

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
 Data File : BF077938.D
 Acq On : 25 Mar 2015 6:00
 Operator : TP/IZ
 Sample : G1615-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16-2

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-BF031115.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	1.264	31	33	36	rVB	1945513	2536289	67.79%	11.334%
2	1.550	56	58	65	rVB	83517	179136	4.79%	0.801%
3	1.641	65	66	74	rVV	508271	852012	22.77%	3.808%
4	1.767	74	77	97	rVB	1955801	3741165	100.00%	16.719%
5	4.864	346	348	355	rVB	95855	130277	3.48%	0.582%
6	5.401	393	395	398	rBV	761566	930371	24.87%	4.158%
7	6.693	506	508	511	rBV	802775	972962	26.01%	4.348%
8	6.830	518	520	523	rBV	1111593	1037229	27.72%	4.635%
9	7.116	543	545	548	rVB	287452	258441	6.91%	1.155%
10	7.299	559	561	564	rBV	757822	783779	20.95%	3.503%
11	7.813	603	606	608	rBV	719040	640263	17.11%	2.861%
12	8.693	681	683	686	rBV	414935	358232	9.58%	1.601%
13	10.042	799	801	803	rBV	1408251	1250685	33.43%	5.589%
14	10.545	843	845	848	rBV	45583	51362	1.37%	0.230%
15	10.865	871	873	875	rBV	437465	418831	11.20%	1.872%
16	11.836	956	958	961	rBV2	544333	728151	19.46%	3.254%
17	12.705	1031	1034	1035	rBV	312940	436795	11.68%	1.952%
18	12.728	1035	1036	1038	rVV	98113	77751	2.08%	0.347%
19	14.202	1163	1165	1167	rBV	195830	196672	5.26%	0.879%
20	14.477	1186	1189	1191	rBV	198162	212928	5.69%	0.952%
21	14.694	1205	1208	1211	rVB	1372110	1344504	35.94%	6.008%
22	14.900	1220	1226	1228	rBV2	31607	59135	1.58%	0.264%
23	15.025	1235	1237	1242	rVB2	33749	48759	1.30%	0.218%
24	15.528	1277	1281	1285	rVB3	18248	39908	1.07%	0.178%
25	15.894	1307	1313	1318	rBV2	93716	249453	6.67%	1.115%
26	15.985	1318	1321	1323	rVV2	457350	747731	19.99%	3.342%
27	16.020	1323	1324	1326	rVV	118998	132960	3.55%	0.594%
28	16.168	1334	1337	1340	rVV3	42320	58049	1.55%	0.259%
29	16.305	1346	1349	1353	rVB3	23962	47465	1.27%	0.212%
30	16.500	1364	1366	1368	rBV	25632	37836	1.01%	0.169%
31	16.660	1378	1380	1384	rVV2	35869	72766	1.95%	0.325%
32	17.128	1418	1421	1424	rVV4	20902	48677	1.30%	0.218%
33	17.323	1435	1438	1443	rBV	157728	394877	10.55%	1.765%
34	17.437	1446	1448	1451	rVB	33883	50353	1.35%	0.225%

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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-BF031115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.528	1454	1456	1459	rBV3	18573	39300	1.05%	0.176%
36	17.654	1464	1467	1470	rVB	83304	113788	3.04%	0.509%
37	17.711	1470	1472	1476	rBV	141812	188445	5.04%	0.842%
38	17.780	1476	1478	1483	rBV	421566	592358	15.83%	2.647%
39	17.940	1490	1492	1496	rBV4	20851	46220	1.24%	0.207%
40	18.363	1527	1529	1532	rVB	26130	39663	1.06%	0.177%
41	18.877	1572	1574	1580	rVB	50883	102372	2.74%	0.457%
42	19.163	1596	1599	1605	rVB2	69498	161704	4.32%	0.723%
43	19.346	1611	1615	1622	rBV	623250	1367957	36.57%	6.113%
44	19.563	1631	1634	1638	rVB	52013	101702	2.72%	0.454%
45	19.654	1638	1642	1647	rVB4	113589	249540	6.67%	1.115%
46	20.100	1677	1681	1686	rVB2	98716	248049	6.63%	1.109%

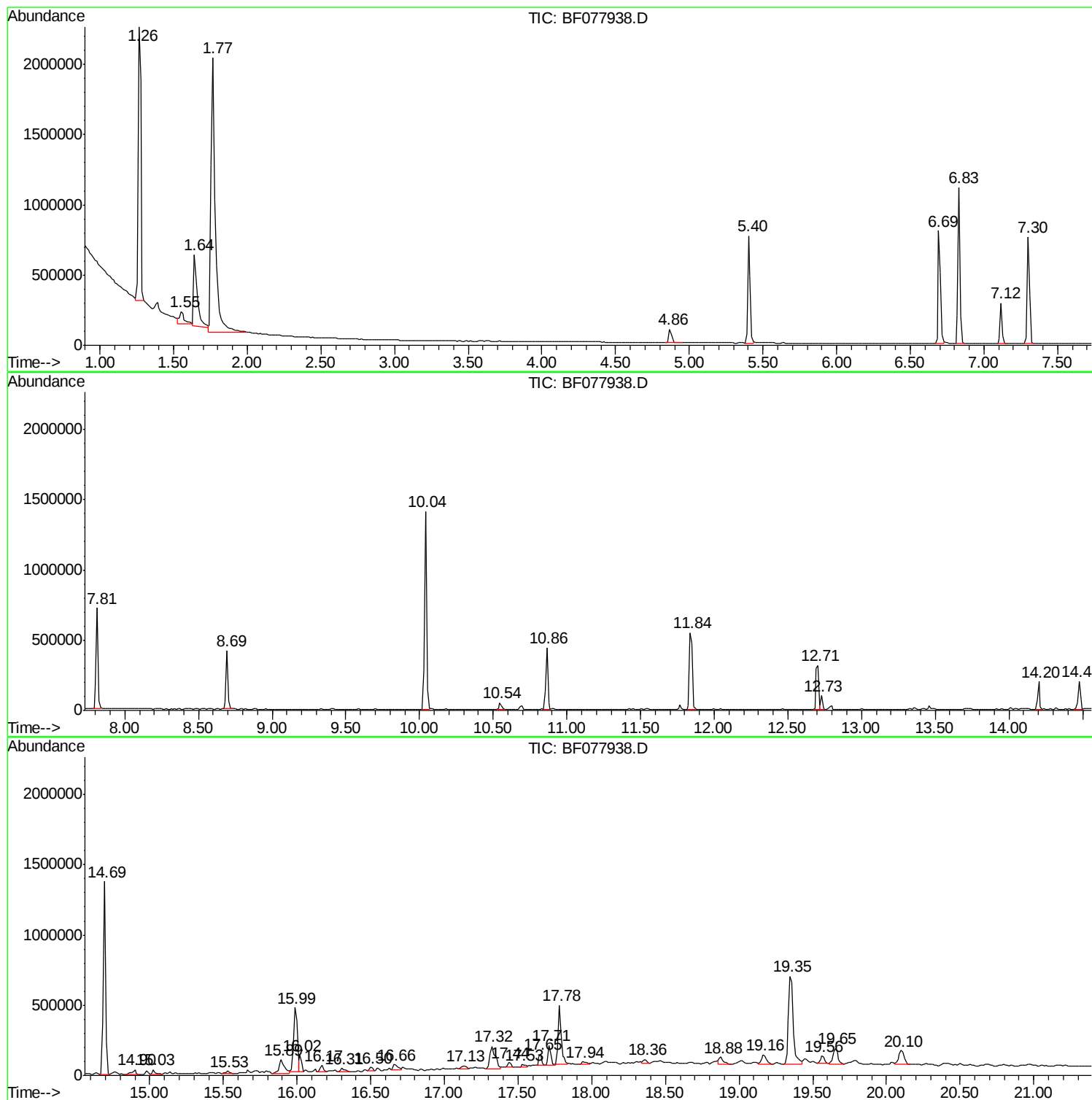
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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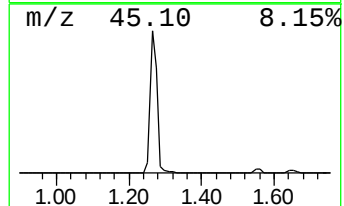
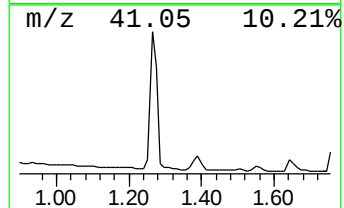
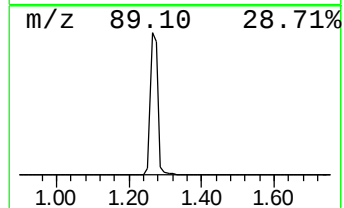
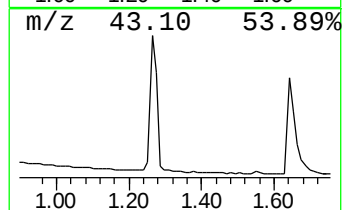
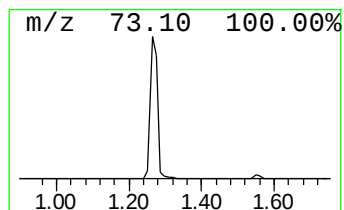
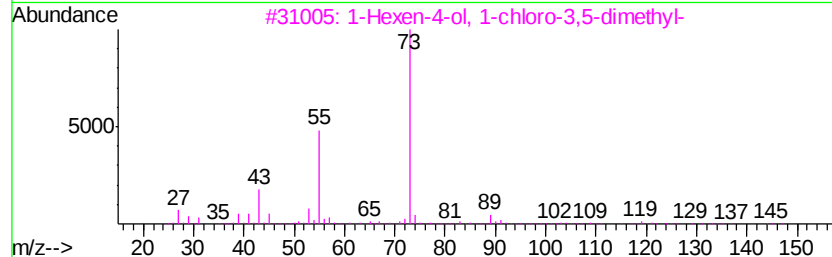
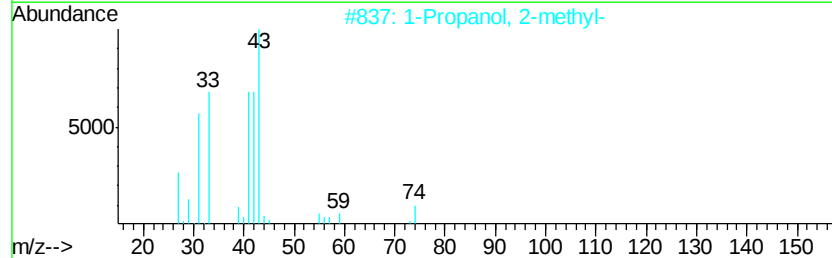
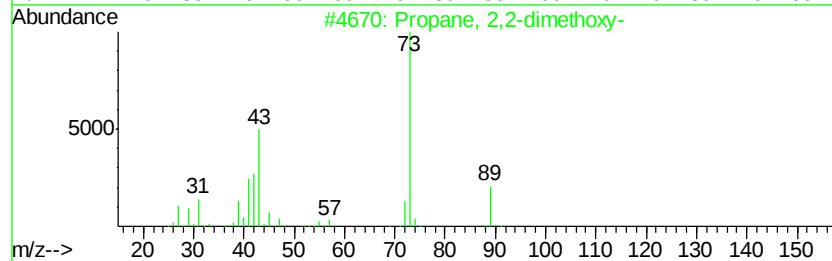
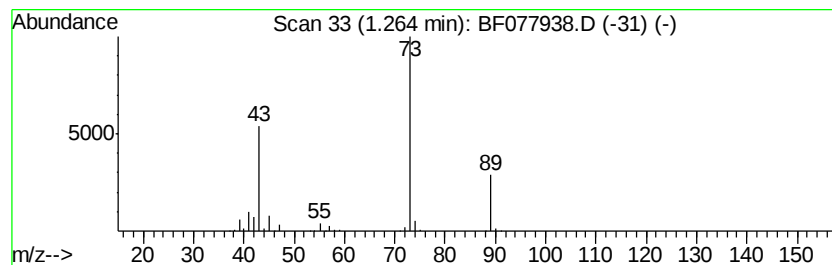
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	196.28 ng	2536290	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9



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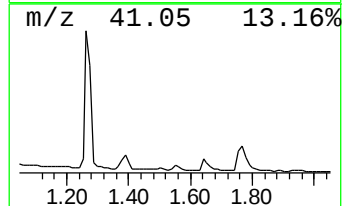
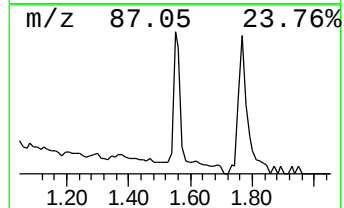
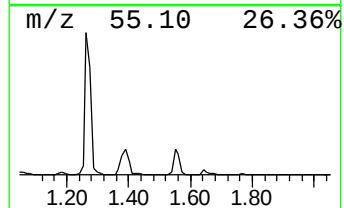
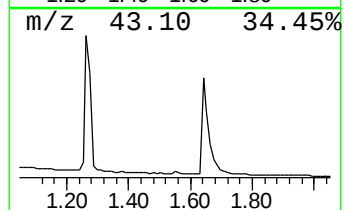
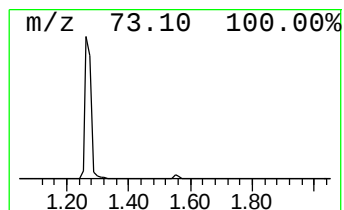
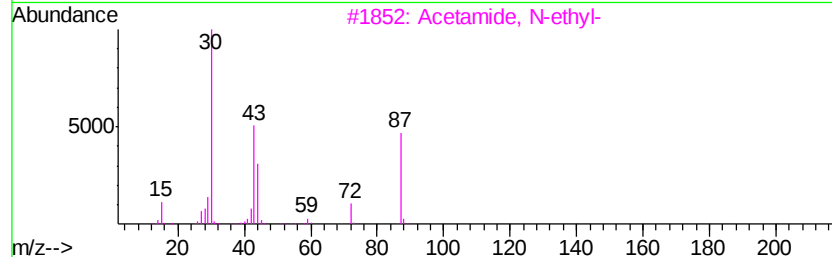
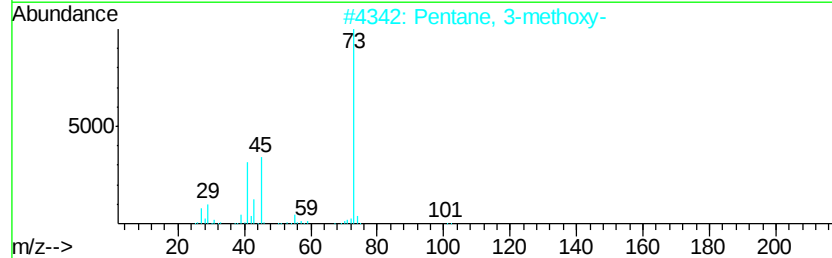
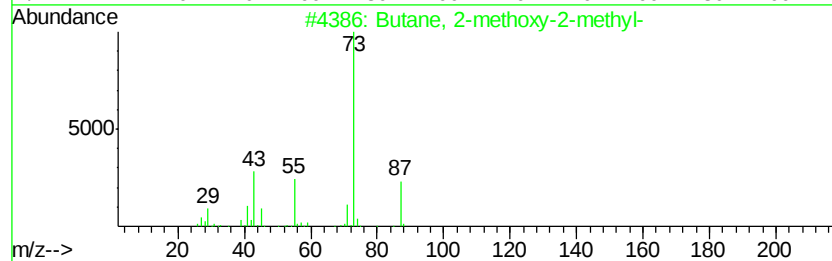
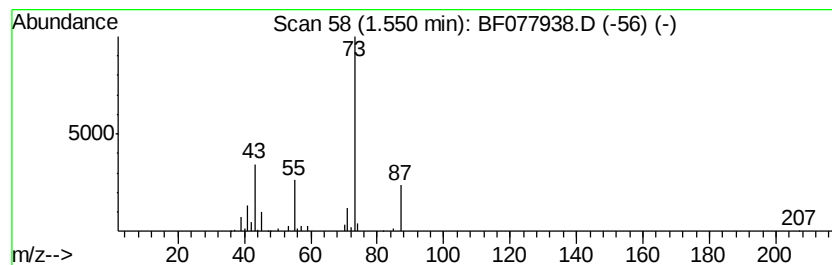
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	13.86 ng	179136	1,4-Dichlorobenzene-d4	7.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78	
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12	
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9	
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9	
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9	



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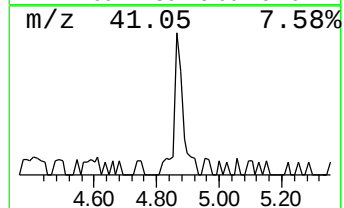
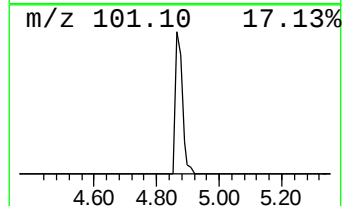
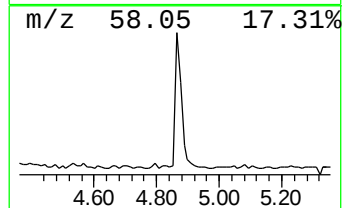
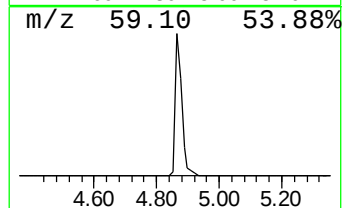
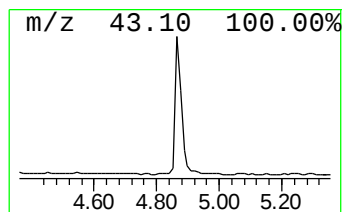
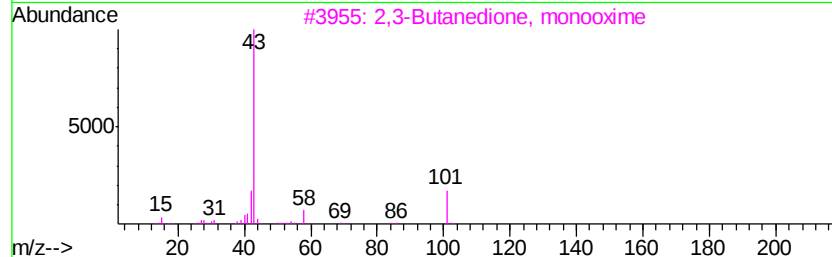
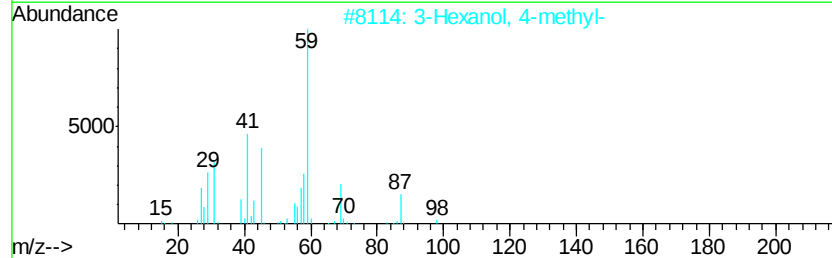
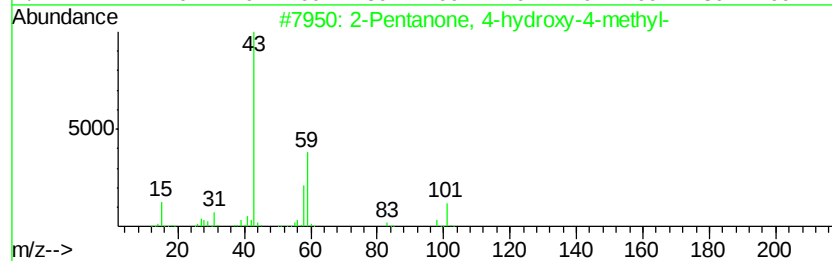
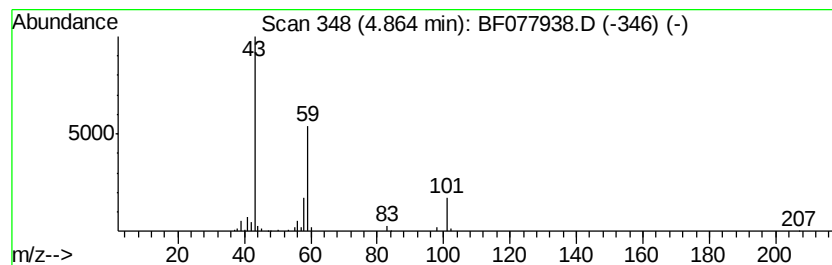
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	10.08 ng	130277	1,4-Dichlorobenzene-d4	7.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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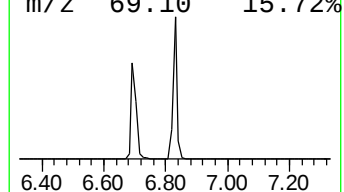
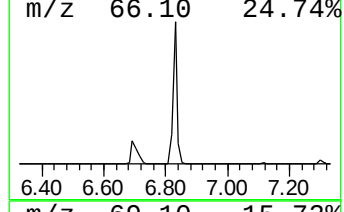
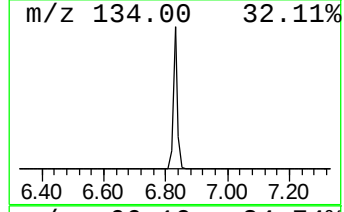
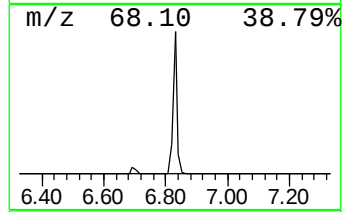
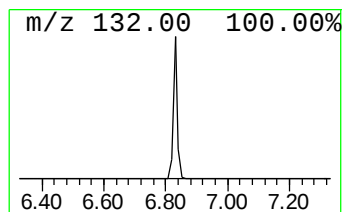
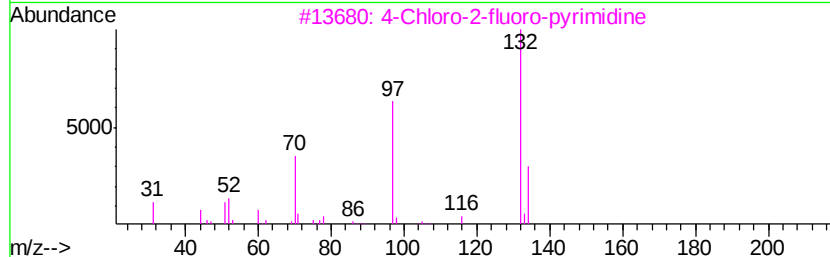
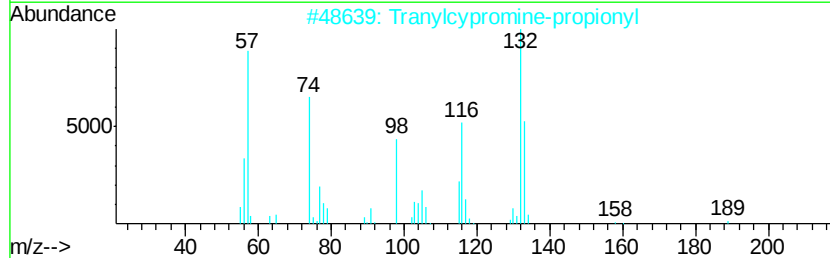
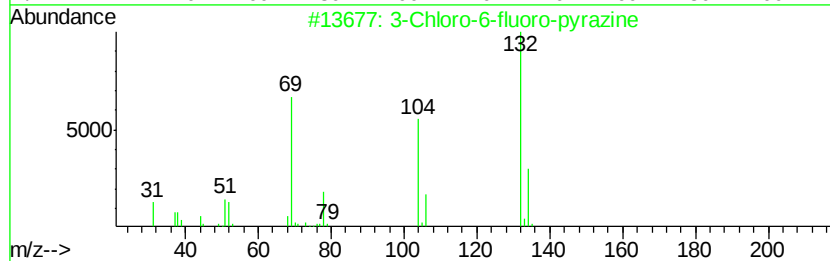
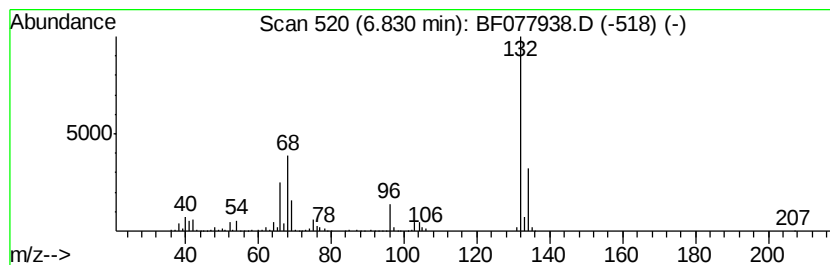
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.83 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	80.27 ng	1037230	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranlylcypropine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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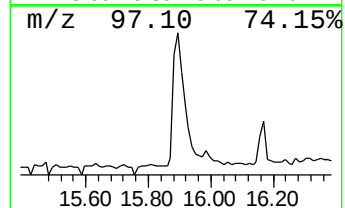
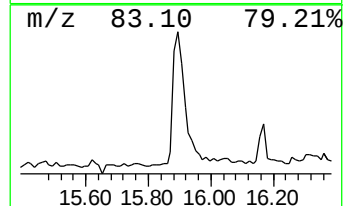
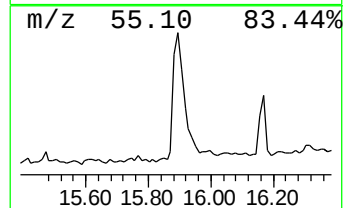
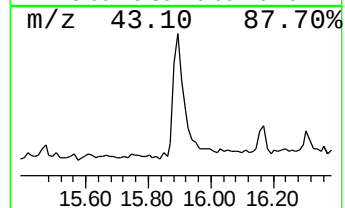
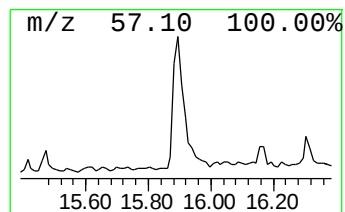
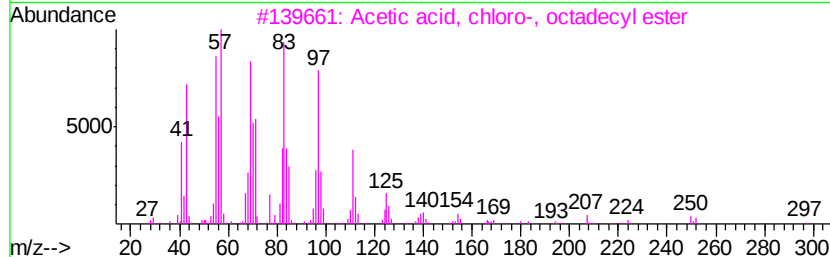
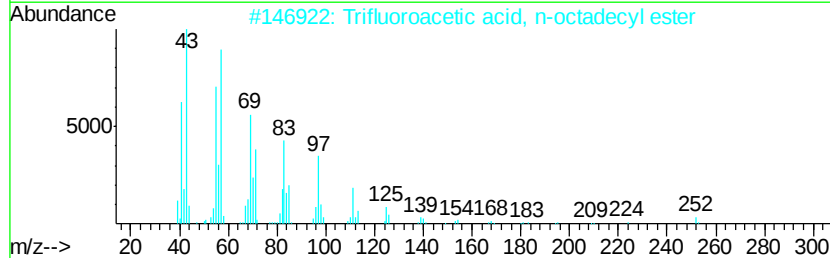
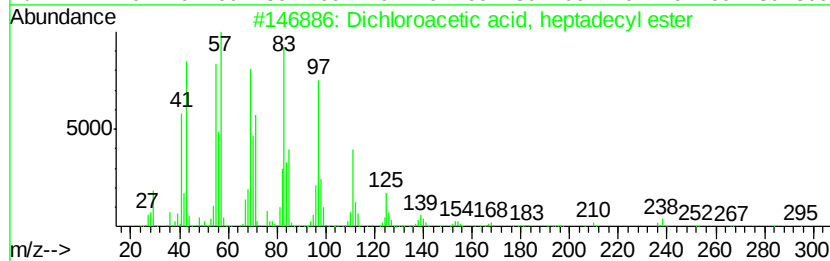
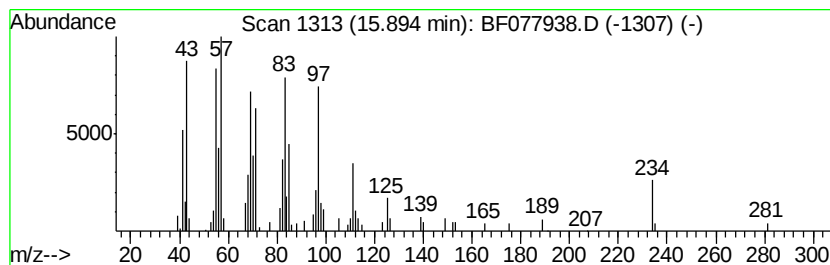
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	6.67 ng	249453	Chrysene-d12	16.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
3		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	83
4		17-Pentatriacontene	491	C35H70	006971-40-0	80
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077938.D
Acq On : 25 Mar 2015 6:00
Operator : TP/IZ
Sample : G1615-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-2

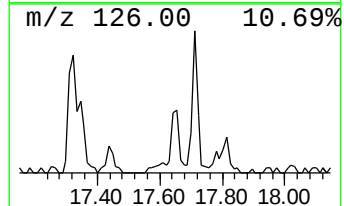
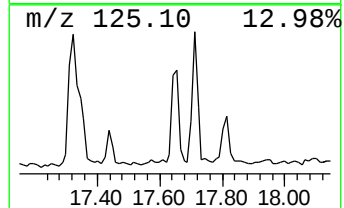
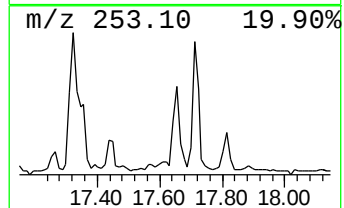
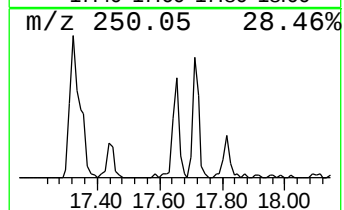
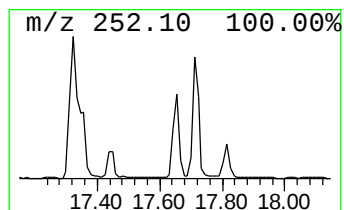
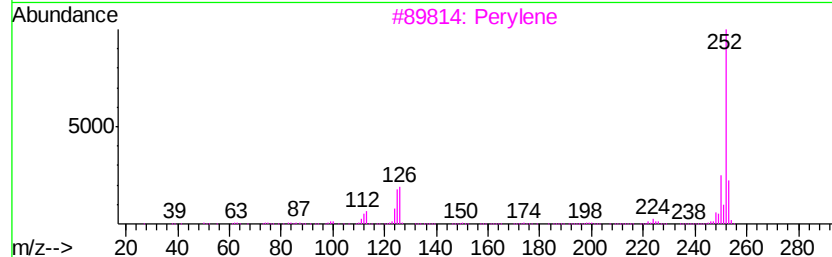
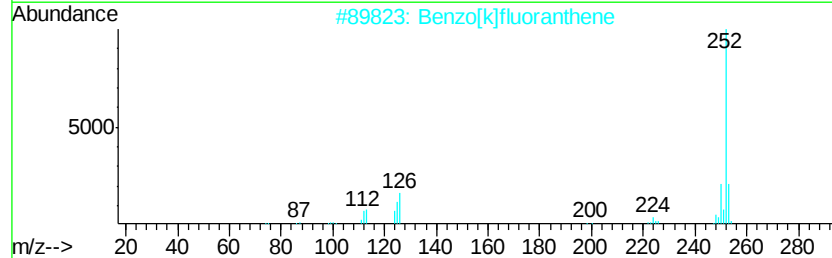
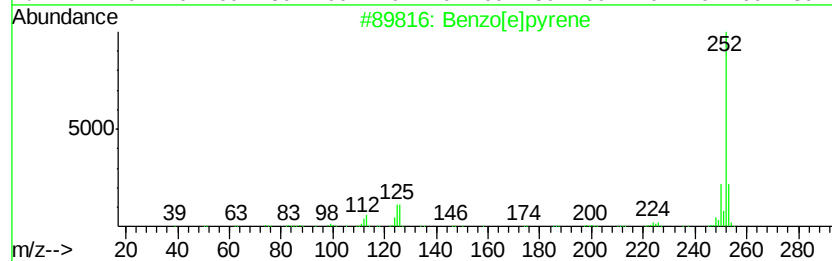
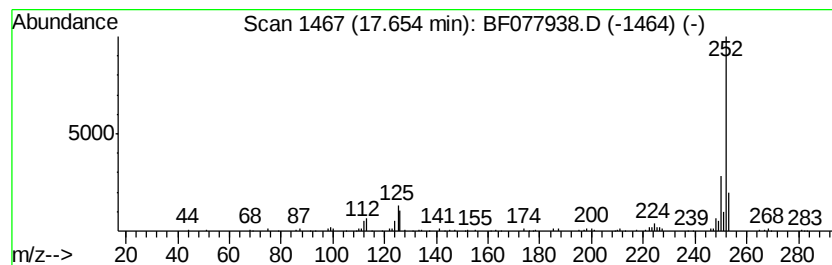
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.65	3.84 ng	113788	Perylene-d12	17.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3		Perylene	252	C20H12	000198-55-0	95
4		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



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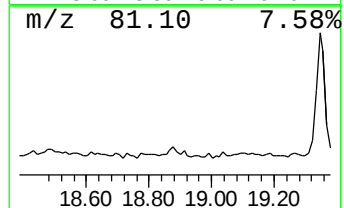
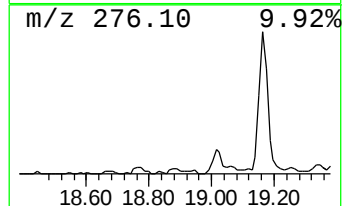
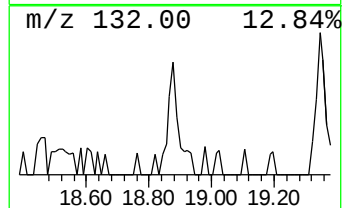
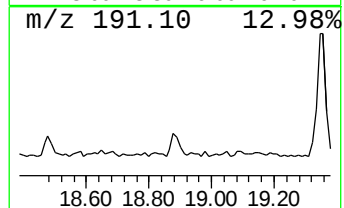
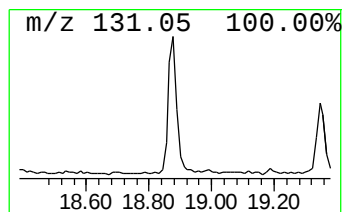
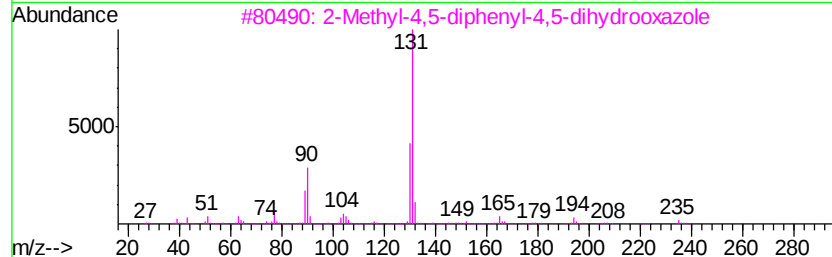
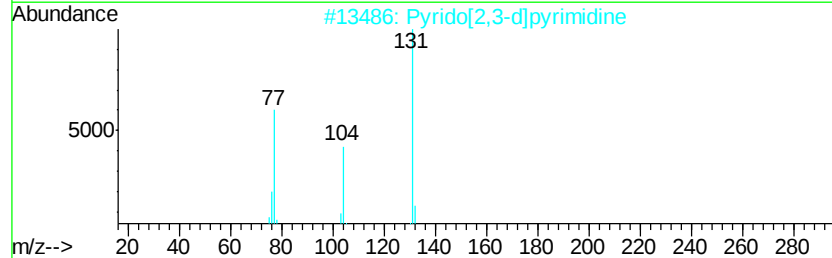
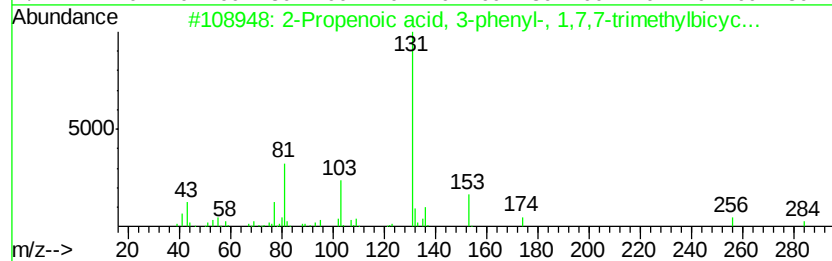
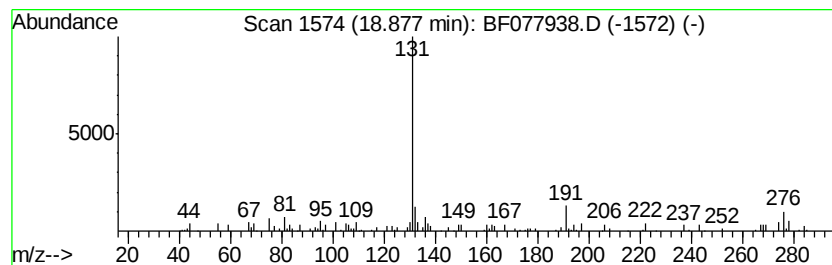
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Propenoic acid, 3-phenyl-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.88	3.46 ng	102372	Perylene-d12	17.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 3-phenyl-, 1,7...	284	C19H24O2	006330-67-2	50
2		Pyrido[2,3-d]pyrimidine	131	C7H5N3	000254-61-5	40
3		2-Methyl-4,5-diphenyl-4,5-dihydr...	237	C16H15NO	133649-09-9	36
4		2-Methyl-1,3-bis(trimethylsiloxy...	262	C12H30O2Si2	122424-36-6	33
5		Silane, [1-(5-ethenyltetrahydro-...	242	C13H26O2Si	057428-80-5	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077938.D
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Operator : TP/IZ
Sample : G1615-04
Misc :
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BNA_F
ClientSampleId :
SB-16-2

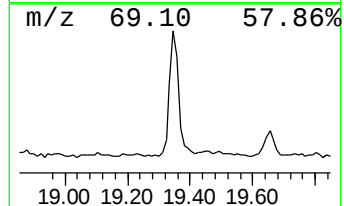
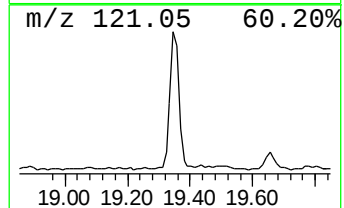
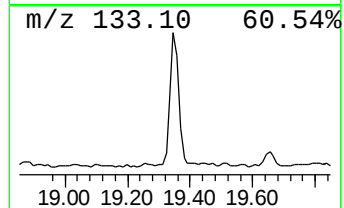
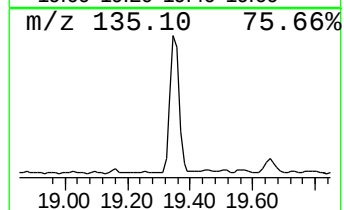
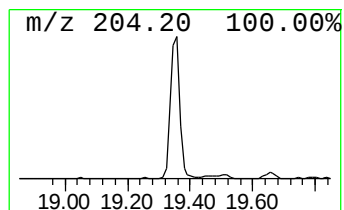
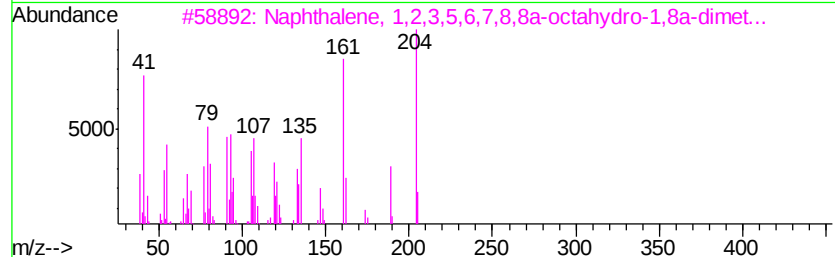
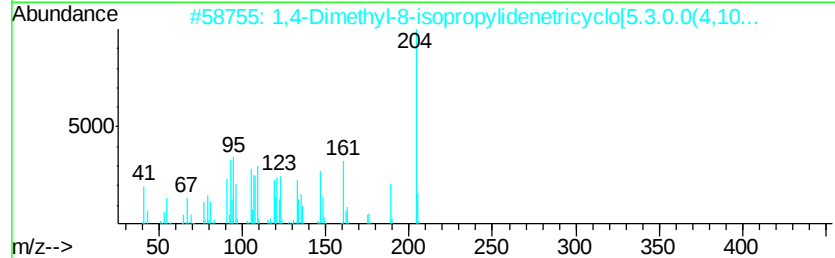
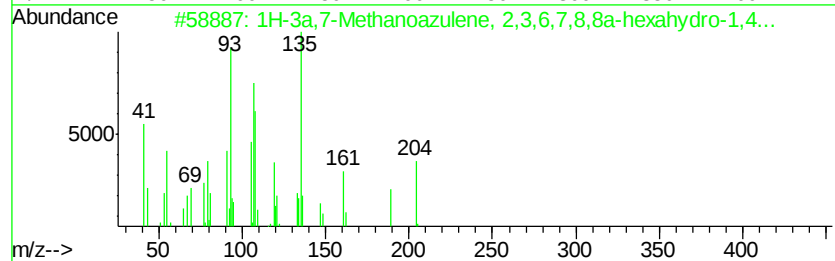
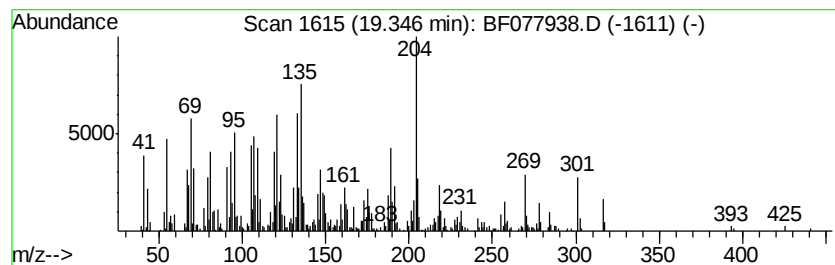
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	46.19 ng	1367960	Perylene-d12	17.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	58
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	46
3		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	46
4		Guaia-3,9-diene	204	C15H24	000489-83-8	43
5		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H200	124957-09-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
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Sample : G1615-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

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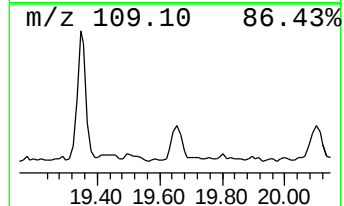
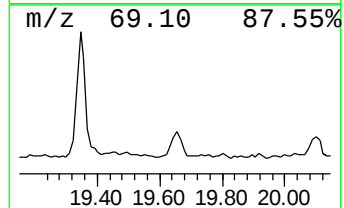
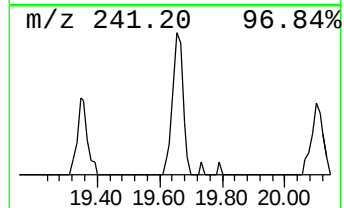
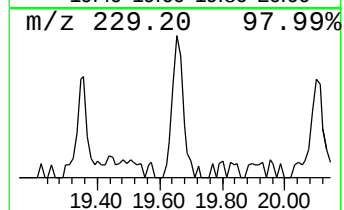
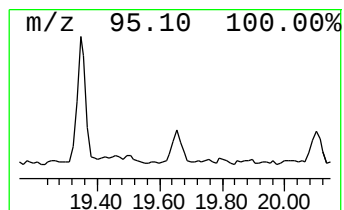
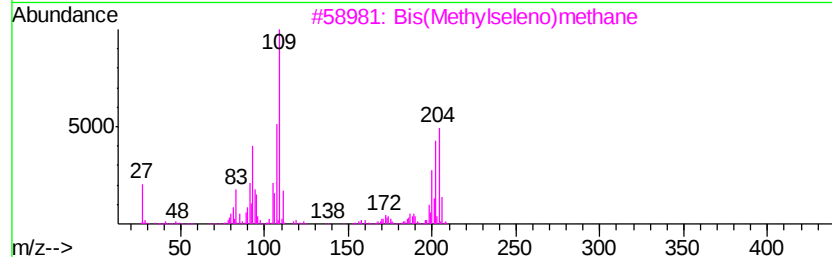
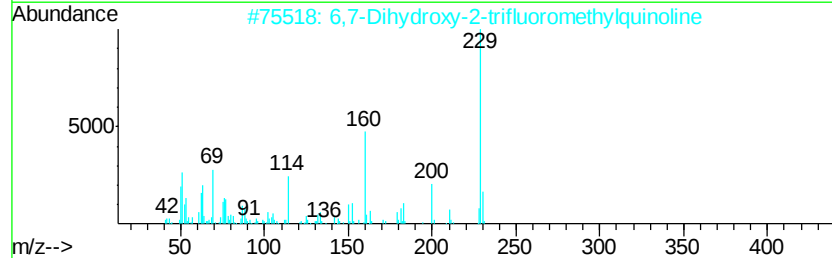
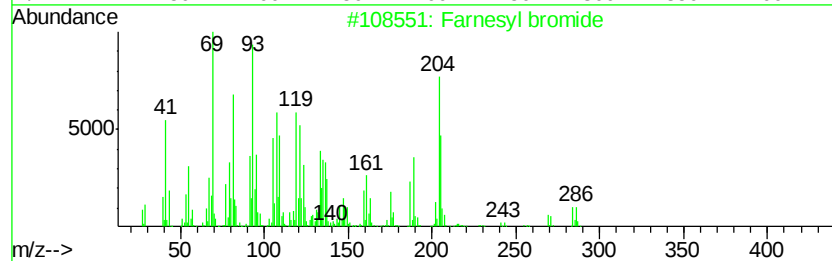
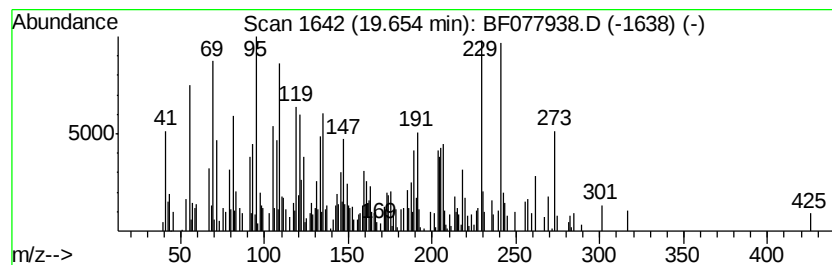
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown19.65 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.65	8.43 ng	249540	Perylene-d12	17.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Farnesyl bromide	284	C15H25Br	006874-67-5	41
2		6,7-Dihydroxy-2-trifluoromethylq...	229	C10H6F3N02	041192-79-4	15
3		Bis(Methylseleno)methane	204	C3H8Se2	056051-03-7	15
4		2-Butyl-3-methyl-5-(2-methylprop...	222	C15H26O	1000281-10-7	15
5		Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	15



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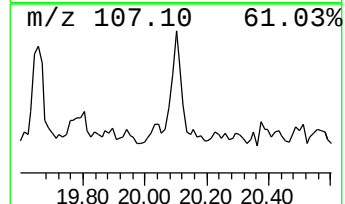
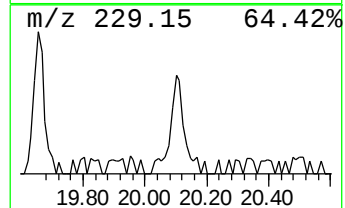
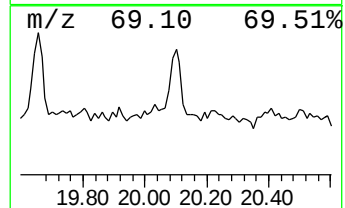
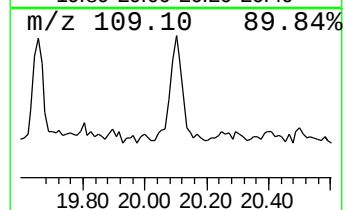
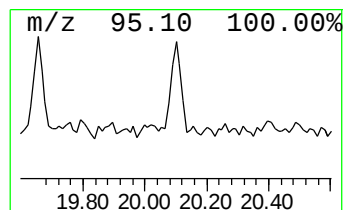
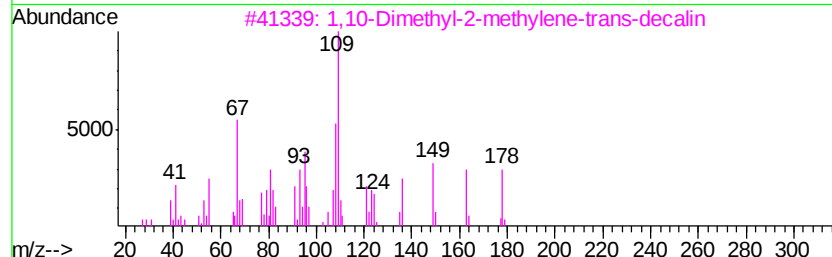
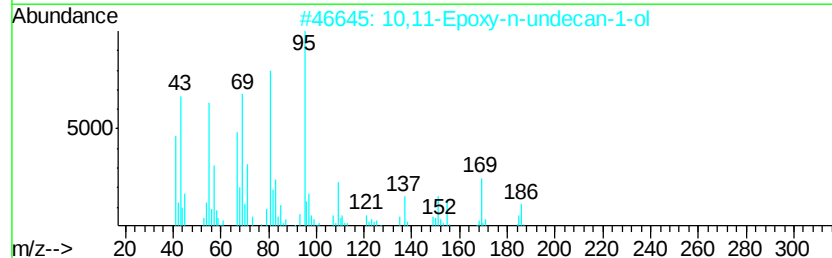
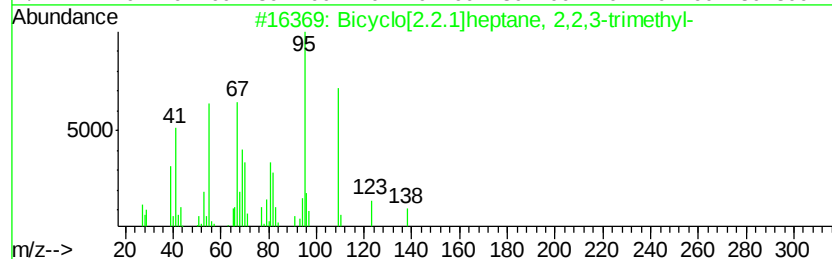
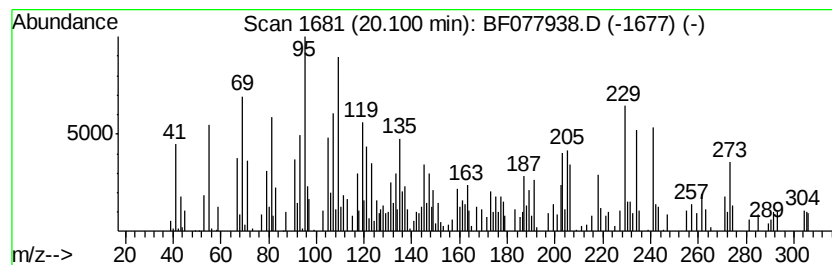
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown20.10 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.10	8.37 ng	248049	Perylene-d12	17.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25
2			10,11-Epoxy-n-undecan-1-ol	186	C11H22O2	015764-66-6	25
3			1,10-Dimethyl-2-methylene-trans-...	178	C13H22	1000103-97-8	15
4			1-Chloro-1-ethyl-3-methyl-1-germ...	206	C7H13ClGe	026311-76-2	15
5			Imidazole-5-propenoic acid, 2-[4...	274	C13H11FN4O2	1000129-48-0	15



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.26	196.3	ng	2536290	1	7.12	258441	20.0
Butane, 2-methoxy...	1.55	13.9	ng	179136	1	7.12	258441	20.0
2-Pentanone, 4-hy...	4.86	10.1	ng	130277	1	7.12	258441	20.0
unknown6.83	6.83	80.3	ng	1037230	1	7.12	258441	20.0
Dichloroacetic ac...	15.89	6.7	ng	249453	5	16.00	747731	20.0
Benzo[e]pyrene	17.65	3.8	ng	113788	6	17.78	592358	20.0
2-Propenoic acid, ...	18.88	3.5	ng	102372	6	17.78	592358	20.0
1H-3a,7-Methanoaz...	19.35	46.2	ng	1367960	6	17.78	592358	20.0
unknown19.65	19.65	8.4	ng	249540	6	17.78	592358	20.0
unknown20.10	20.10	8.4	ng	248049	6	17.78	592358	20.0