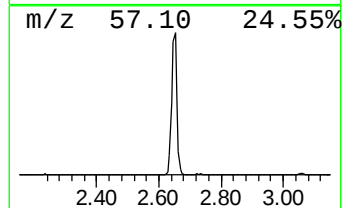
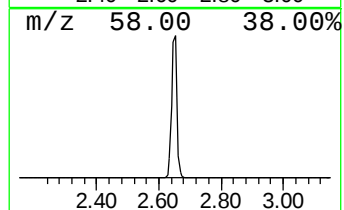
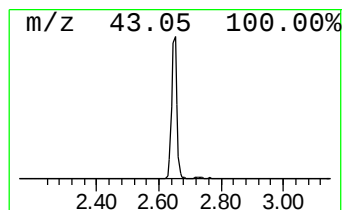
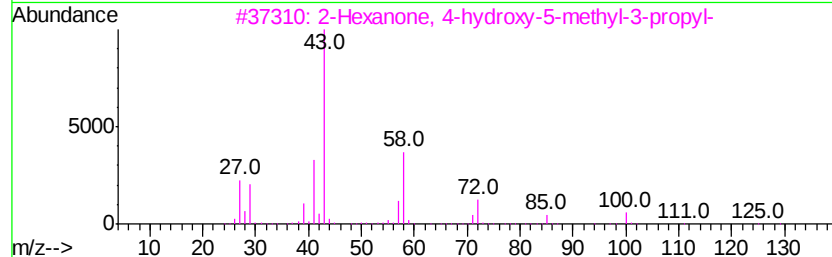
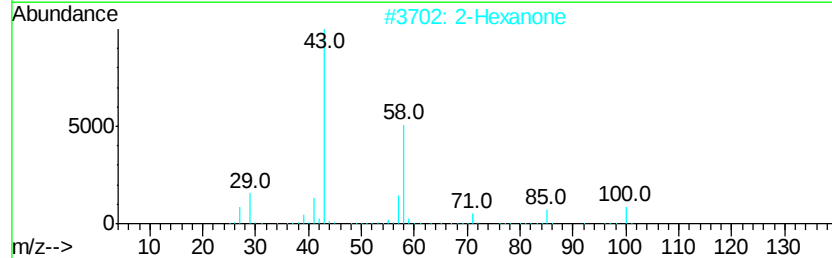
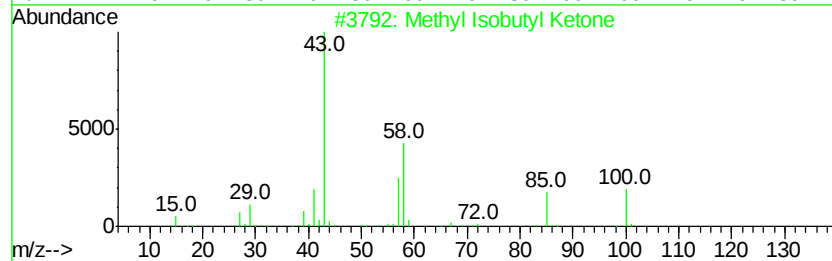
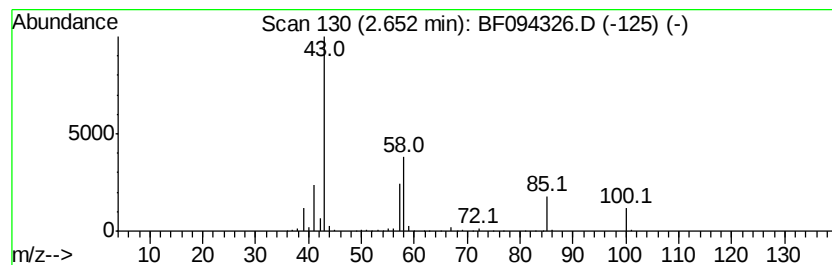
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.65	18.43 ng	868271	1,4-Dichlorobenzene-d4	5.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	86
2		2-Hexanone	100	C6H12O	000591-78-6	78
3		2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	45
4		Pentanal, 2,2-dimethyl-	114	C7H14O	014250-88-5	38
5		3-Penten-2-one, 4-(acetyloxy)-, ...	142	C7H10O3	038365-58-1	38



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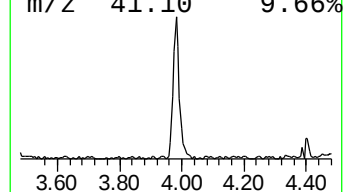
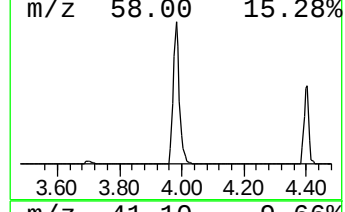
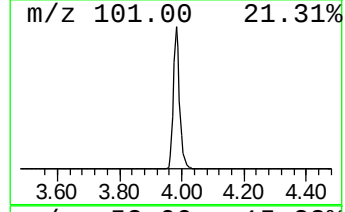
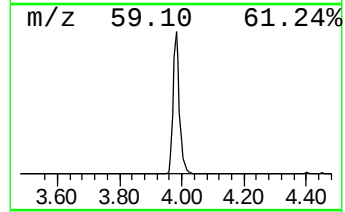
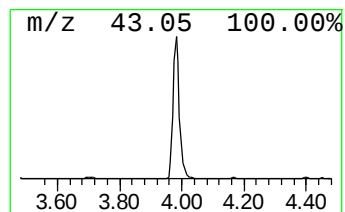
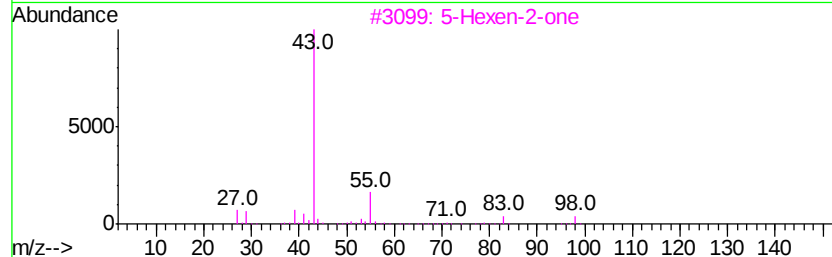
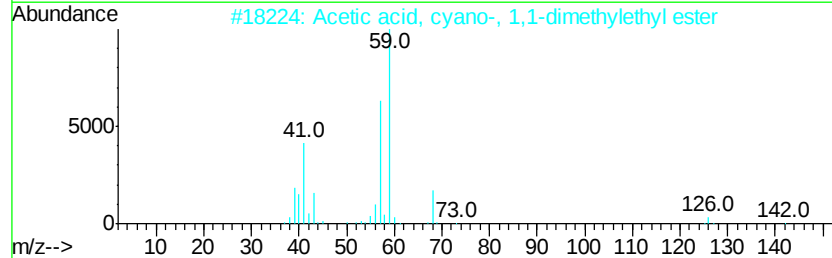
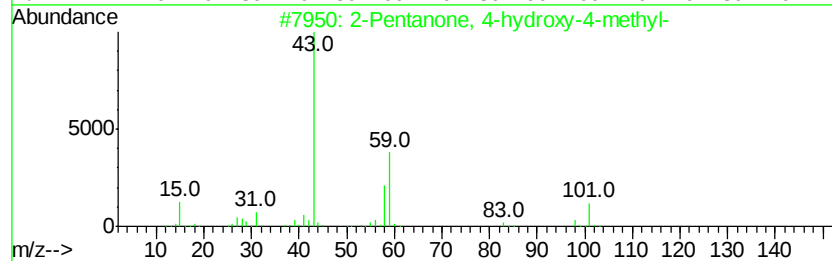
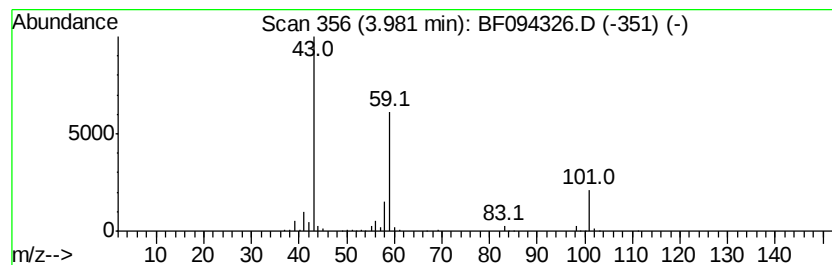
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	21.23 ng	1000200	1,4-Dichlorobenzene-d4	5.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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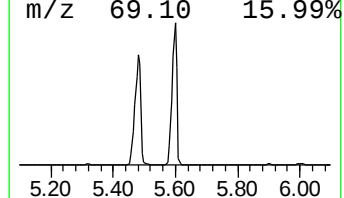
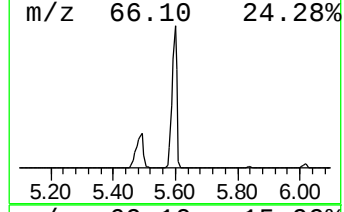
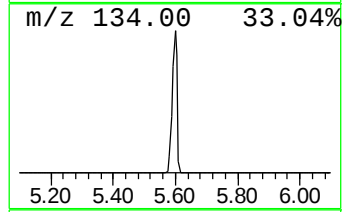
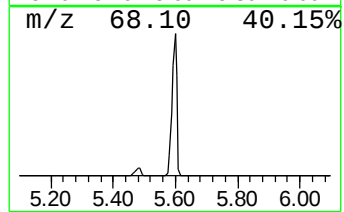
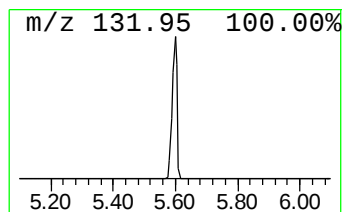
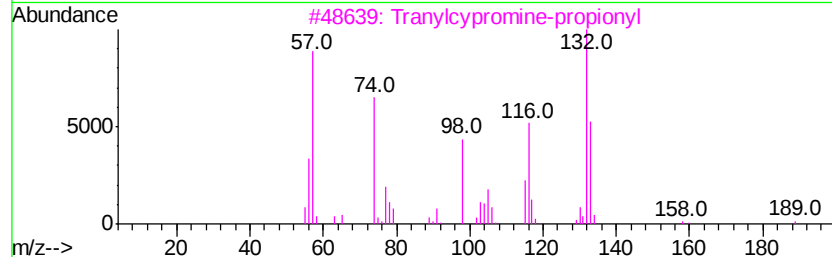
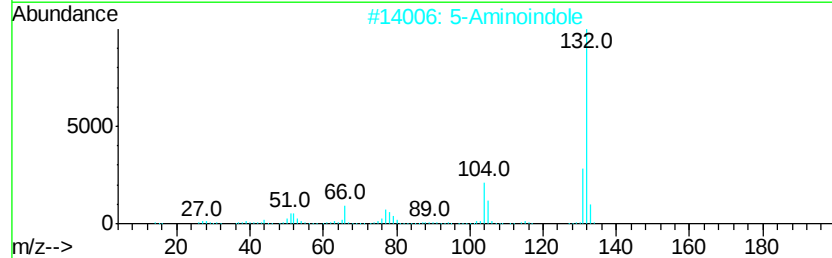
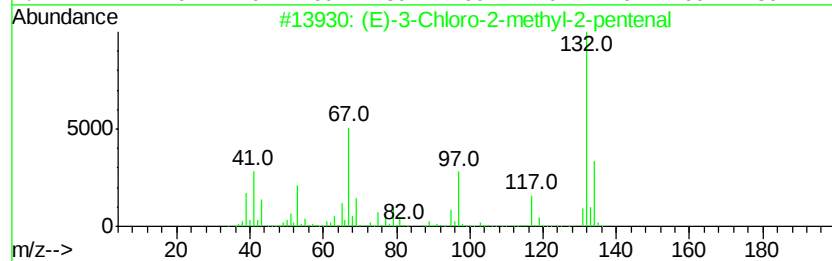
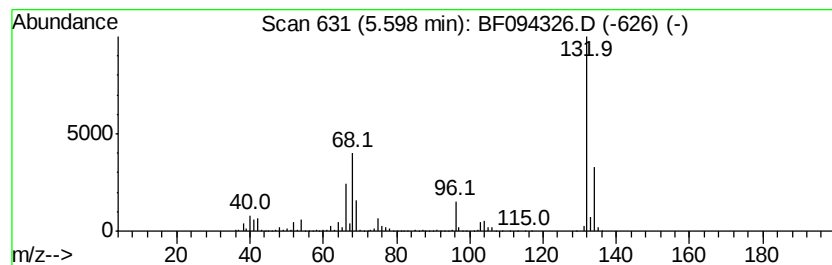
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	98.00 ng	4615990	1,4-Dichlorobenzene-d4	5.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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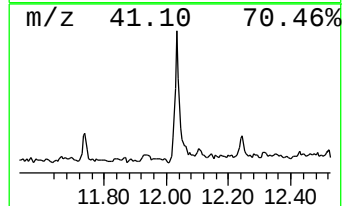
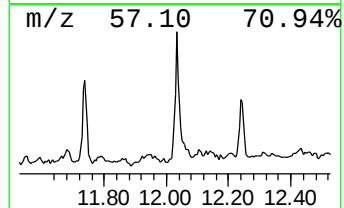
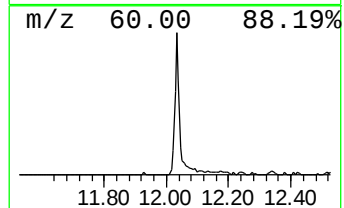
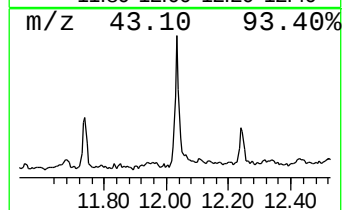
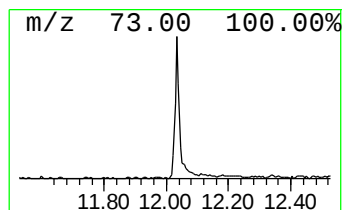
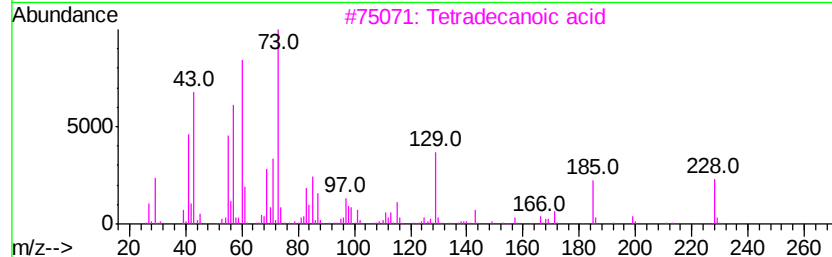
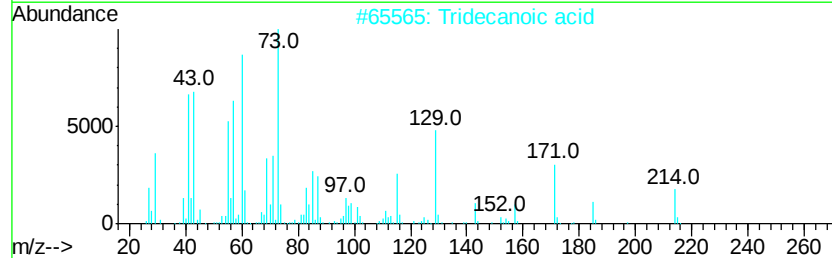
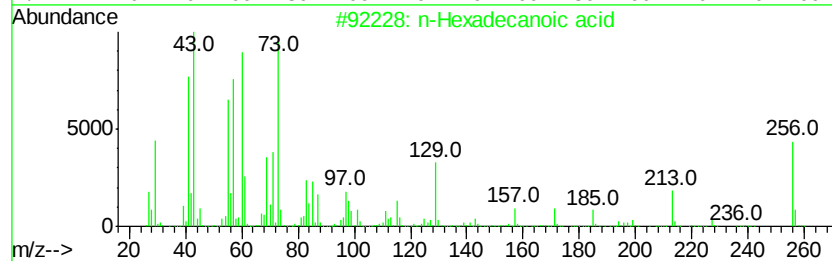
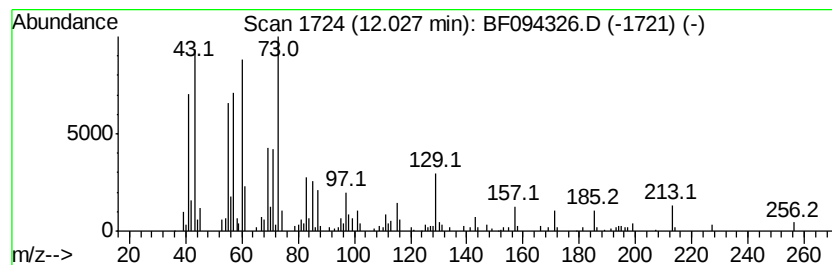
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	7.11 ng	416372	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	46
5		Tetradecane	198	C14H30	000629-59-4	11



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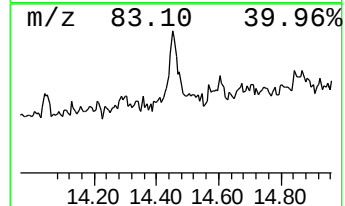
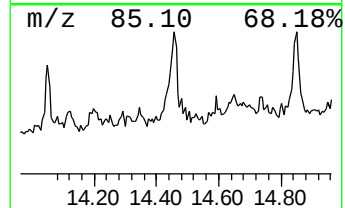
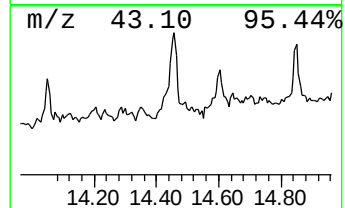
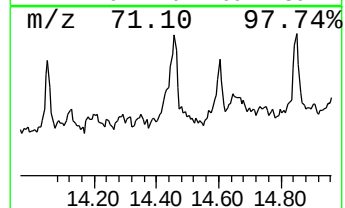
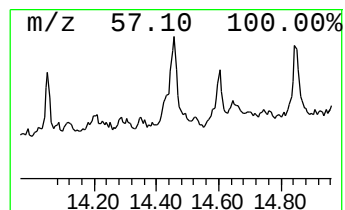
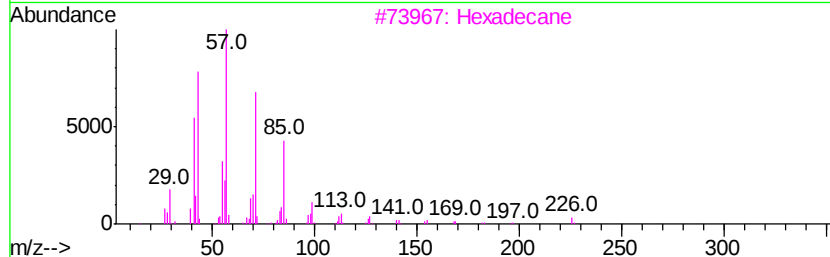
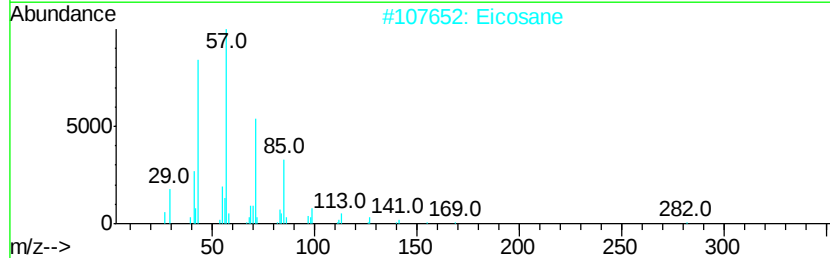
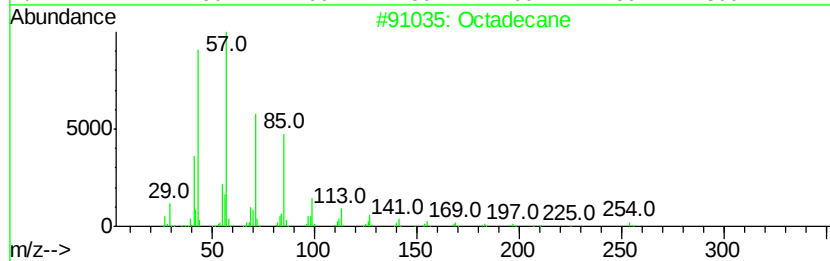
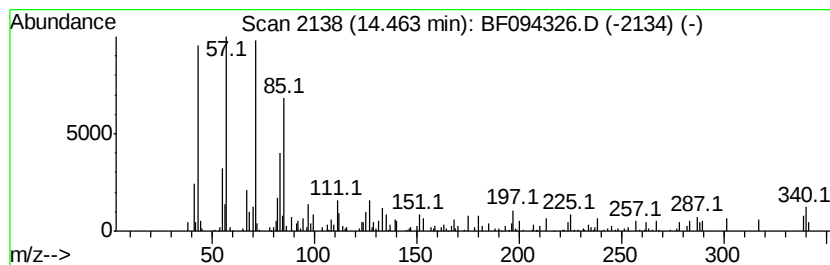
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BNA_F
ClientSampleId :
GRID-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.46	4.21 ng	184622	Chrysene-d12		14.55		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	78
2			Eicosane	282	C20H42	000112-95-8	64
3			Hexadecane	226	C16H34	000544-76-3	55
4			Nonadecane	268	C19H40	000629-92-5	52
5			Tetradecane	198	C14H30	000629-59-4	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
Data File : BF094326.D
Acq On : 10 Apr 2017 22:06
Operator : SJ/MA
Sample : I2595-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-4

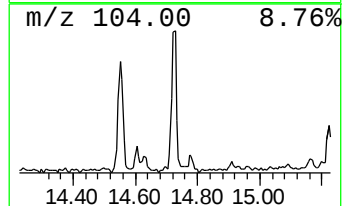
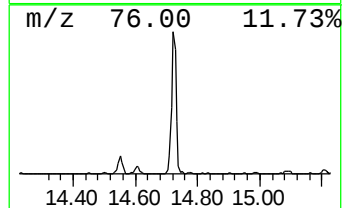
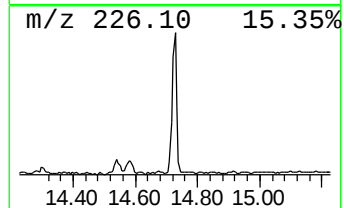
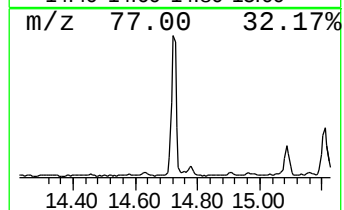
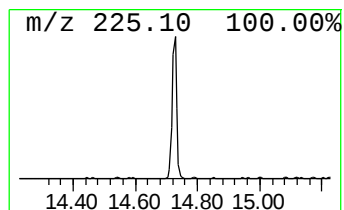
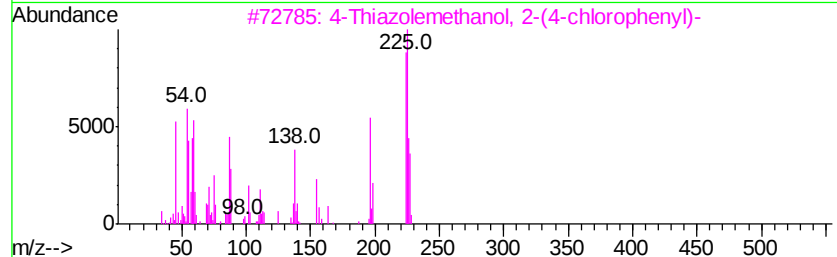
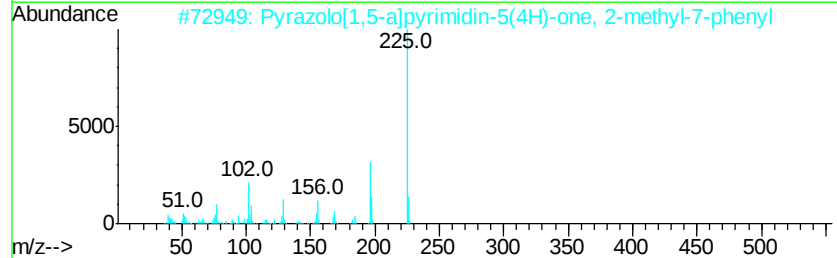
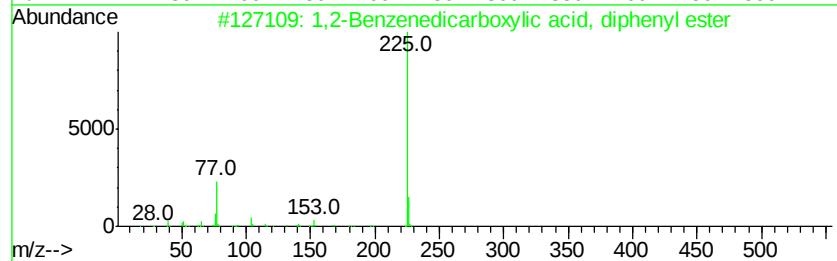
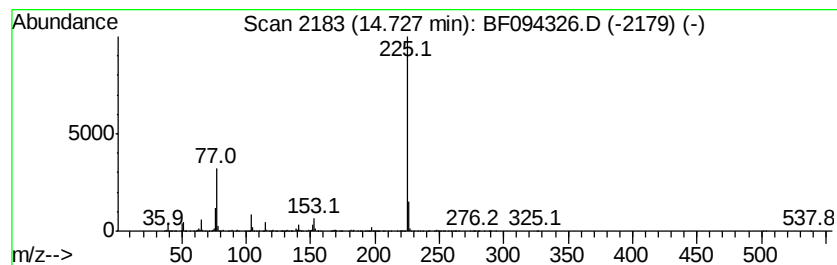
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	12.12 ng	531590	Chrysene-d12	14.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, di...	318	C20H14O4	000084-62-8	90
2		Pyrazolo[1,5-a]pyrimidin-5(4H)-o...	225	C13H11N3O	309949-80-2	72
3		4-Thiazolemethanol, 2-(4-chlorop...	225	C10H8ClNOS	036093-99-9	37
4		Benzene, 1-nitro-4-(2-phenylethe...	225	C14H11NO2	004003-94-5	36
5		Benzene, 1-nitro-3-(2-phenylethe...	225	C14H11NO2	004714-26-5	36



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041017\
Data File : BF094326.D
Acq On : 10 Apr 2017 22:06
Operator : SJ/MA
Sample : I2595-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-4

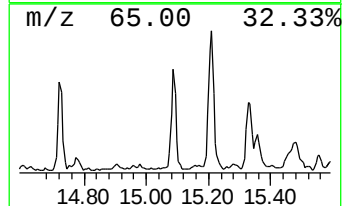
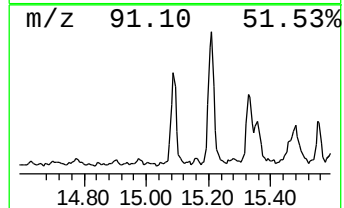
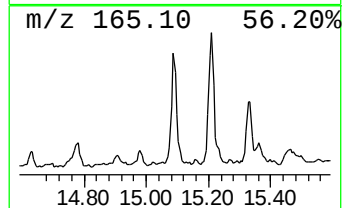
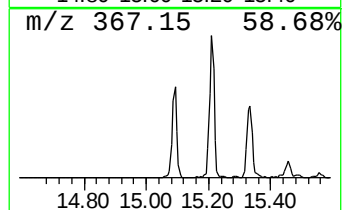
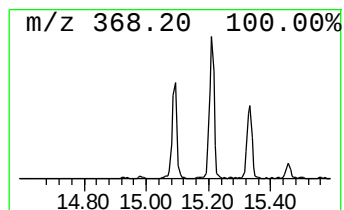
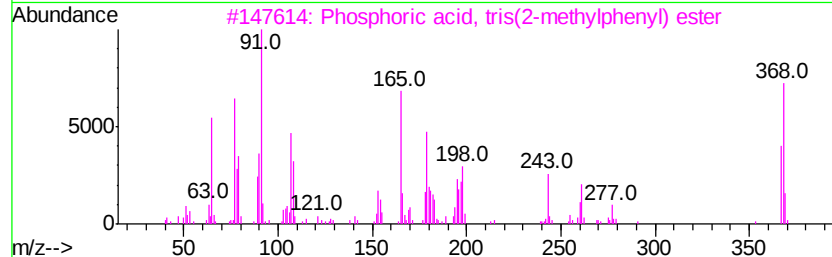
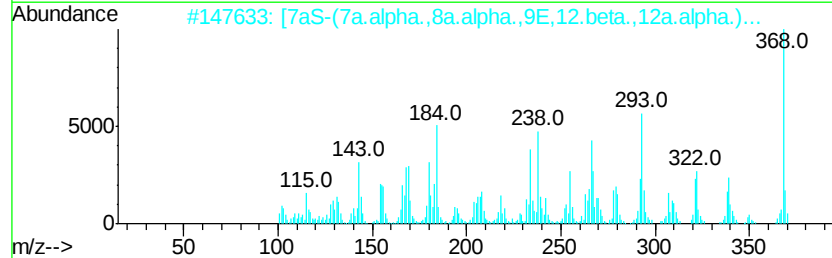
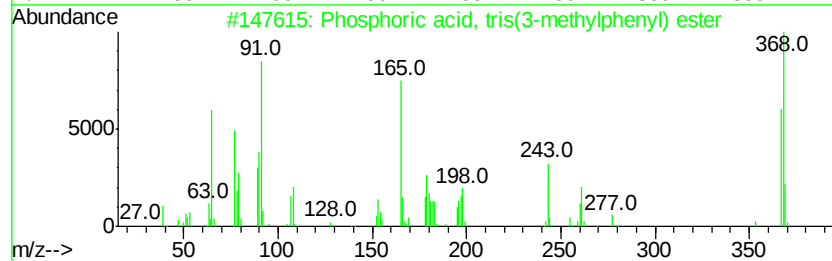
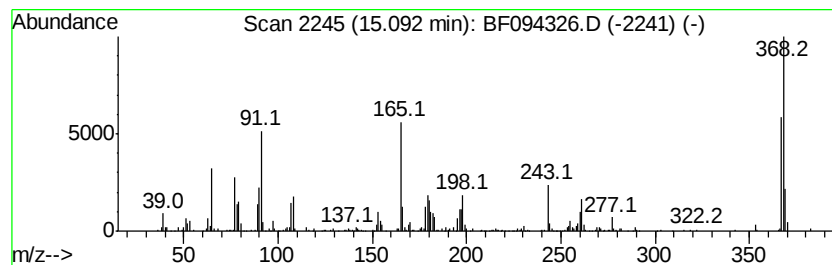
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Phosphoric acid, tris(3-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	9.11 ng	399628	Chrysene-d12	14.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phosphoric acid, tris(3-methylph...	368	C21H21O4P	000563-04-2	99
2		[7aS-(7a.alpha.,8a.alpha.,9E,12....	368	C21H24N2O4	030809-15-5	92
3		Phosphoric acid, tris(2-methylph...	368	C21H21O4P	000078-30-8	90
4		Phosphoric acid, tris(4-methylph...	368	C21H21O4P	000078-32-0	70
5		Carbamic acid, (2-methylphenyl)-...	165	C9H11NO2	014983-92-7	23



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
Data File : BF094326.D
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Operator : SJ/MA
Sample : I2595-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-4

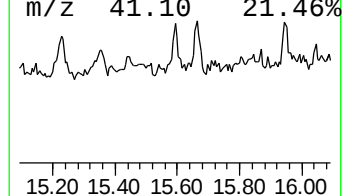
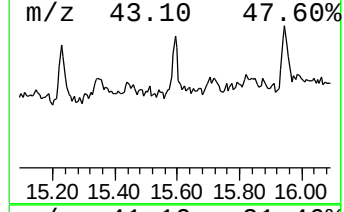
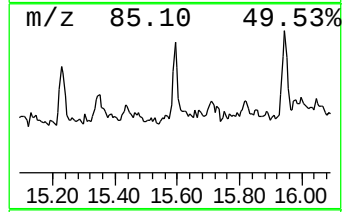
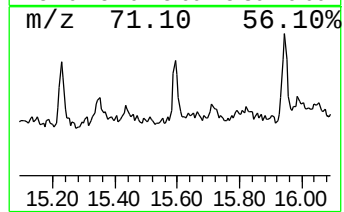
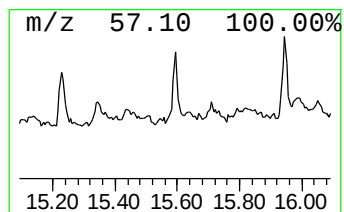
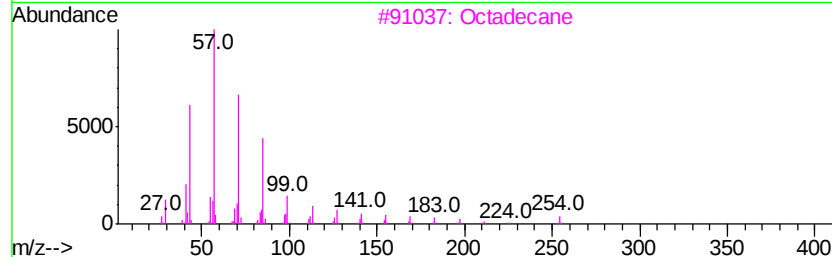
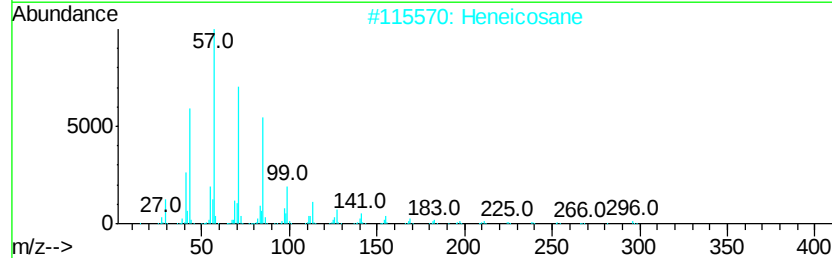
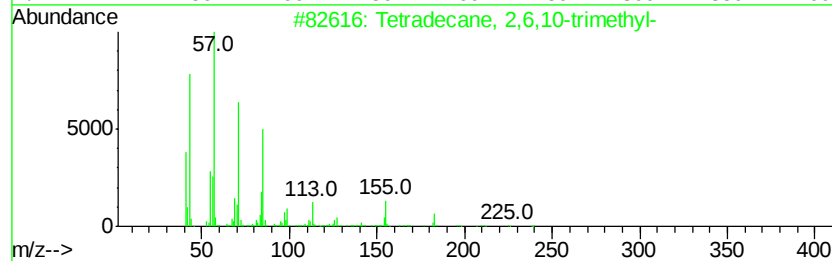
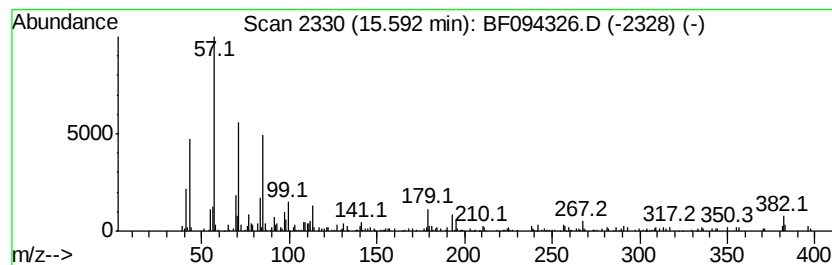
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetradecane, 2,6,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	5.12 ng	201040	Perylene-d12	16.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
2		Heneicosane	296	C21H44	000629-94-7	83
3		Octadecane	254	C18H38	000593-45-3	81
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5		Triacontane	422	C30H62	000638-68-6	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041017\
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Acq On : 10 Apr 2017 22:06
Operator : SJ/MA
Sample : I2595-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methyl Isobutyl K...	2.65	18.4	ng	868271	1	5.84	942075	20.0
2-Pentanone, 4-hy...	3.98	21.2	ng	1000200	1	5.84	942075	20.0
unknown5.60	5.60	98.0	ng	4615990	1	5.84	942075	20.0
n-Hexadecanoic acid	12.03	7.1	ng	416372	4	11.30	1171260	20.0
Octadecane	14.46	4.2	ng	184622	5	14.55	877265	20.0
1,2-Benzenedicarb...	14.73	12.1	ng	531590	5	14.55	877265	20.0
Phosphoric acid, ...	15.09	9.1	ng	399628	5	14.55	877265	20.0
Tetradecane, 2,6,...	15.59	5.1	ng	201040	6	16.18	785629	20.0