

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
 Data File : BF095316.D
 Acq On : 22 May 2017 16:18
 Operator : SJ/MA
 Sample : I3157-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WEST

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.954	509	513	520	rVB3	15969	27373	1.04%	0.119%
2	5.119	537	541	559	rBV	119895	323775	12.32%	1.411%
3	5.725	640	644	678	rBV	890196	2116948	80.57%	9.226%
4	6.489	770	774	779	rBV	27128	40149	1.53%	0.175%
5	6.936	845	850	860	rBV	120008	166767	6.35%	0.727%
6	7.301	905	912	928	rBV	1332555	2302204	87.62%	10.033%
7	7.419	928	932	943	rVB	1542421	2552033	97.13%	11.122%
8	7.760	986	990	999	rBV	353777	438671	16.70%	1.912%
9	7.854	1004	1006	1011	rVB	24447	29059	1.11%	0.127%
10	7.995	1025	1030	1033	rBV	1552676	1830988	69.69%	7.980%
11	8.030	1033	1036	1045	rVB	251641	331141	12.60%	1.443%
12	8.183	1058	1062	1066	rBV	33304	42013	1.60%	0.183%
13	8.289	1075	1080	1088	rBV2	47673	89533	3.41%	0.390%
14	8.401	1095	1099	1110	rVB	29610	42452	1.62%	0.185%
15	8.625	1130	1137	1139	rBV2	151363	202017	7.69%	0.880%
16	8.660	1139	1143	1166	rVB	920263	1532893	58.34%	6.681%
17	9.001	1197	1201	1206	rBV	73307	89938	3.42%	0.392%
18	9.272	1244	1247	1260	rVB	100098	142167	5.41%	0.620%
19	9.372	1260	1264	1267	rBV	158307	195396	7.44%	0.852%
20	9.777	1329	1333	1346	rBV	352254	643397	24.49%	2.804%
21	9.883	1347	1351	1361	rVB4	27567	54736	2.08%	0.239%
22	11.113	1551	1560	1570	rBV	19449	38169	1.45%	0.166%
23	11.548	1629	1634	1655	rBV	1771674	2627358	100.00%	11.450%
24	12.248	1749	1753	1772	rBV	215859	367762	14.00%	1.603%
25	12.613	1810	1815	1826	rBV2	465043	741728	28.23%	3.233%
26	13.442	1950	1956	1961	rBV	34212	42538	1.62%	0.185%
27	13.807	2011	2018	2021	rBV	16204	29426	1.12%	0.128%
28	13.907	2030	2035	2055	rBV	868626	1550726	59.02%	6.758%
29	14.212	2083	2087	2089	rBV	33972	39240	1.49%	0.171%
30	14.236	2089	2091	2097	rVB2	24336	29675	1.13%	0.129%
31	14.942	2207	2211	2215	rBV2	23589	27709	1.05%	0.121%
32	15.012	2219	2223	2244	rVB	409347	697618	26.55%	3.040%
33	15.965	2379	2385	2394	rBV6	23755	62074	2.36%	0.271%
34	17.330	2612	2617	2638	rBV	2024058	2424494	92.28%	10.566%

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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	18.571	2819	2828	2844	rBV3	35946	129955	4.95%	0.566%
36	18.683	2844	2847	2865	rVV	320435	553224	21.06%	2.411%
37	20.365	3128	3133	3141	rBV	206891	360261	13.71%	1.570%
38	23.841	3713	3724	3729	rVB9	10623	29994	1.14%	0.131%

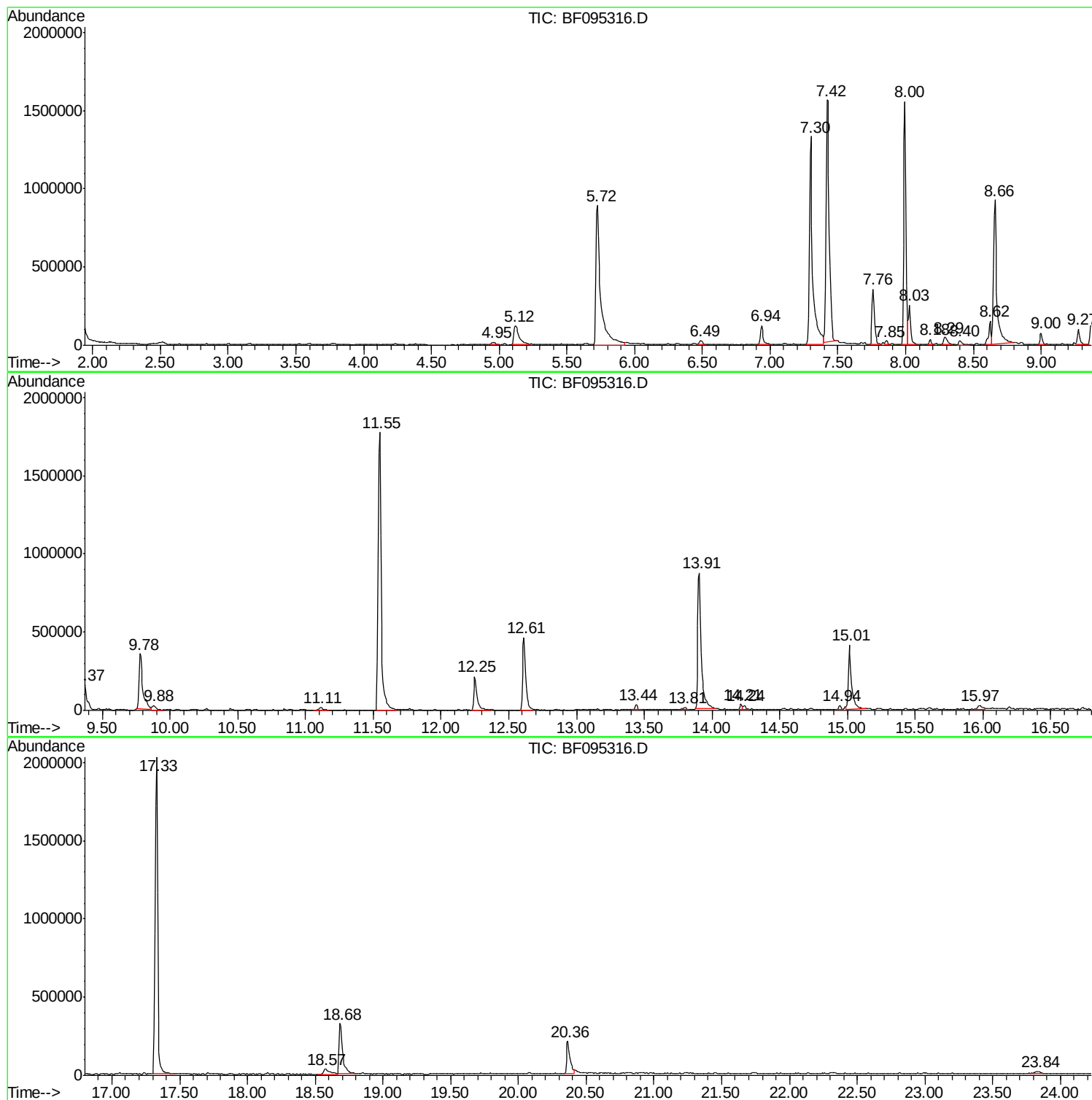
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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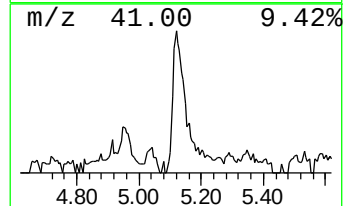
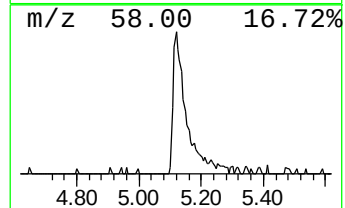
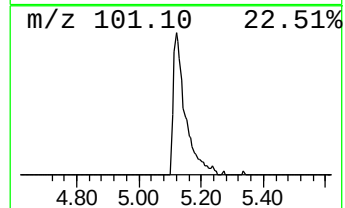
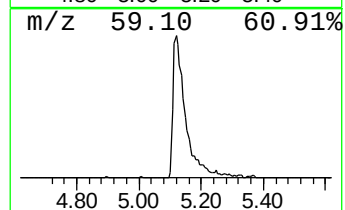
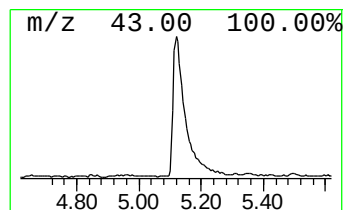
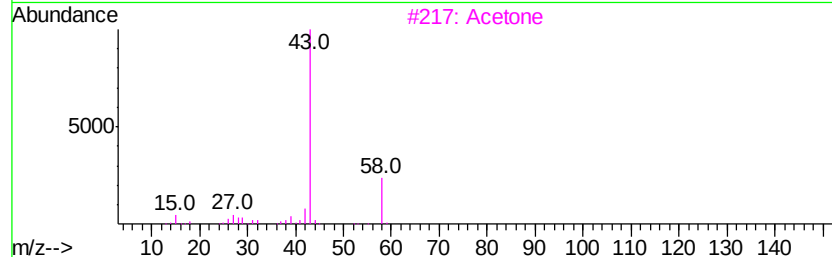
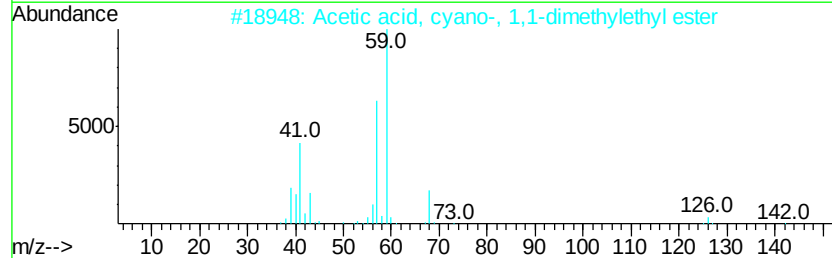
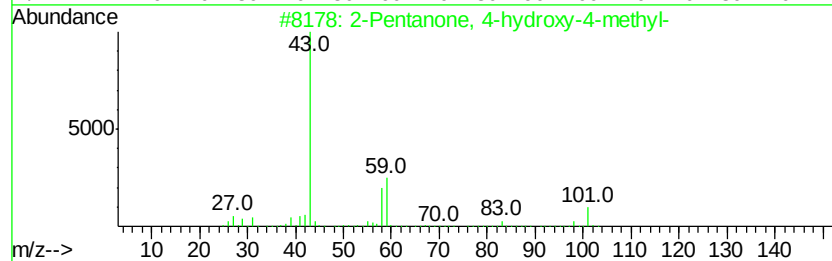
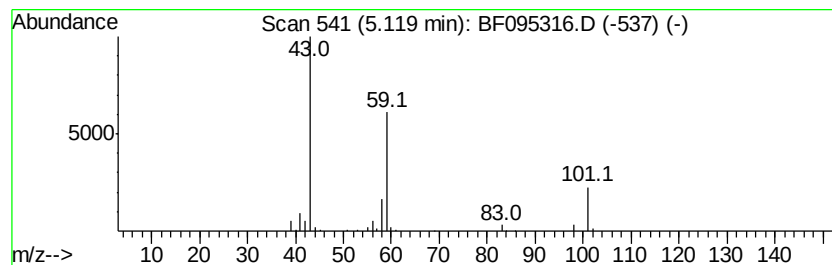
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	14.76 ng	323775	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Acetone	58	C3H6O	000067-64-1	14
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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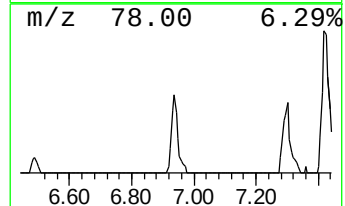
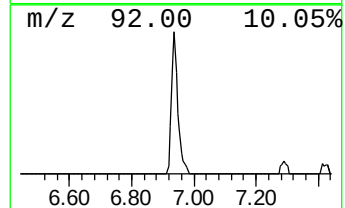
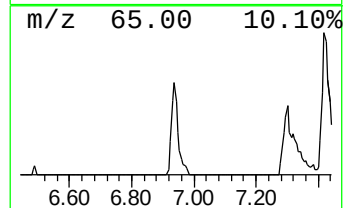
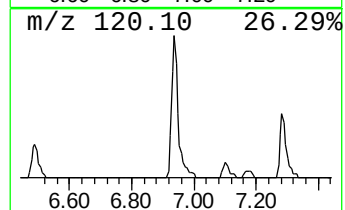
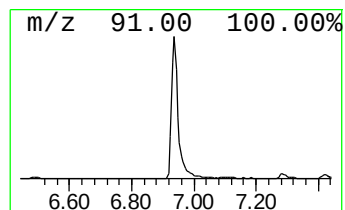
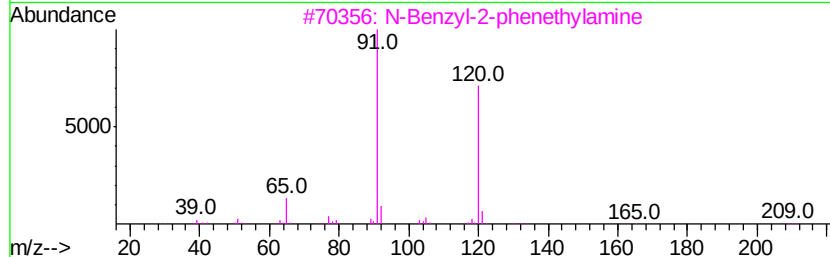
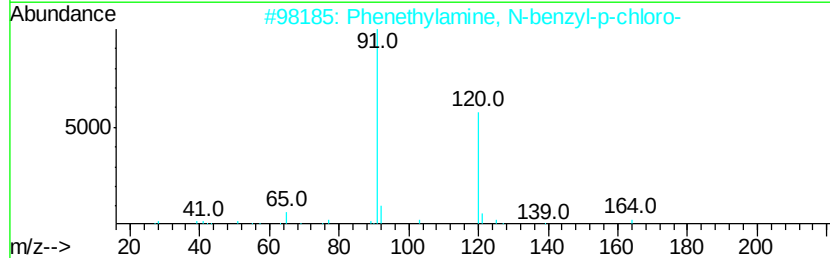
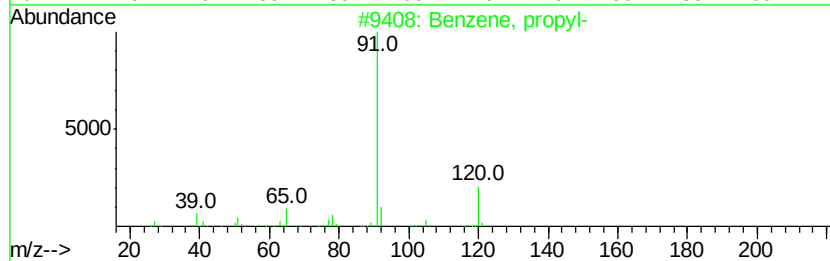
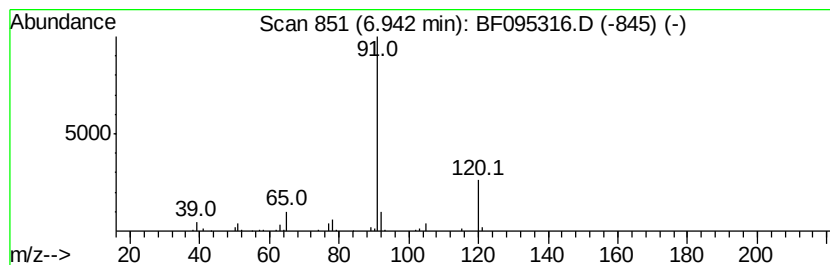
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Benzene, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	7.60 ng	166767	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, propyl-	120	C9H12	000103-65-1	90
2		Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	72
3		N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	64
4		Propanenitrile, 3-[(phenylmethyl)...	160	C10H12N2	000706-03-6	64
5		Phosphonous dichloride, (phenylm...	192	C7H7Cl2P	004545-85-1	50



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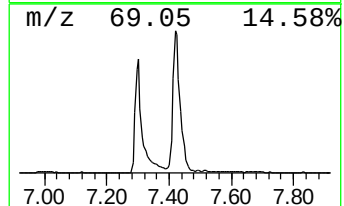
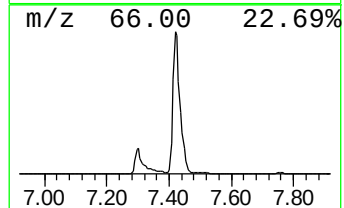
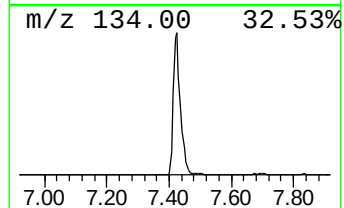
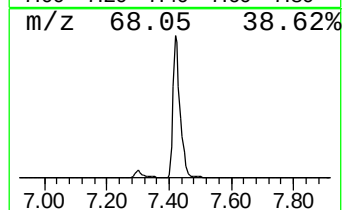
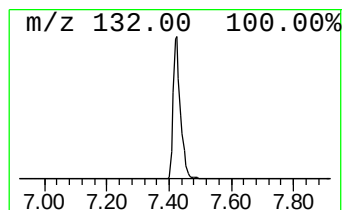
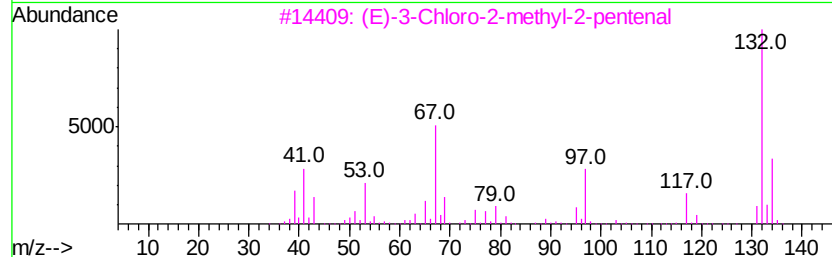
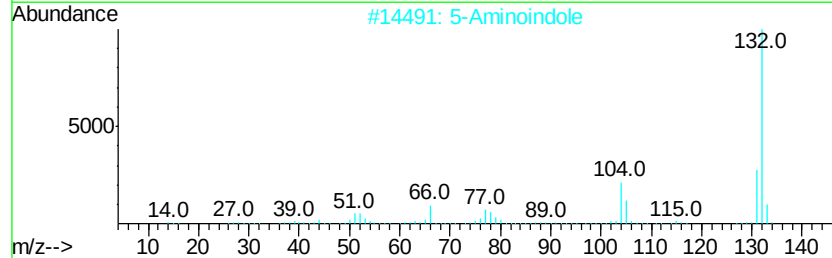
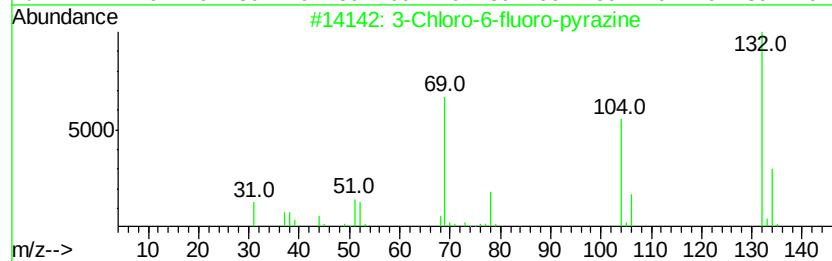
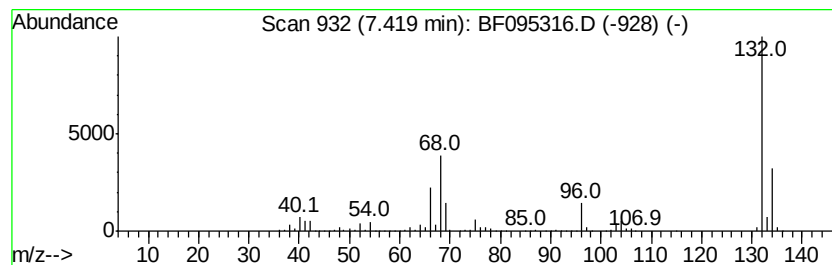
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	116.35 ng	2552030	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Xenon	132	Xe	007440-63-3	9



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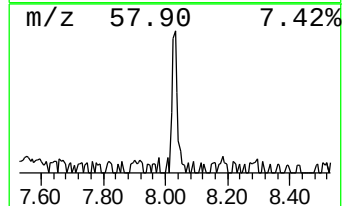
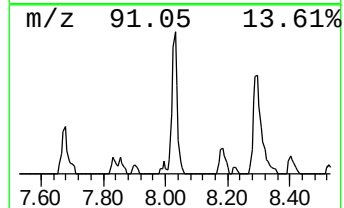
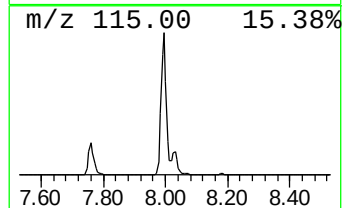
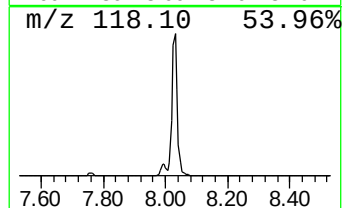
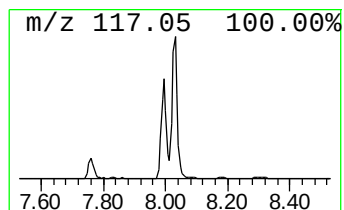
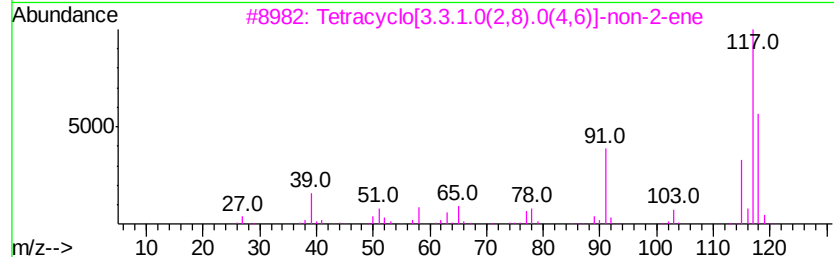
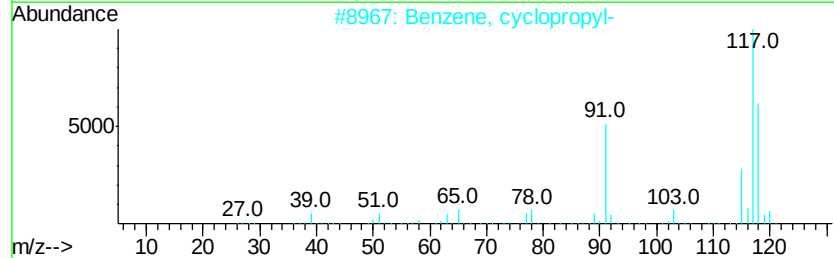
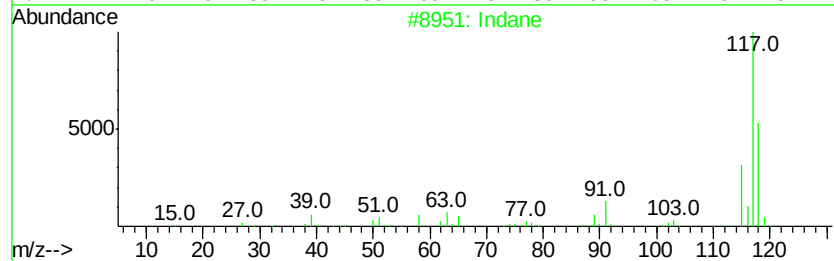
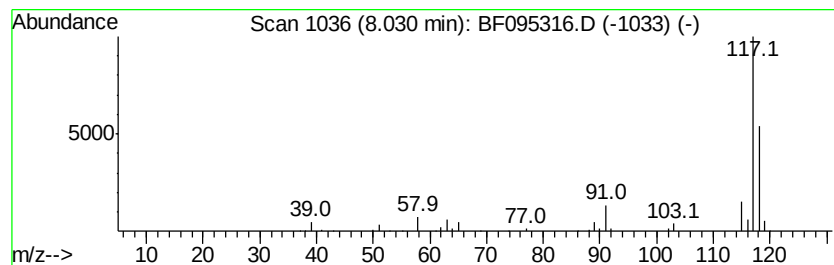
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.03	15.10 ng	331141	1,4-Dichlorobenzene-d4	7.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	90
2	Benzene, cyclopropyl-		118	C9H10	000873-49-4	86
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-	...	118	C9H10	1000191-13-7	78
4	1,3-Methanopentalene, 1,2,3,5-te...		118	C9H10	128600-88-4	72
5	Benzeneethanol, .beta.-ethenyl-....		162	C11H14O	040596-14-3	59



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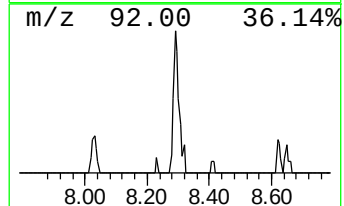
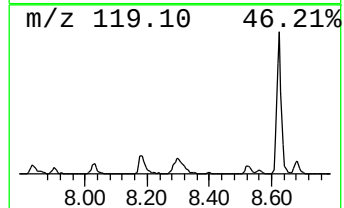
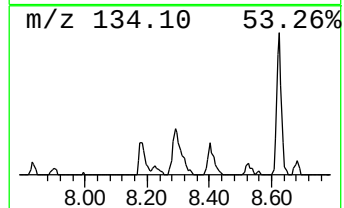
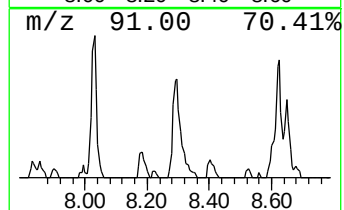
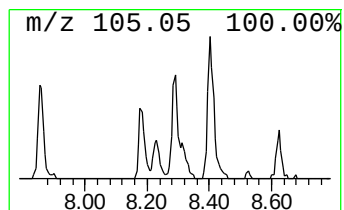
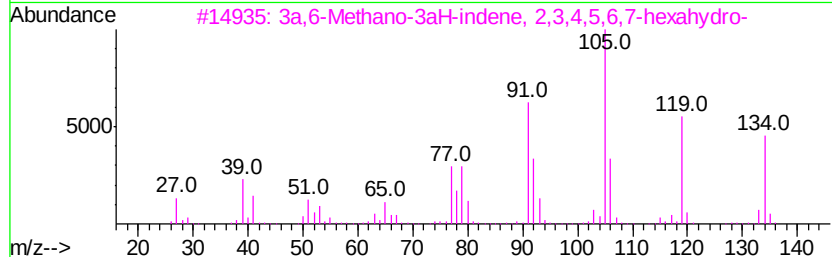
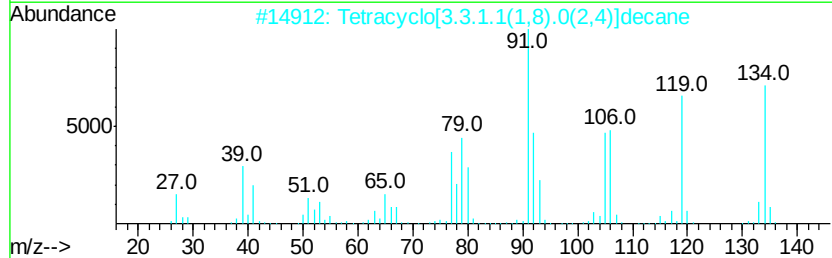
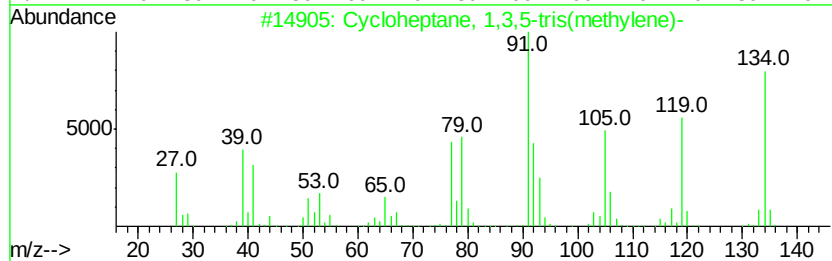
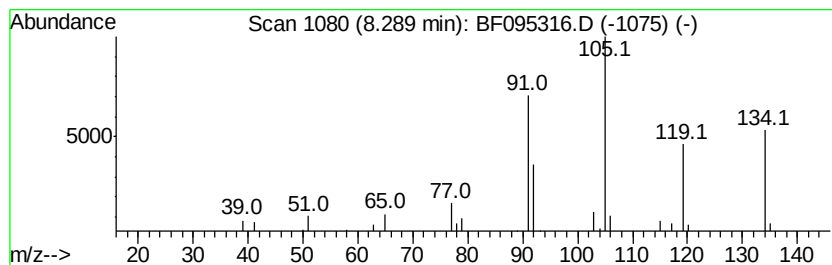
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Peak Number 6 Cycloheptane, 1,3,5-tris(me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	4.08 ng	89533	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloheptane, 1,3,5-tris(methyle...	134	C10H14	068284-24-2	76
2		Tetracyclo[3.3.1.1(1,8).0(2,4)]d...	134	C10H14	1000185-58-7	58
3		3a,6-Methano-3aH-indene, 2,3,4,5...	134	C10H14	098640-10-9	50
4		p-Isopropenylphenol	134	C9H10O	004286-23-1	49
5		Benzaldehyde, 3-ethyl-	134	C9H10O	034246-54-3	49



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Sample : I3157-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WEST

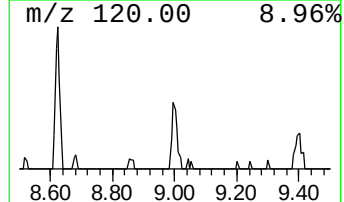
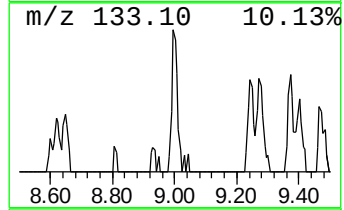
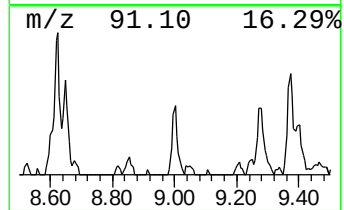
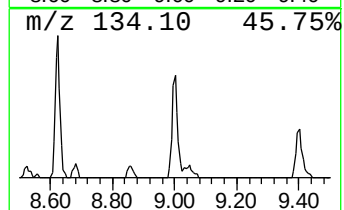
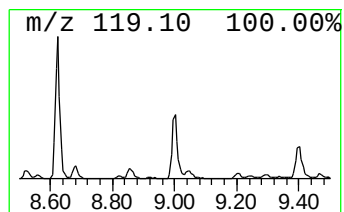
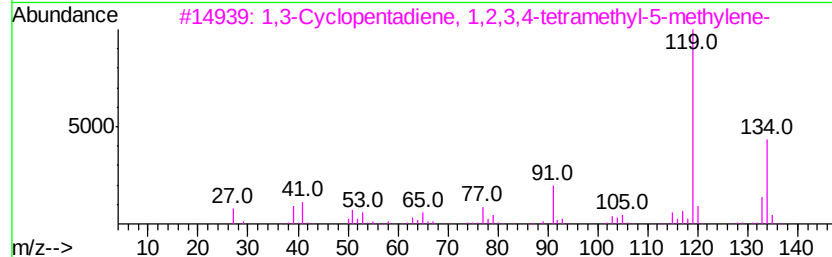
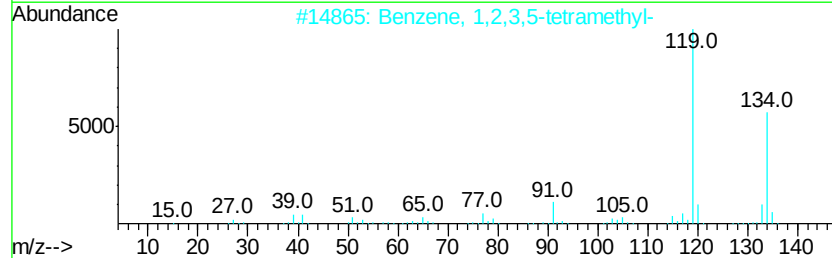
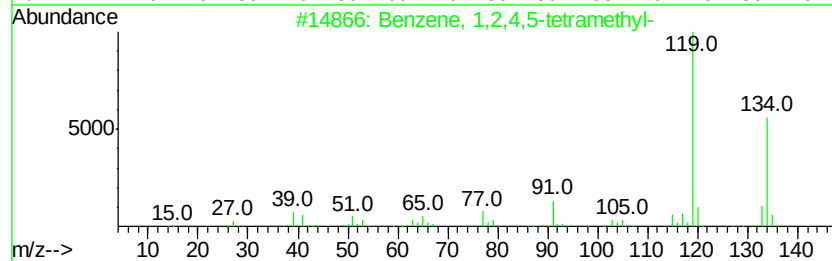
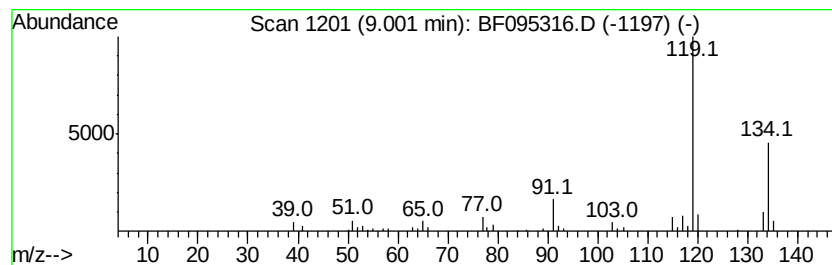
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.00	2.80 ng	89938	Napthalene-d8	9.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94
4		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
5		o-Cymene	134	C10H14	000527-84-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095316.D
Acq On : 22 May 2017 16:18
Operator : SJ/MA
Sample : I3157-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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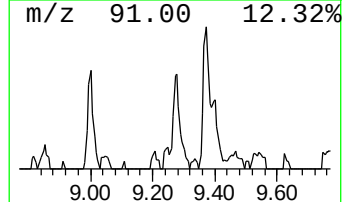
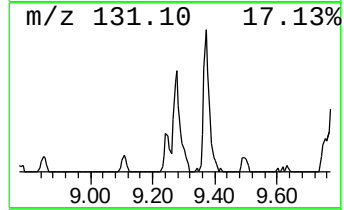
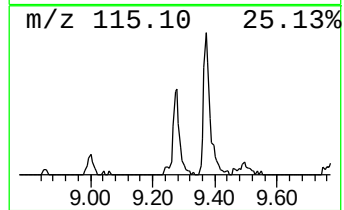
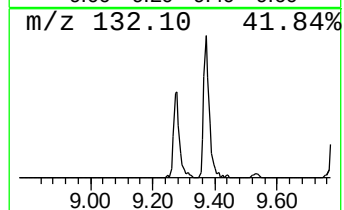
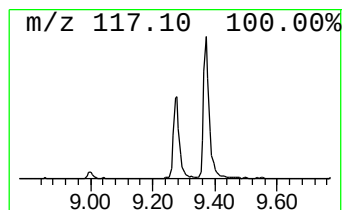
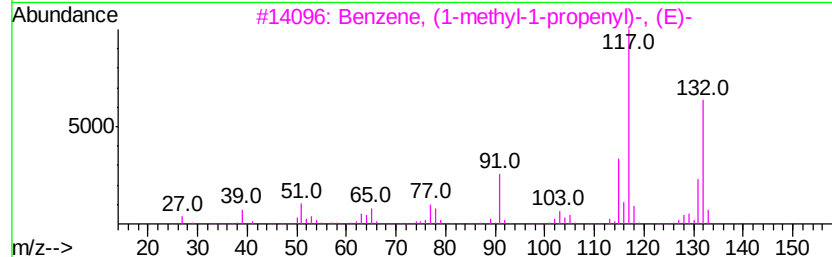
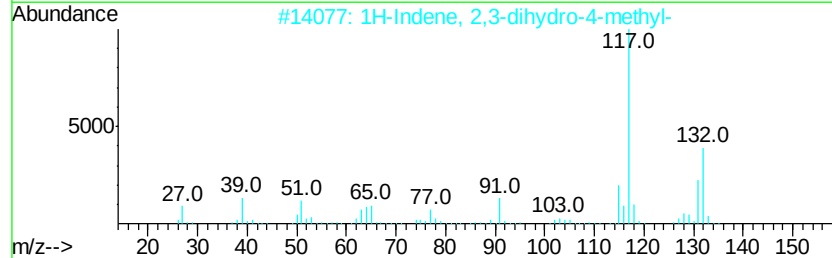
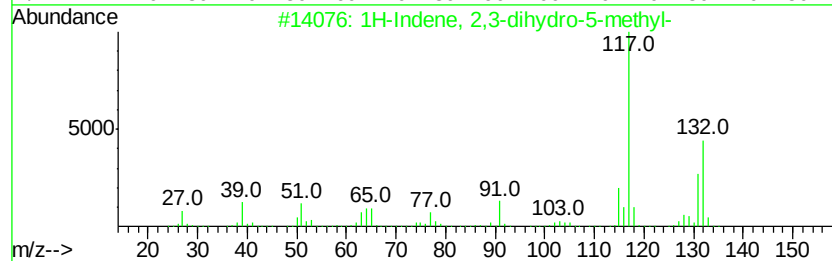
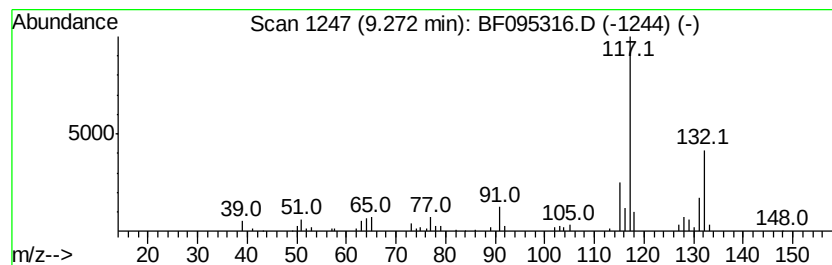
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	4.42 ng	142167	Napthalene-d8	9.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
2		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
4		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
Data File : BF095316.D
Acq On : 22 May 2017 16:18
Operator : SJ/MA
Sample : I3157-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WEST

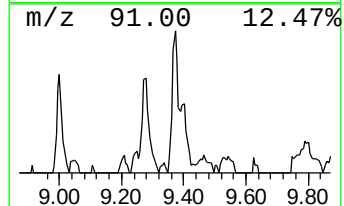
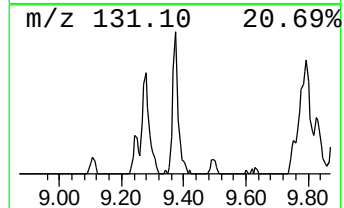
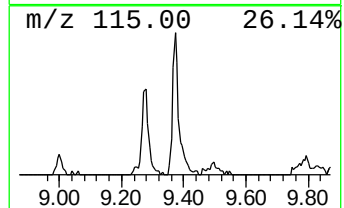
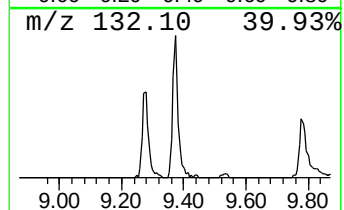
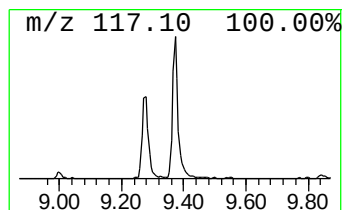
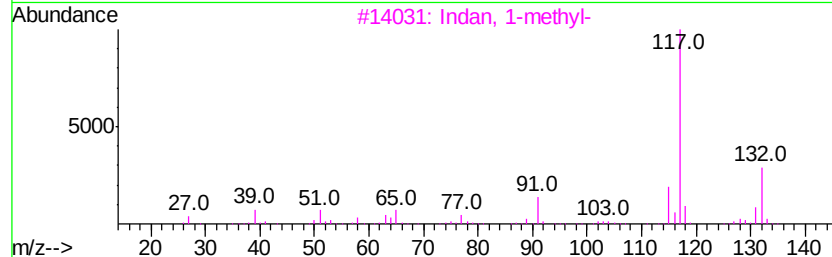
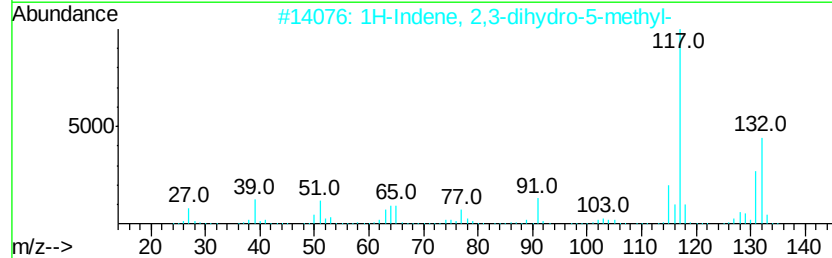
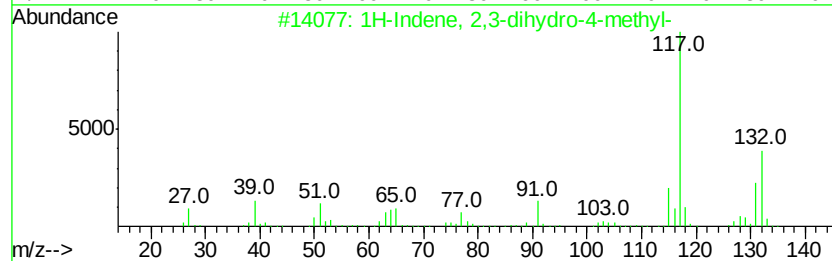
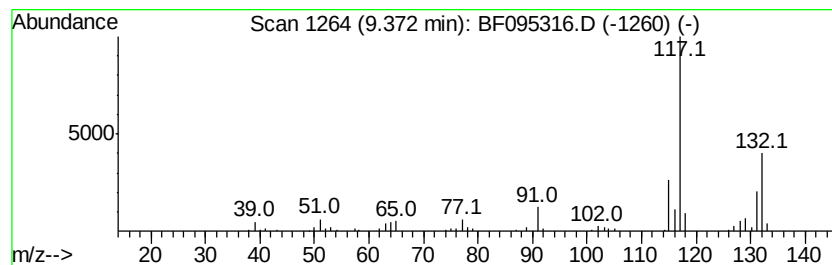
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.37	6.07 ng	195396	Napthalene-d8	9.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3		Indan, 1-methyl-	132	C10H12	000767-58-8	87
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	86
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
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Sample : I3157-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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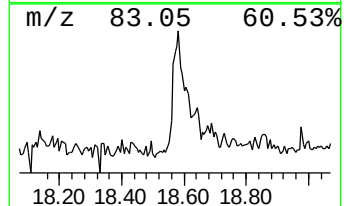
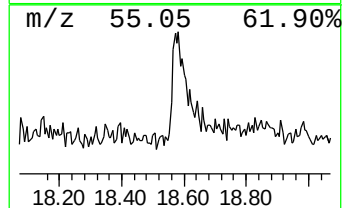
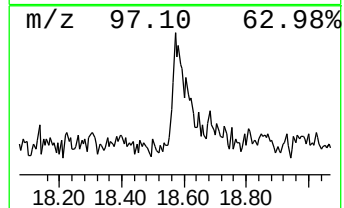
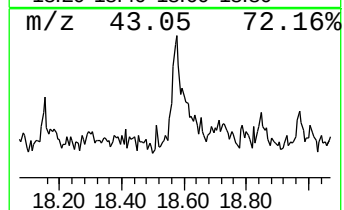
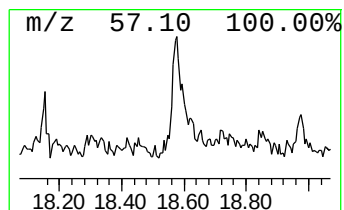
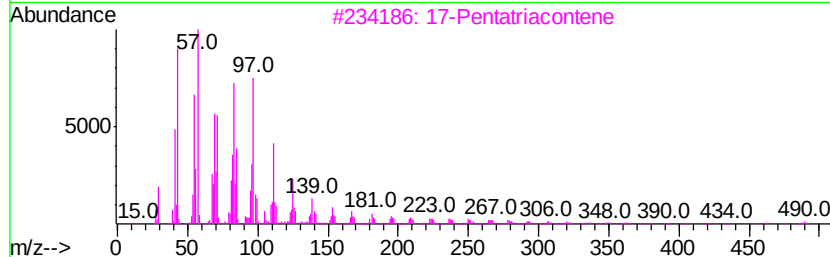
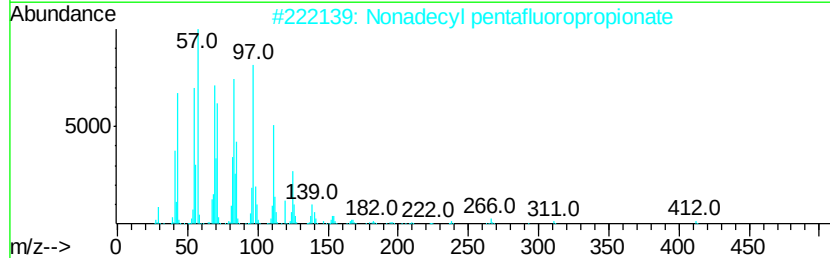
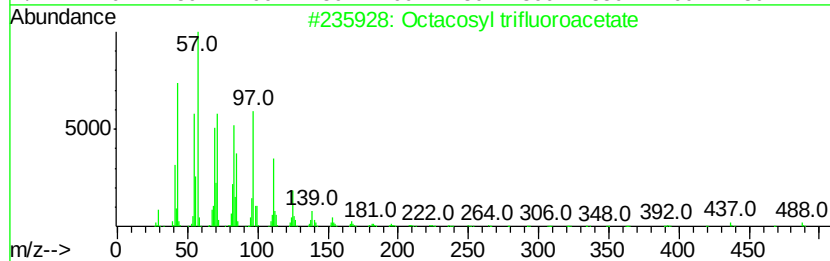
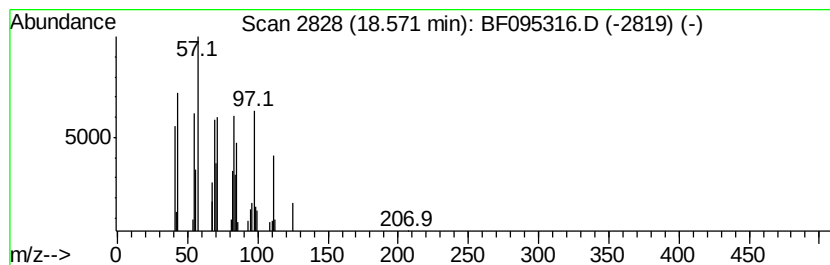
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	4.70 ng	129955	Chrysene-d12	18.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Tetracosyl heptafluorobutyrte	550	C28H49F7O2	1000351-83-7	87
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87



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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...	5.12	14.8	ng	323775	1	7.76	438671	20.0
Benzene, propyl-	6.94	7.6	ng	166767	1	7.76	438671	20.0
unknown7.42	7.42	116.3	ng	2552030	1	7.76	438671	20.0
Indane	8.03	15.1	ng	331141	1	7.76	438671	20.0
Cycloheptane, 1,3...	8.29	4.1	ng	89533	1	7.76	438671	20.0
Benzene, 1,2,4,5-...	9.00	2.8	ng	89938	2	9.78	643397	20.0
1H-Indene, 2,3-di...	9.27	4.4	ng	142167	2	9.78	643397	20.0
1H-Indene, 2,3-di...	9.37	6.1	ng	195396	2	9.78	643397	20.0
Octacosyl trifluo...	18.57	4.7	ng	129955	5	18.68	553224	20.0