

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
 Data File : BF085687.D
 Acq On : 23 Mar 2016 5:32
 Operator : UM/SJ
 Sample : H1858-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRACK-D-GRID-12A

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-BF031816.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	5.019	236	239	251	rBV	796432	1249057	25.51%	3.123%
2	5.441	272	276	278	rBV	2953339	3918448	80.03%	9.797%
3	5.830	308	310	314	rVB	93744	123072	2.51%	0.308%
4	6.470	363	366	369	rBV	2600989	3922542	80.11%	9.807%
5	6.607	375	378	380	rBV	3159968	4086573	83.47%	10.217%
6	6.836	395	398	400	rBV	658854	817091	16.69%	2.043%
7	6.984	409	411	414	rBV	2497976	3116576	63.65%	7.792%
8	7.396	444	447	449	rBV	1976314	2733168	55.82%	6.833%
9	7.499	452	456	459	rVV	76431	107902	2.20%	0.270%
10	8.116	507	510	512	rBV	1348046	1168173	23.86%	2.921%
11	9.202	601	605	607	rBV	3605354	4896148	100.00%	12.241%
12	9.590	637	639	641	rBV	879168	808671	16.52%	2.022%
13	9.808	655	658	660	rVB	90038	96937	1.98%	0.242%
14	9.865	661	663	666	rVB	1058863	1141904	23.32%	2.855%
15	10.070	679	681	684	rVB3	26346	56633	1.16%	0.142%
16	10.299	700	701	703	rVB	175601	157318	3.21%	0.393%
17	10.516	718	720	724	rBV	61999	115403	2.36%	0.289%
18	10.665	729	733	735	rBV2	2017292	2798255	57.15%	6.996%
19	10.779	741	743	749	rBV	139868	268308	5.48%	0.671%
20	11.225	780	782	783	rBV	89730	105108	2.15%	0.263%
21	11.351	791	793	795	rBV	1303271	1156205	23.61%	2.891%
22	11.419	796	799	802	rVB3	27882	72216	1.47%	0.181%
23	11.648	817	819	821	rVB	62982	52161	1.07%	0.130%
24	11.876	838	839	842	rBV2	180441	228552	4.67%	0.571%
25	11.956	844	846	851	rVB3	28782	54696	1.12%	0.137%
26	12.562	896	899	900	rBV	137643	155591	3.18%	0.389%
27	12.665	906	908	915	rBV3	143741	235161	4.80%	0.588%
28	12.791	916	919	920	rVB	109852	139589	2.85%	0.349%
29	12.939	929	932	934	rBV	3519452	3707809	75.73%	9.270%
30	13.831	1008	1010	1015	rVB2	119866	172023	3.51%	0.430%
31	13.979	1020	1023	1029	rVV	773260	942786	19.26%	2.357%
32	14.997	1110	1112	1116	rBV	120381	217740	4.45%	0.544%
33	15.282	1135	1137	1140	rVB	68777	84978	1.74%	0.212%
34	15.340	1140	1142	1145	rBV	60124	72723	1.49%	0.182%

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TRACK-D-GRID-12A

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	15.397	1145	1147	1154	rBV	488344	731633	14.94%	1.829%
36	16.780	1266	1268	1273	rVB3	30211	72134	1.47%	0.180%
37	17.568	1335	1337	1344	rVB7	48396	143614	2.93%	0.359%
38	17.694	1344	1348	1350	rBV4	33406	70212	1.43%	0.176%

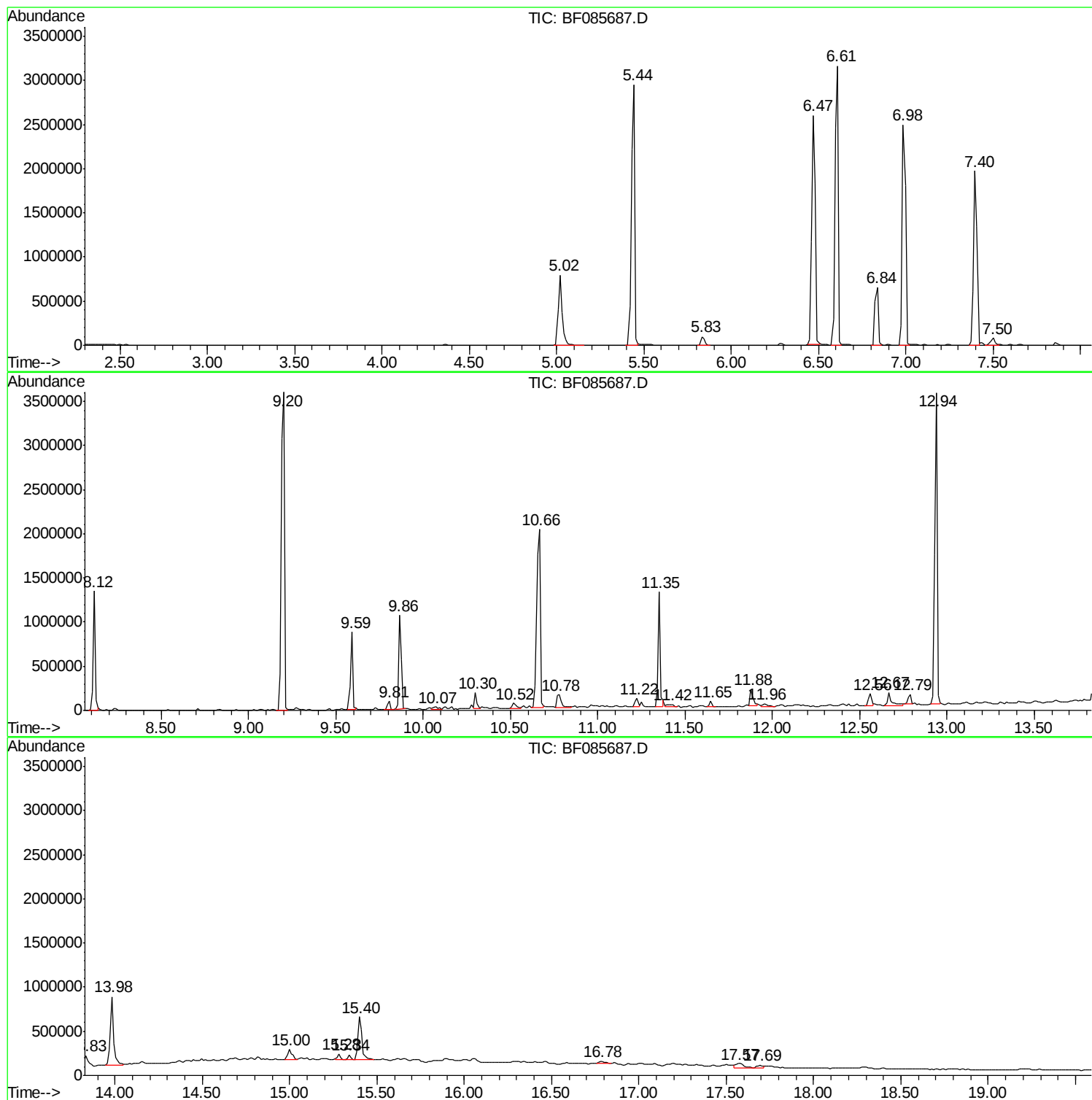
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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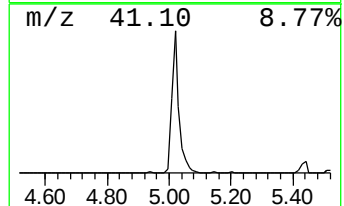
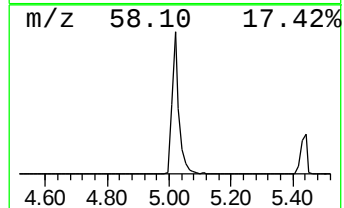
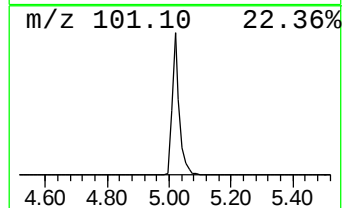
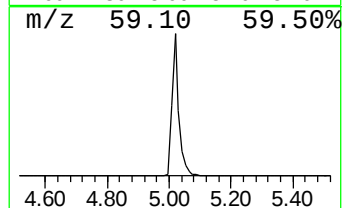
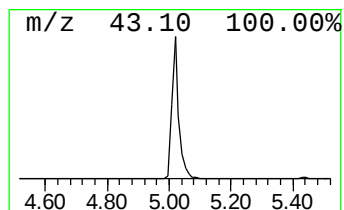
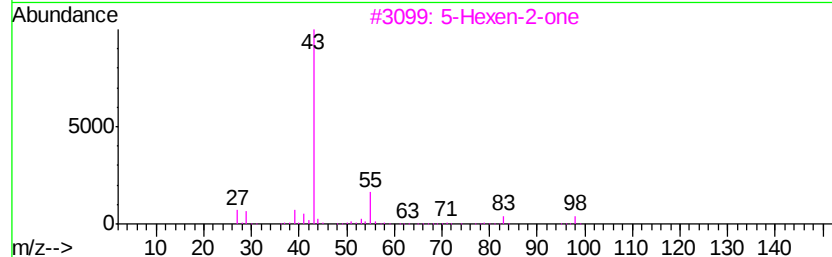
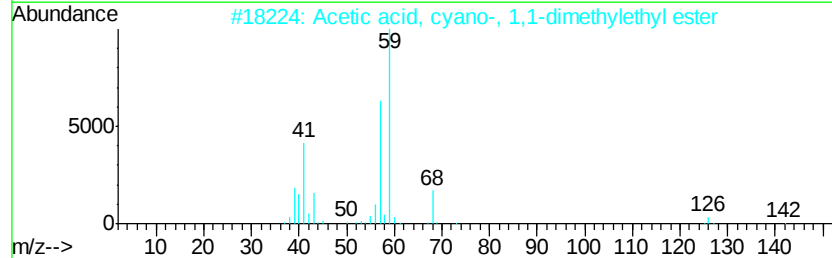
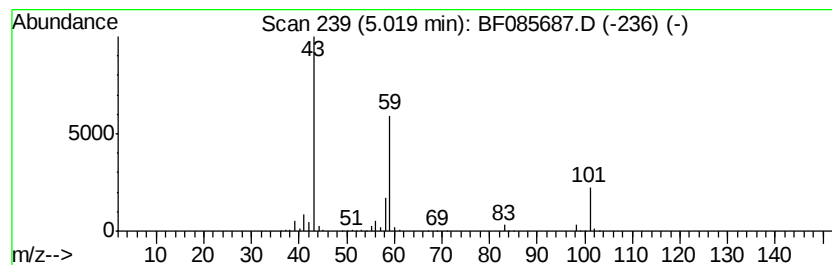
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	30.57 ng	1249060	1,4-Dichlorobenzene-d4	6.84

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, cyano-, 1,1-dimethy...	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		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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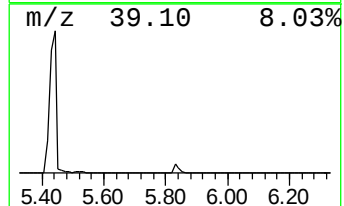
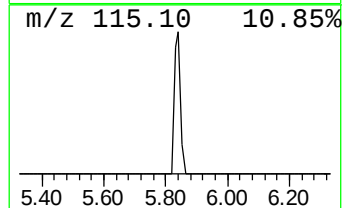
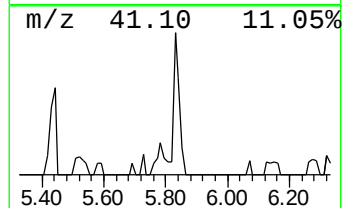
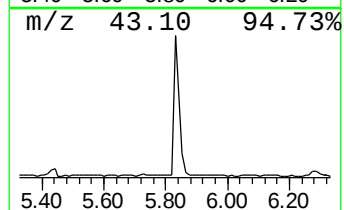
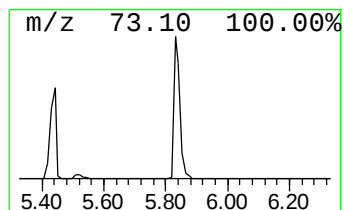
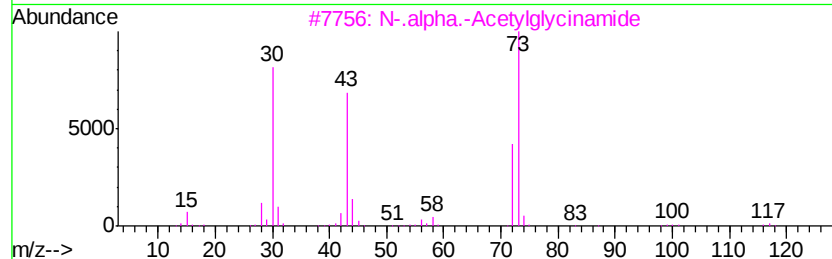
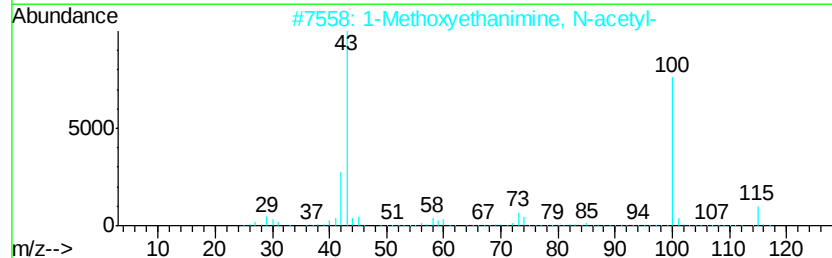
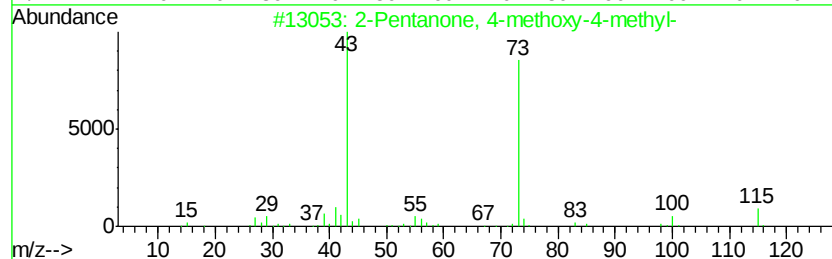
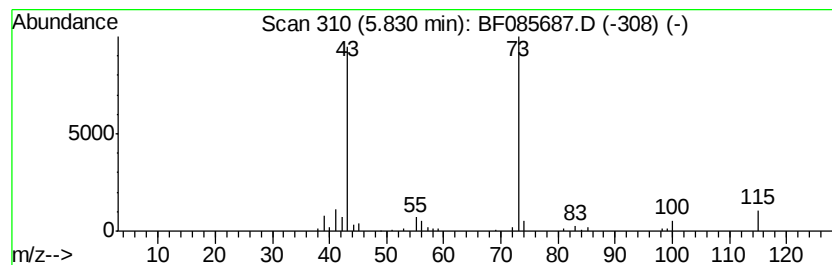
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.83	3.01 ng	123072	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	38
3		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10



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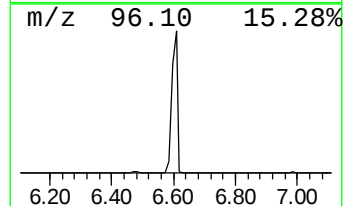
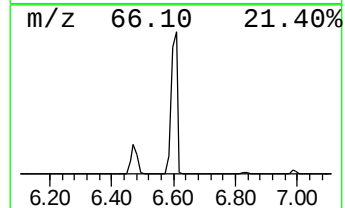
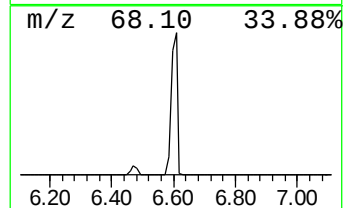
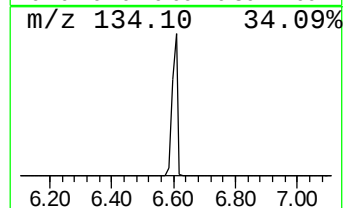
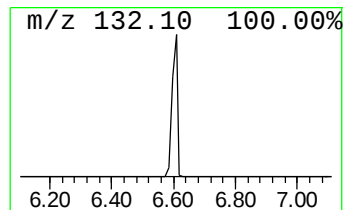
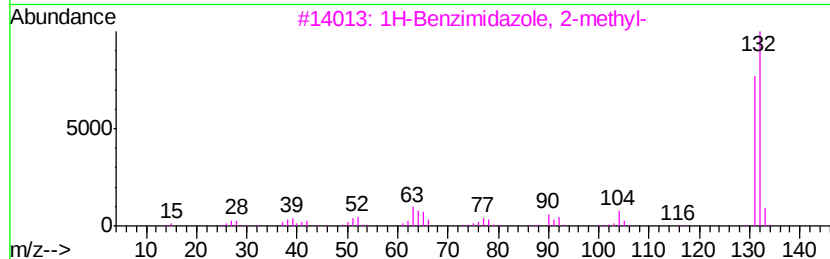
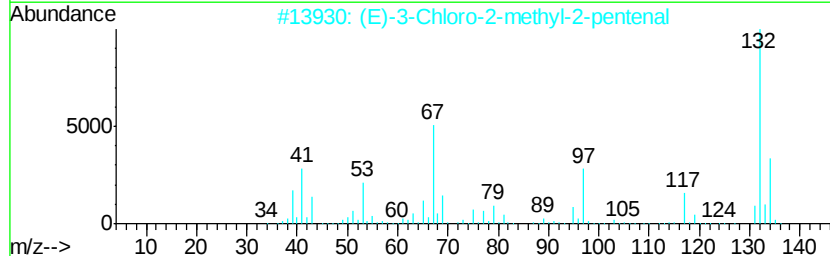
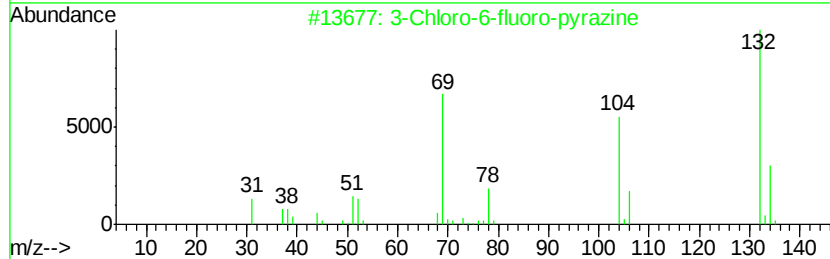
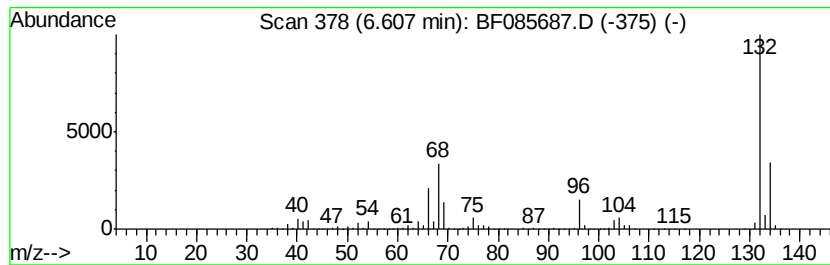
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	100.03 ng	4086570	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9



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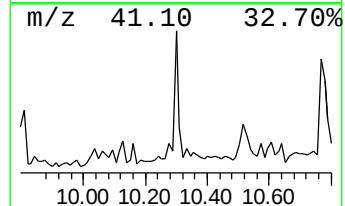
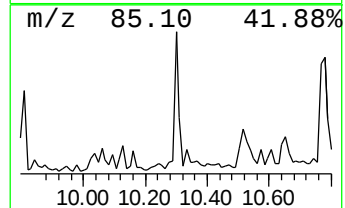
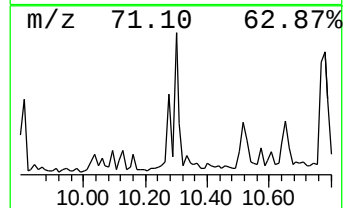
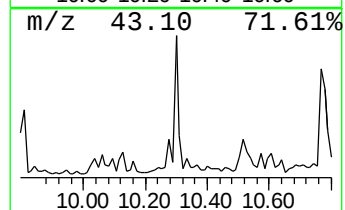
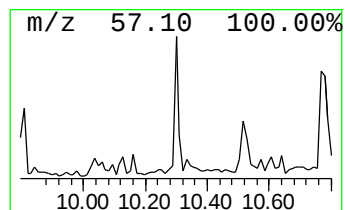
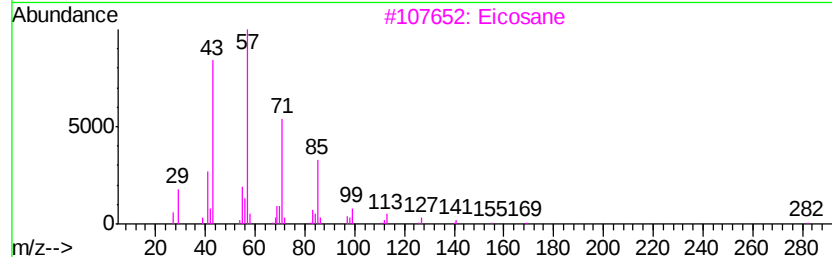
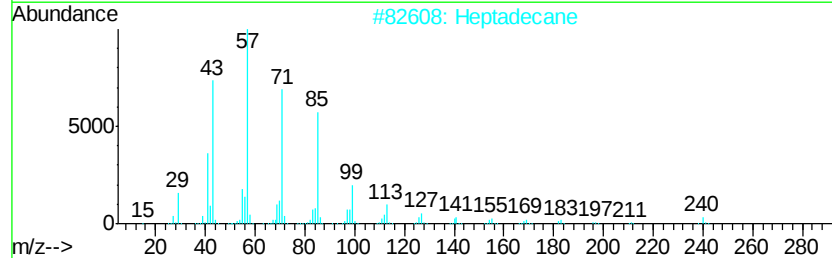
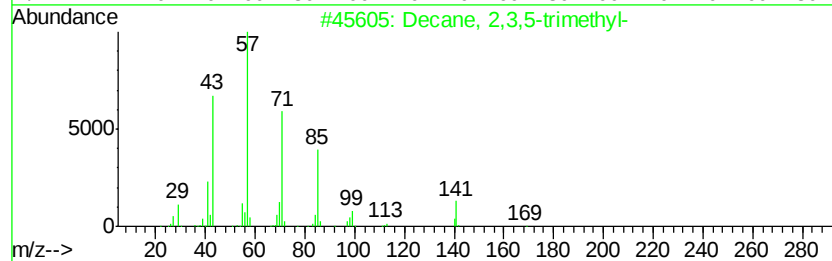
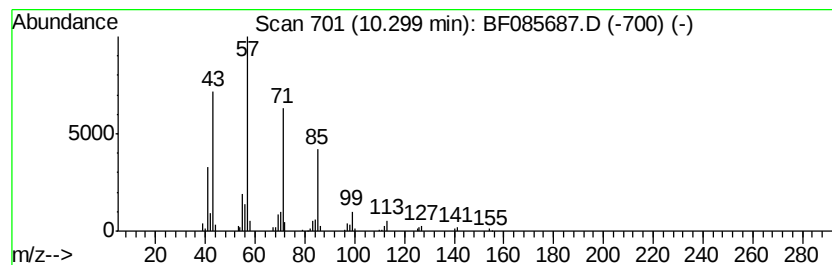
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Decane, 2,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	2.76 ng	157318	Acenaphthene-d10	9.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83	
2	Heptadecane	240	C17H36	000629-78-7	83	
3	Eicosane	282	C20H42	000112-95-8	83	
4	Hexadecane	226	C16H34	000544-76-3	80	
5	Tetradecane	198	C14H30	000629-59-4	72	



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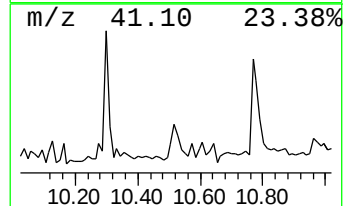
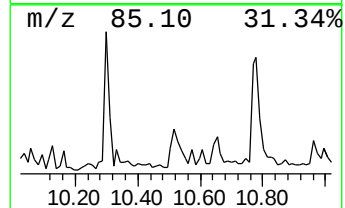
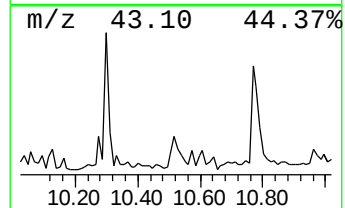
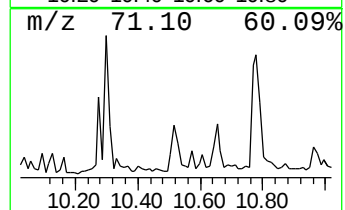
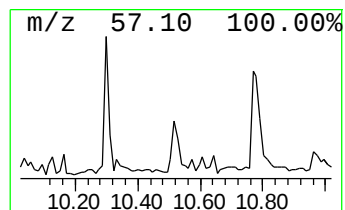
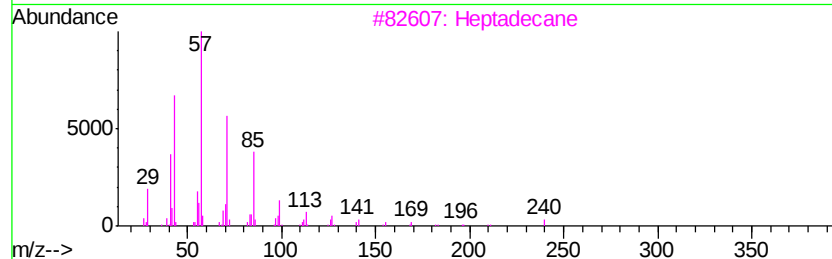
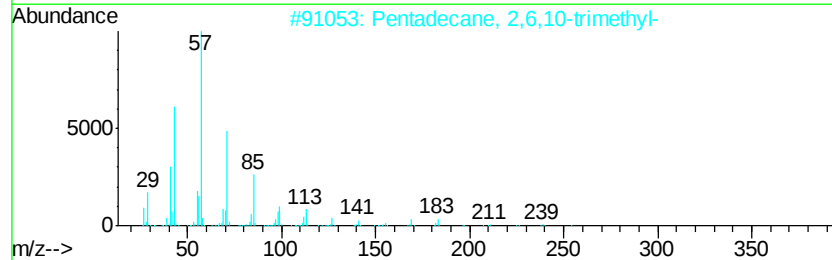
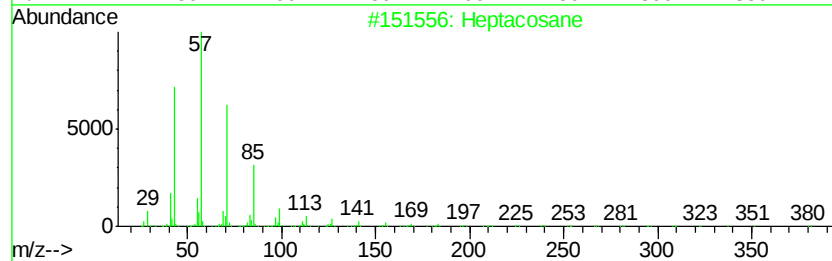
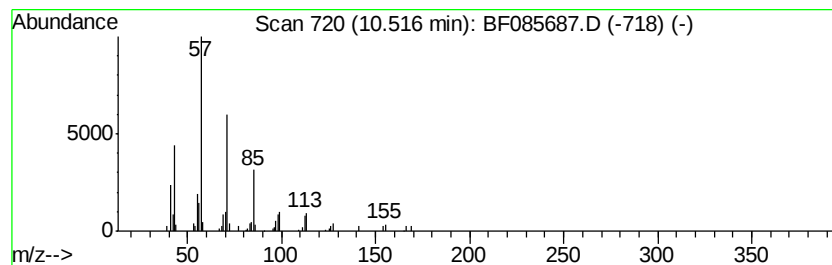
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Peak Number 6 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	2.02 ng	115403	Acenaphthene-d10	9.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	90
2	Pentadecane, 2,6,10-trimethyl-	254 C18H38	003892-00-0	90
3	Heptadecane	240 C17H36	000629-78-7	90
4	Eicosane	282 C20H42	000112-95-8	87
5	Octadecane	254 C18H38	000593-45-3	86



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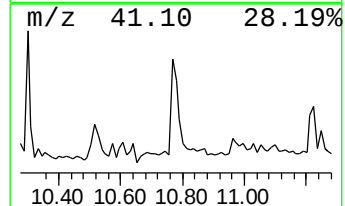
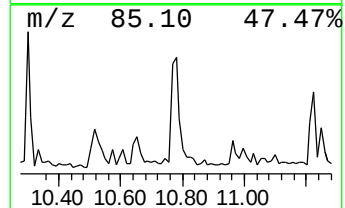
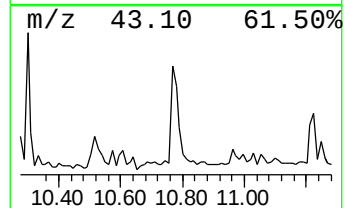
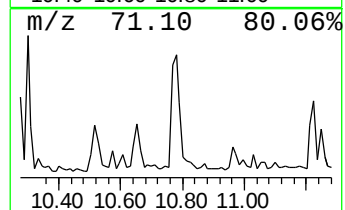
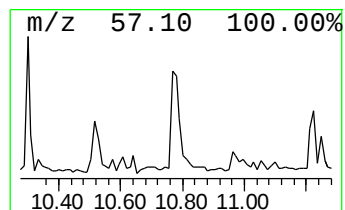
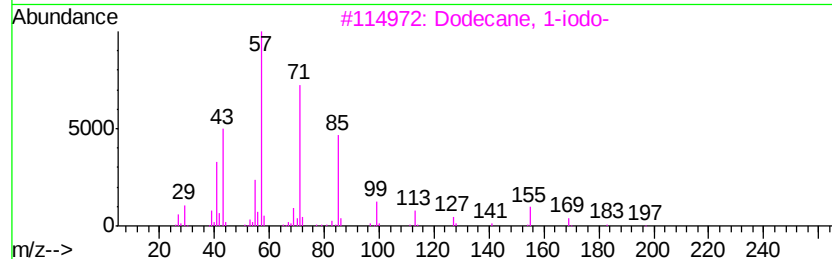
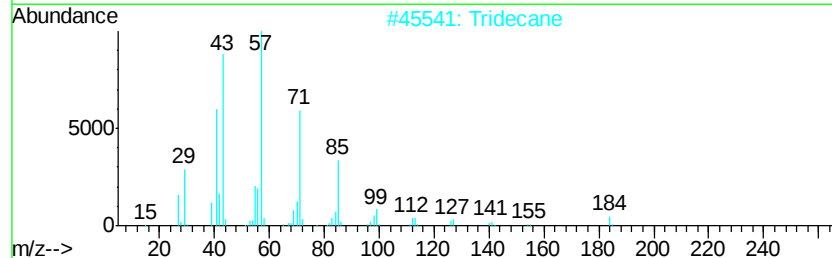
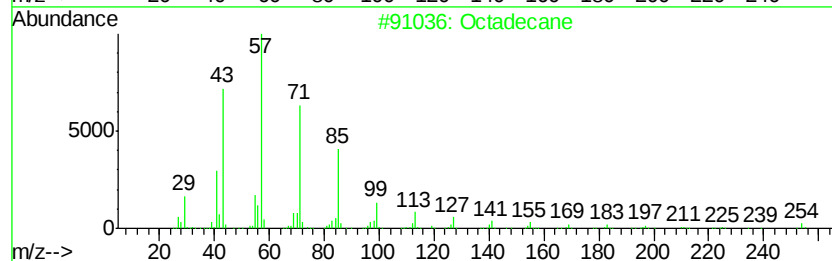
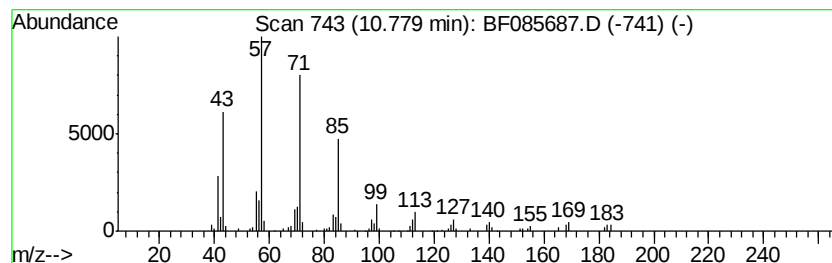
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	4.64 ng	268308	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	90
2	Tridecane		184	C13H28	000629-50-5	87
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	87
4	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	86
5	Eicosane		282	C20H42	000112-95-8	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085687.D
Acq On : 23 Mar 2016 5:32
Operator : UM/SJ
Sample : H1858-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

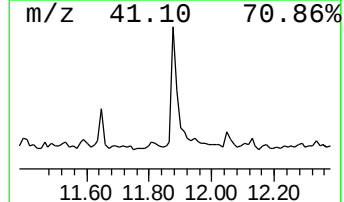
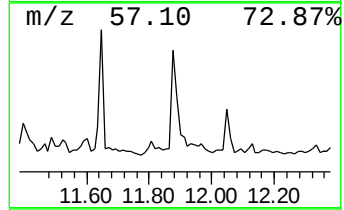
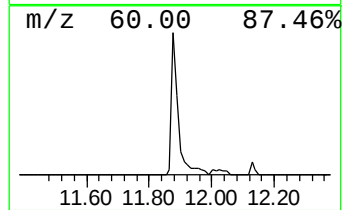
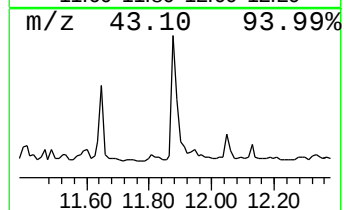
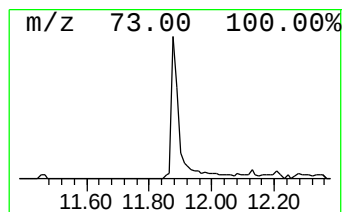
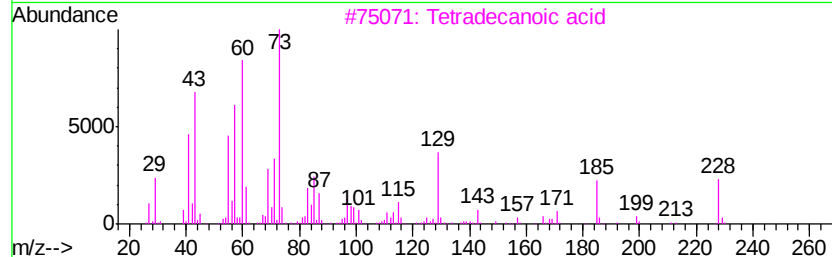
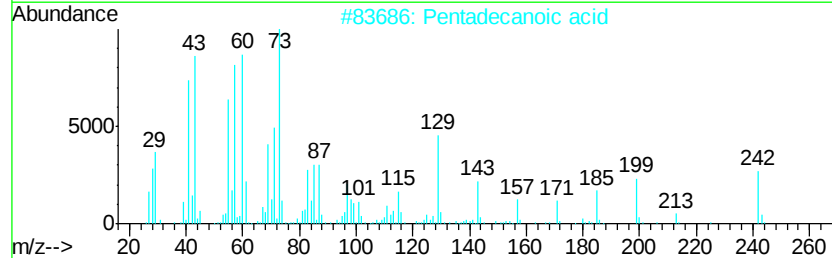
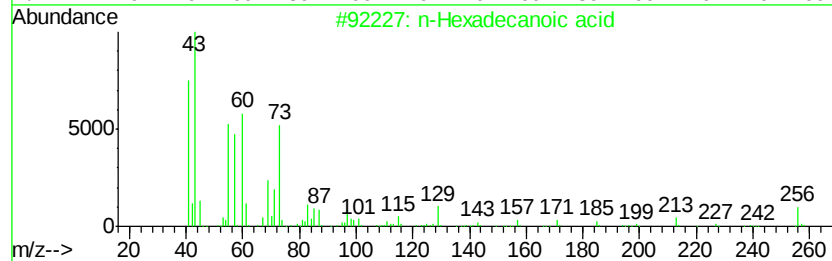
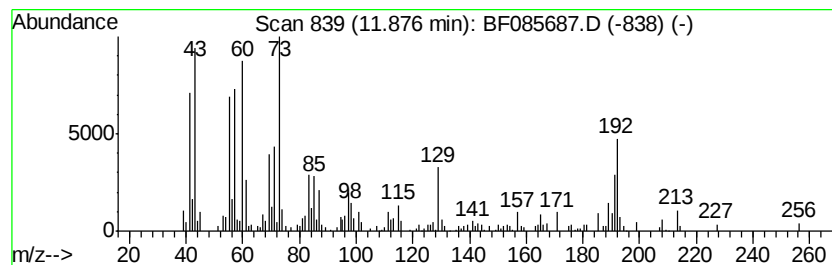
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.88	3.95 ng	228552	Phenanthrene-d10		11.35
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Nonanoic acid	158	C9H18O2	000112-05-0	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
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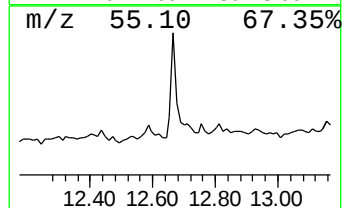
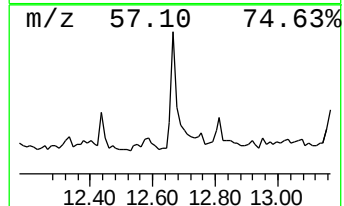
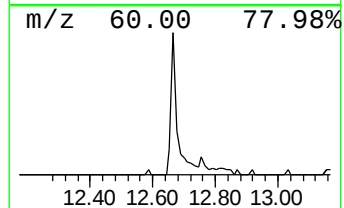
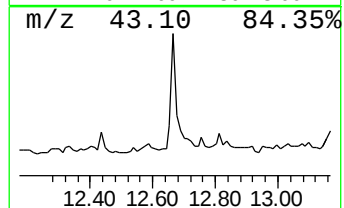
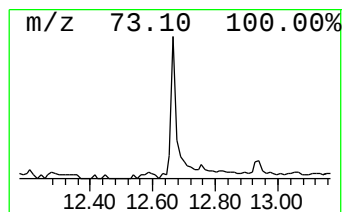
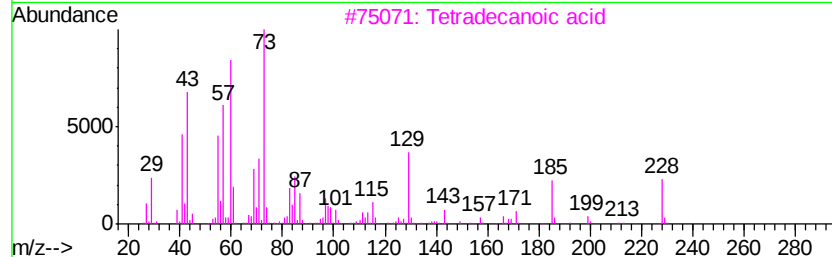
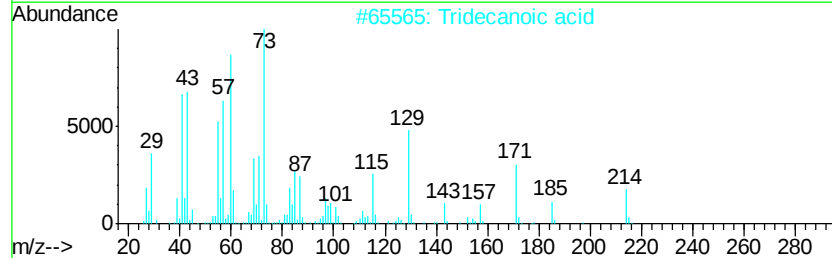
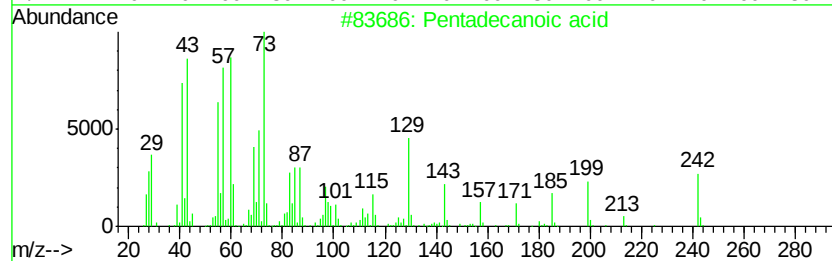
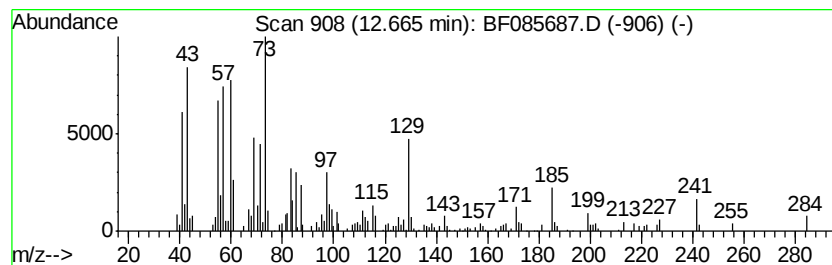
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	4.99 ng	235161	Chrysene-d12	13.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2		Tridecanoic acid	214	C13H26O2	000638-53-9	80
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	68
5		Undecanoic acid	186	C11H22O2	000112-37-8	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
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Acq On : 23 Mar 2016 5:32
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Sample : H1858-01
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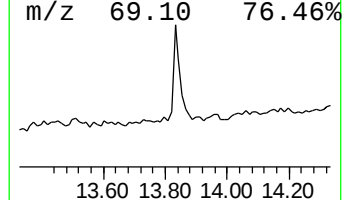
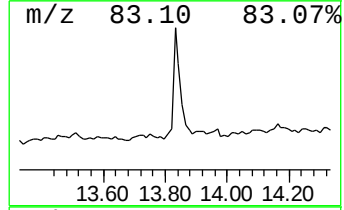
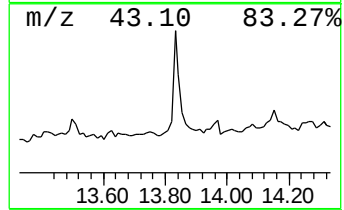
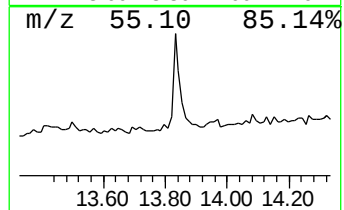
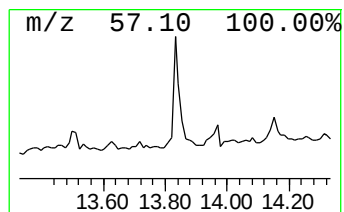
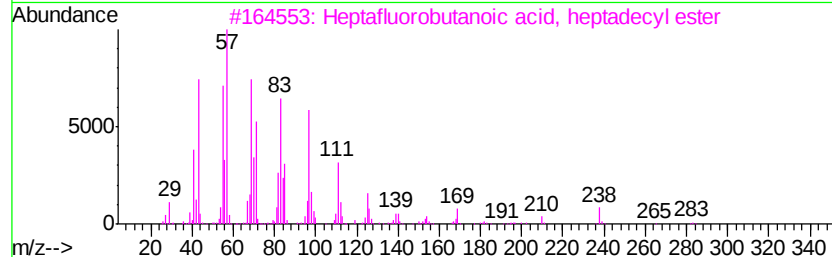
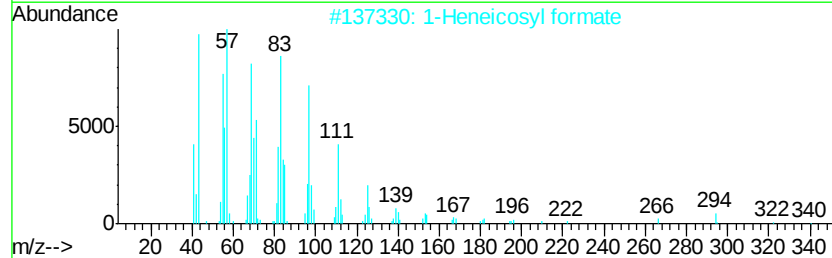
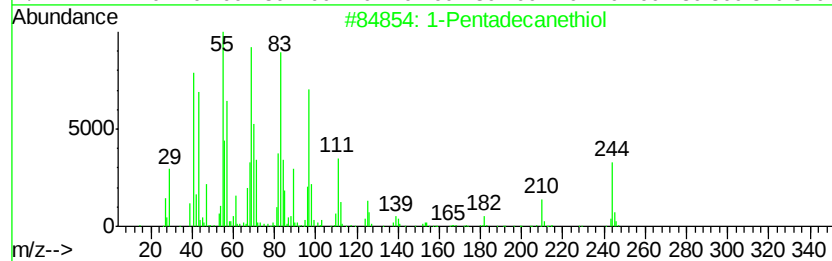
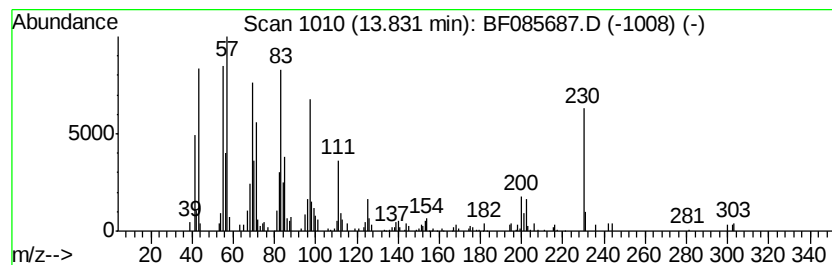
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Pentadecanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.83	3.65 ng	172023	Chrysene-d12	13.98		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3		Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	89
4		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	87
5		Trichloroacetic acid, pentadecyl ester	372	C17H31Cl3O2	074339-53-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
Data File : BF085687.D
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Operator : UM/SJ
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Misc :
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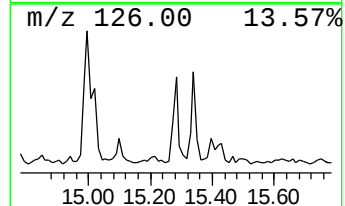
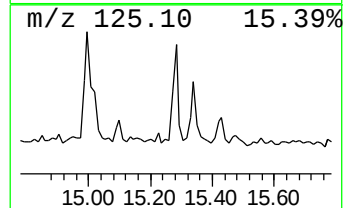
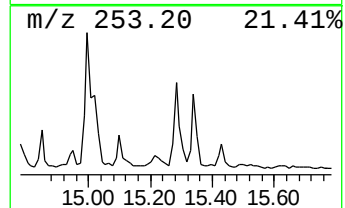
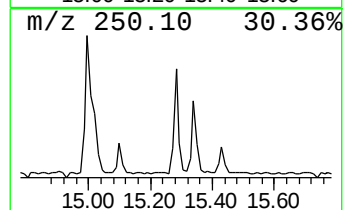
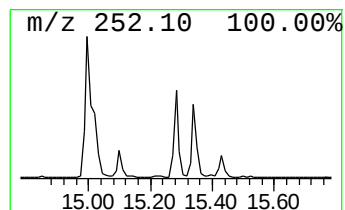
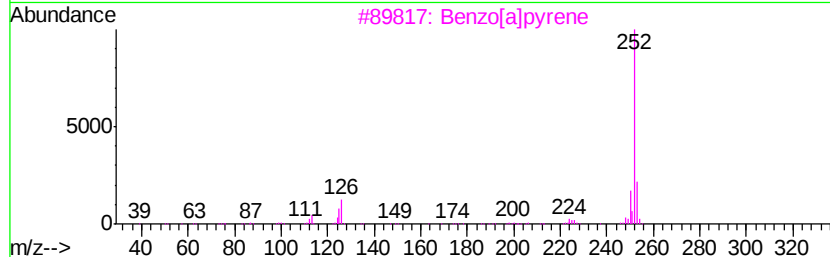
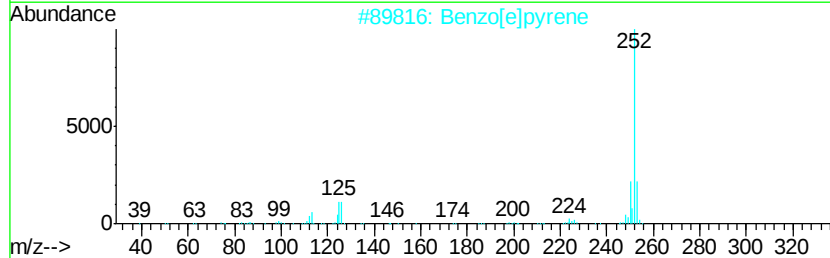
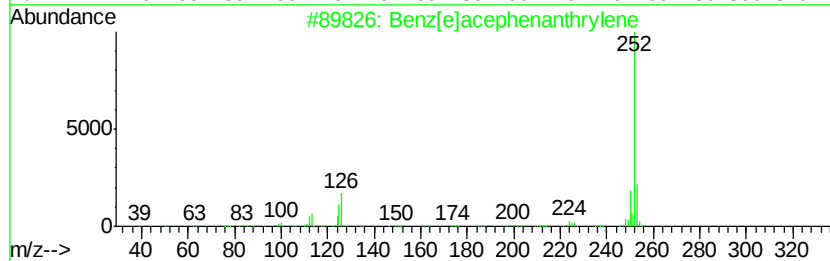
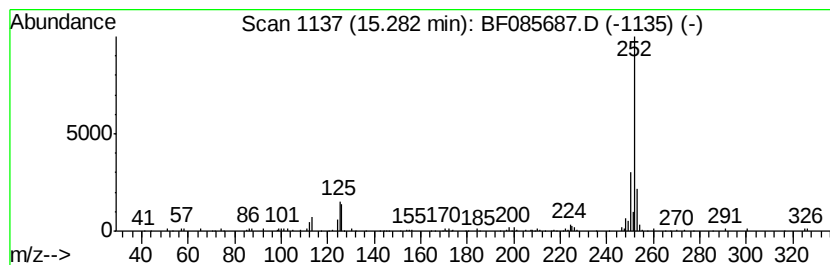
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benz[e]acephenanthrylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.32 ng	84978	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[a]pyrene	252	C20H12	000050-32-8	97
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95



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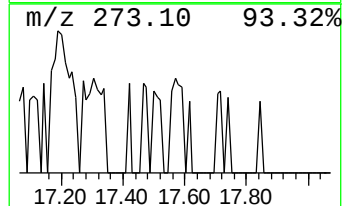
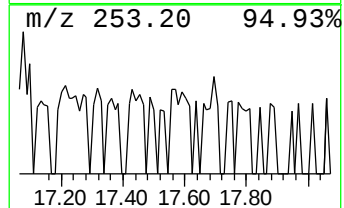
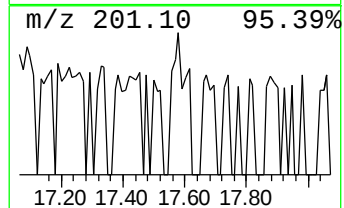
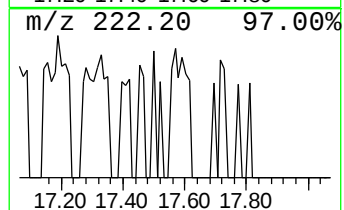
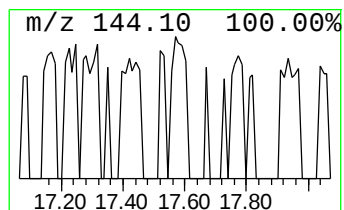
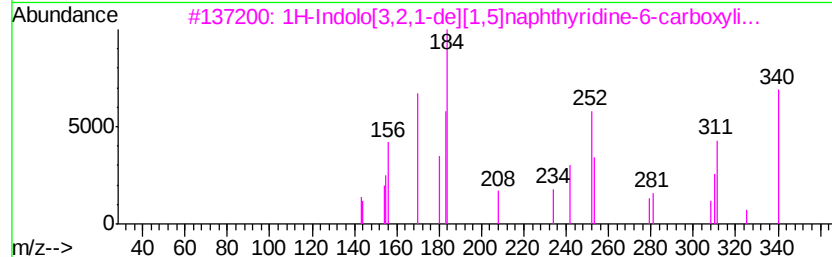
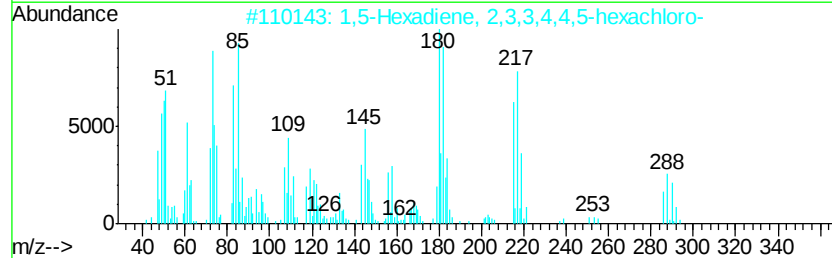
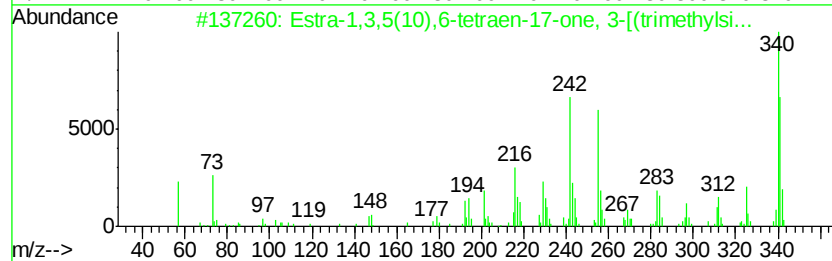
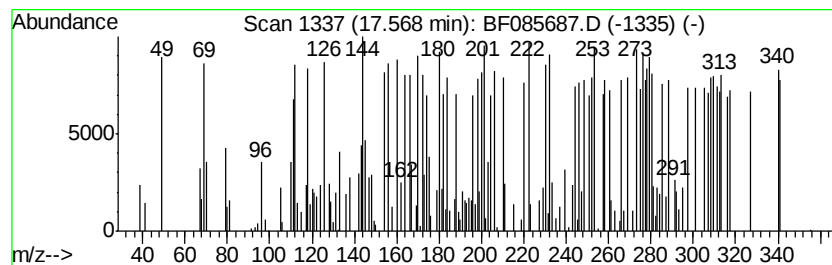
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.57 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	3.93 ng	143614	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estra-1,3,5(10),6-tetraen-17-one...	340	C21H28O2Si	069688-26-2	25		
2	1,5-Hexadiene, 2,3,3,4,4,5-hexac...	286	C6H4Cl6	108562-66-9	22		
3	1H-Indolo[3,2,1-de][1,5]naphthyr...	340	C20H24N2O3	030809-33-7	11		
4	4,6-Dichloro-2-(3-trifluoromethy...	308	C10H5Cl2F3N4	002394-87-8	11		
5	Chloromethylphosphonic dichloride	166	CH2Cl3OP	001983-26-2	9		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
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Acq On : 23 Mar 2016 5:32
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Sample : H1858-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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2-Pentanone, 4-me...	5.83	3.0	ng	123072	1	6.84	817091	20.0
unknown6.61	6.61	100.0	ng	4086570	1	6.84	817091	20.0
Decane, 2,3,5-tri...	10.30	2.8	ng	157318	3	9.86	1141900	20.0
Heptacosane	10.52	2.0	ng	115403	3	9.86	1141900	20.0
Octadecane	10.78	4.6	ng	268308	4	11.35	1156210	20.0
n-Hexadecanoic acid	11.88	4.0	ng	228552	4	11.35	1156210	20.0
Pentadecanoic acid	12.67	5.0	ng	235161	5	13.98	942786	20.0
1-Pentadecanethiol	13.83	3.6	ng	172023	5	13.98	942786	20.0
Benz[e]acephenant...	15.28	2.3	ng	84978	6	15.40	731633	20.0
unknown17.57	17.57	3.9	ng	143614	6	15.40	731633	20.0