

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021315\
 Data File : BF077316.D
 Acq On : 13 Feb 2015 19:41
 Operator : TP/IZ
 Sample : G1294-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1003-20(0-2)

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-BF021215.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	1.275	32	34	38	rBV	20904	41213	4.69%	0.480%
2	1.333	38	39	49	rVB	162860	292157	33.27%	3.405%
3	3.481	224	227	240	rBV	73822	221020	25.17%	2.576%
4	4.487	313	315	336	rBV	274370	695977	79.24%	8.112%
5	5.379	390	393	398	rBB	3968	9531	1.09%	0.111%
6	6.922	526	528	531	rBV	372305	615790	70.11%	7.178%
7	6.990	531	534	548	rVB	454974	878266	100.00%	10.237%
8	7.505	576	579	588	rBB	83520	166416	18.95%	1.940%
9	7.813	603	606	618	rBB	334376	563839	64.20%	6.572%
10	8.808	690	693	711	rBV	265282	455482	51.86%	5.309%
11	10.408	830	833	842	rBV	138001	237583	27.05%	2.769%
12	11.905	962	964	968	rBV	12840	26224	2.99%	0.306%
13	13.059	1062	1065	1069	rBV	532828	845580	96.28%	9.856%
14	14.145	1157	1160	1166	rBB	27574	46231	5.26%	0.539%
15	14.522	1190	1193	1199	rBB	147327	257253	29.29%	2.999%
16	15.860	1307	1310	1313	rVB	12883	21771	2.48%	0.254%
17	16.237	1340	1343	1346	rBV	69874	117605	13.39%	1.371%
18	16.294	1346	1348	1356	rVB	315603	455240	51.83%	5.306%
19	16.808	1390	1393	1398	rBV2	6965	15909	1.81%	0.185%
20	17.426	1445	1447	1450	rBV	172875	251428	28.63%	2.931%
21	17.551	1456	1458	1463	rVB	4169	9327	1.06%	0.109%
22	17.631	1463	1465	1468	rVB	6954	9766	1.11%	0.114%
23	18.134	1505	1509	1511	rBV	7128	11841	1.35%	0.138%
24	18.477	1535	1539	1541	rBV3	4358	9365	1.07%	0.109%
25	19.140	1595	1597	1599	rVB	14967	18871	2.15%	0.220%
26	19.414	1619	1621	1624	rVB	17511	26257	2.99%	0.306%
27	19.689	1642	1645	1648	rBV	752418	828290	94.31%	9.655%
28	20.123	1679	1683	1685	rBV4	7159	16876	1.92%	0.197%
29	20.352	1701	1703	1706	rBV	41969	61346	6.98%	0.715%
30	20.512	1713	1717	1718	rBV4	4770	9015	1.03%	0.105%
31	20.557	1718	1721	1723	rVV	9198	13768	1.57%	0.160%
32	20.946	1752	1755	1762	rBV	297215	428168	48.75%	4.991%
33	21.095	1767	1768	1770	rVV	7659	10101	1.15%	0.118%
34	21.163	1770	1774	1776	rVV5	7469	15796	1.80%	0.184%

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Instrument :
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ClientSampleId :
1003-20(0-2)

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-BF021215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.357	1788	1791	1793	rBV	18531	28049	3.19%	0.327%
36	21.563	1807	1809	1810	rBV2	8266	12016	1.37%	0.140%
37	21.643	1814	1816	1817	rBV2	11202	16860	1.92%	0.197%
38	21.746	1823	1825	1830	rVB5	26190	47005	5.35%	0.548%
39	22.112	1854	1857	1860	rVB3	17882	33832	3.85%	0.394%
40	22.466	1886	1888	1890	rBV2	34712	44807	5.10%	0.522%
41	22.535	1890	1894	1896	rBV4	17678	45831	5.22%	0.534%
42	22.580	1896	1898	1901	rBV	210772	255813	29.13%	2.982%
43	22.820	1917	1919	1922	rBV2	27511	57799	6.58%	0.674%
44	23.163	1946	1949	1952	rBV3	69657	146863	16.72%	1.712%
45	23.461	1972	1975	1977	rBV2	50127	94863	10.80%	1.106%
46	23.518	1978	1980	1985	rVB2	31600	79827	9.09%	0.930%
47	26.661	2253	2255	2260	rBV5	12926	32238	3.67%	0.376%

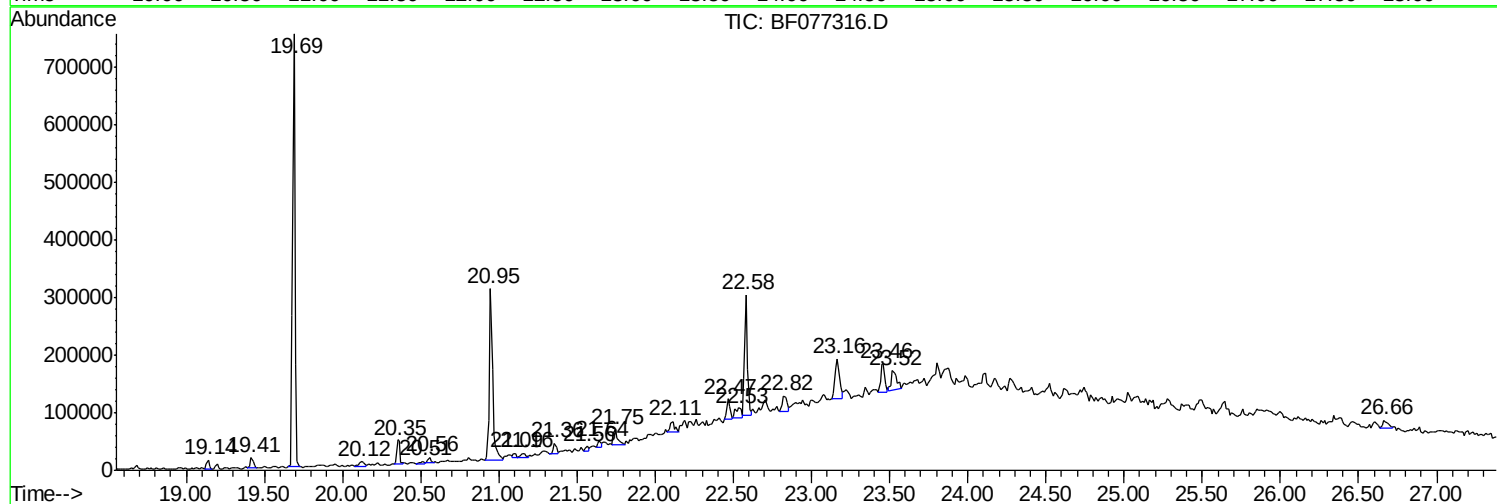
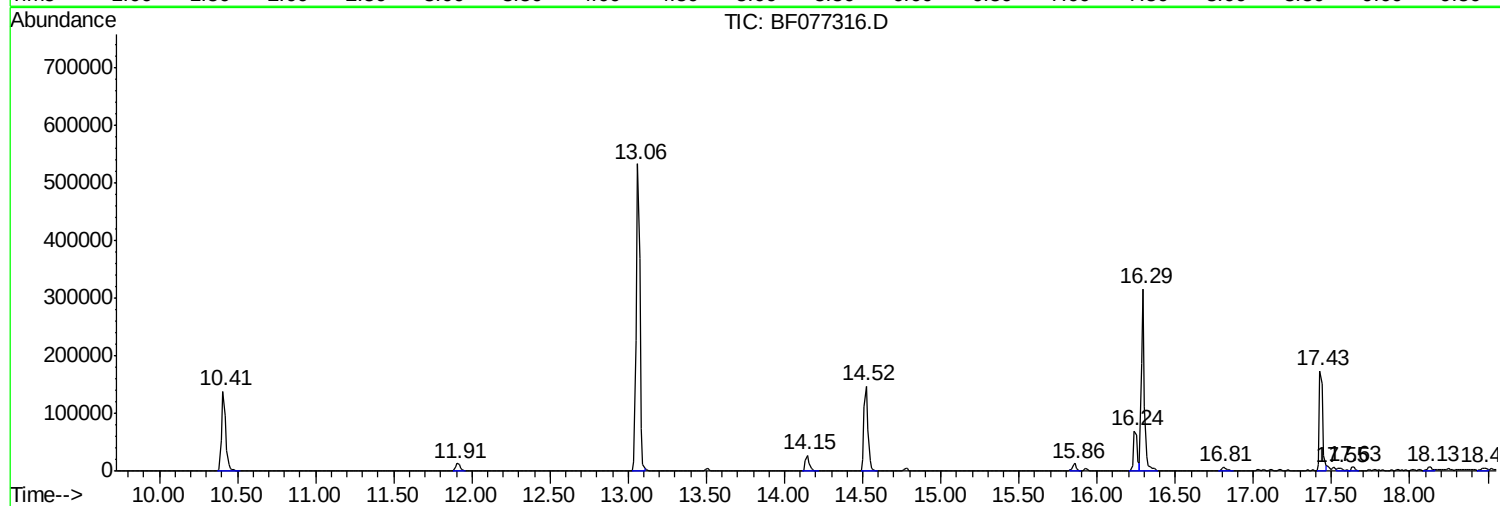
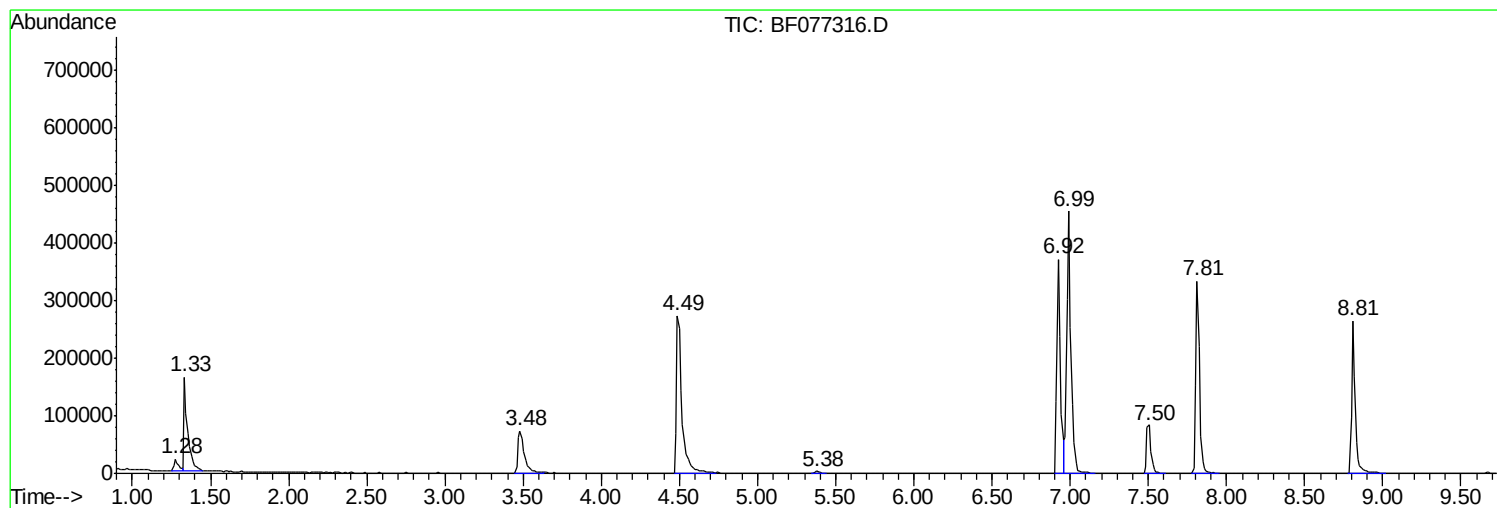
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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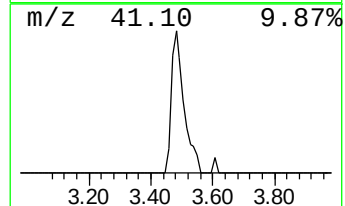
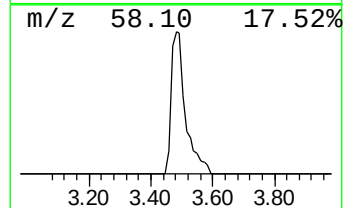
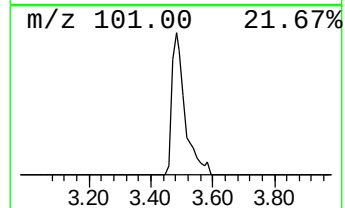
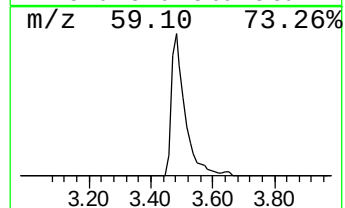
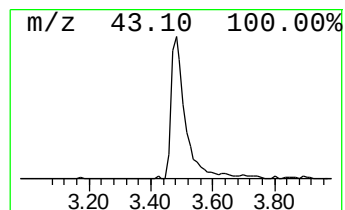
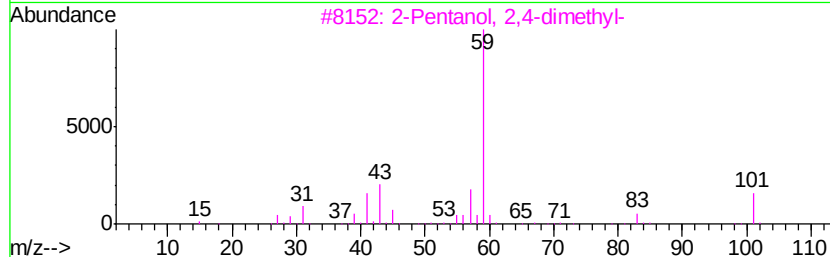
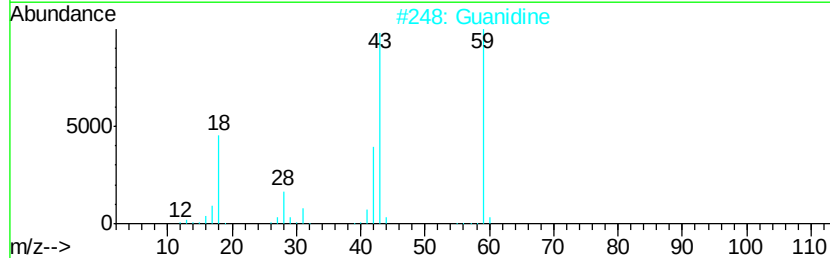
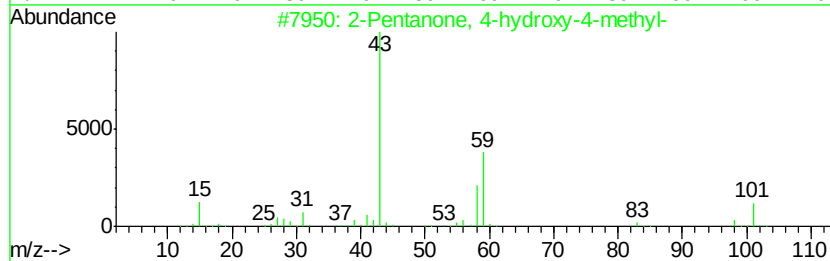
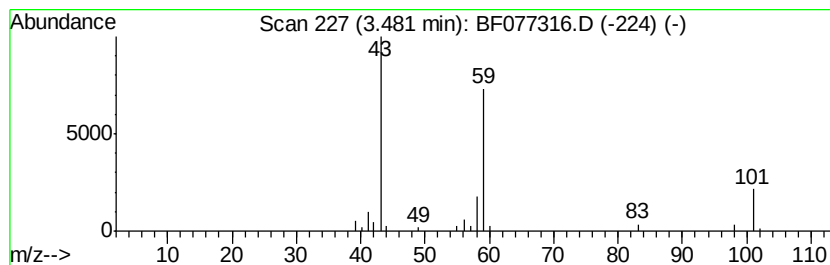
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.48	26.56 ng	221020	1,4-Dichlorobenzene-d4	7.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	50
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	39
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28



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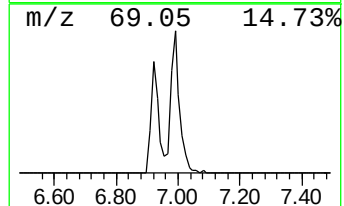
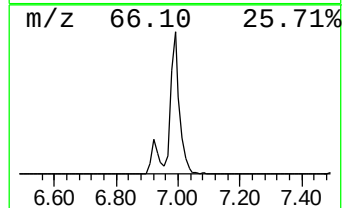
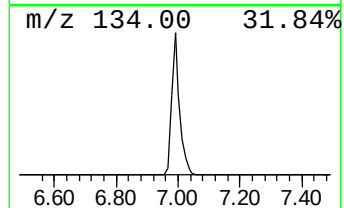
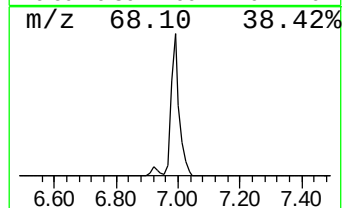
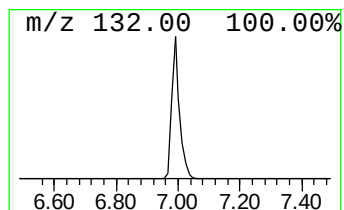
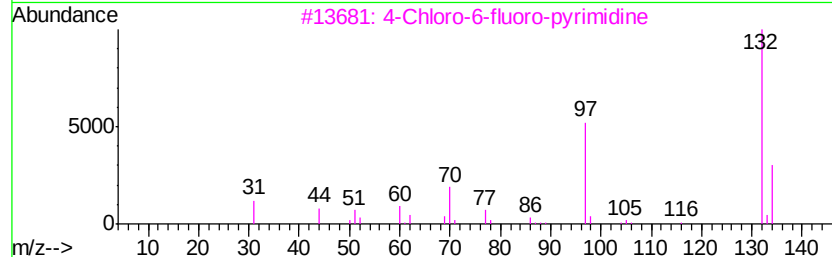
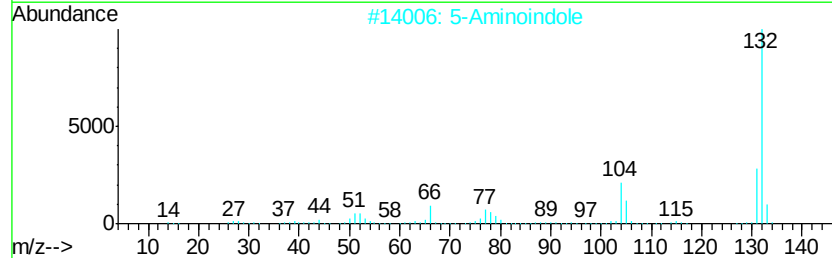
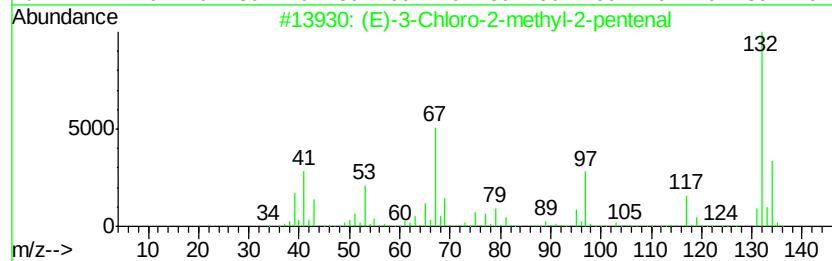
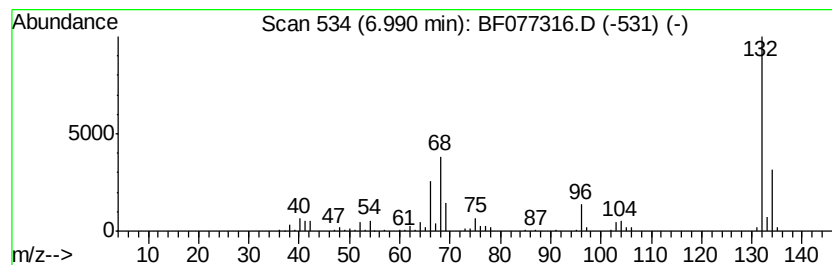
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	105.55 ng	878266	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	10
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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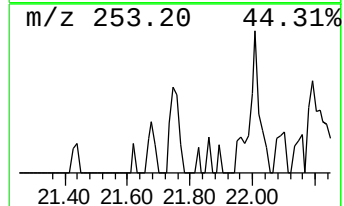
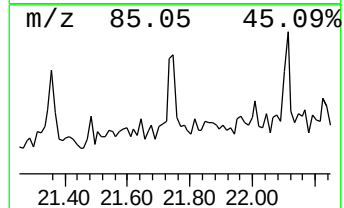
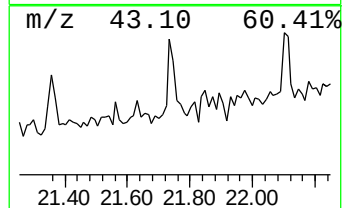
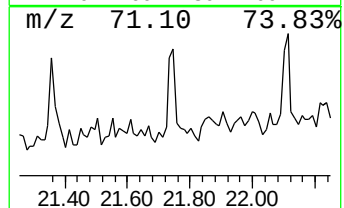
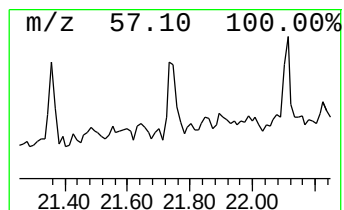
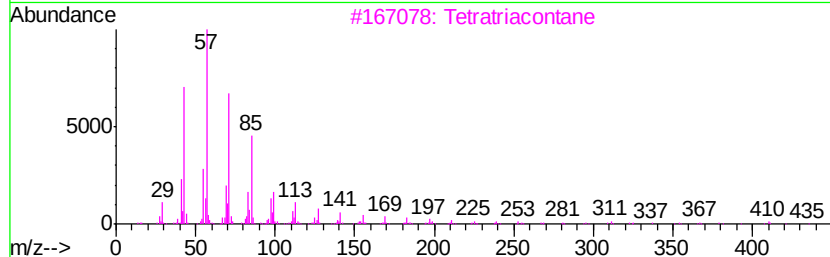
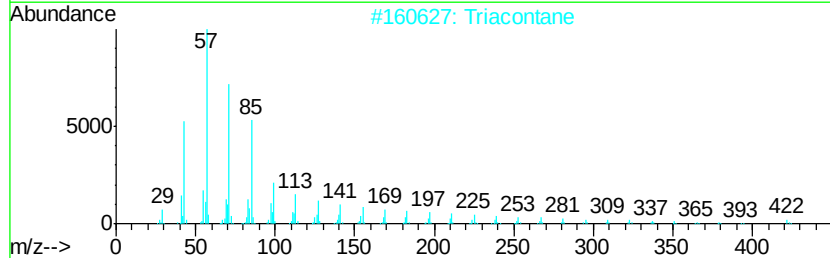
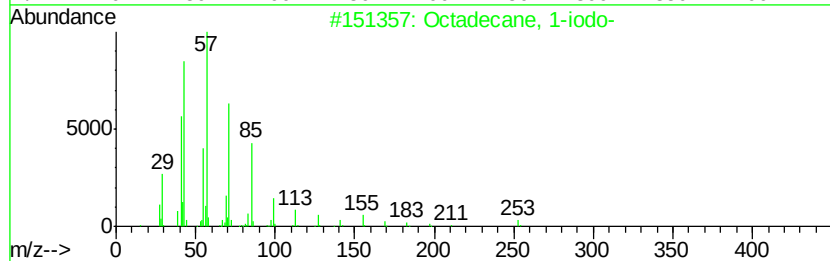
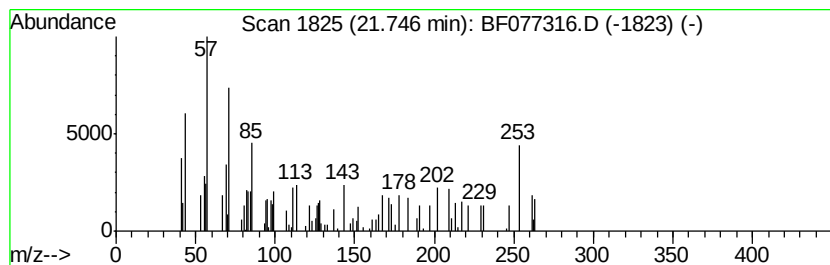
Instrument :
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ClientSampleId :
1003-20(0-2)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.75 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.75	2.20 ng	47005	Chrysene-d12	20.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	43
2	Triacontane	422	C30H62	000638-68-6	38
3	Tetratriacontane	479	C34H70	014167-59-0	38
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	38
5	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	38



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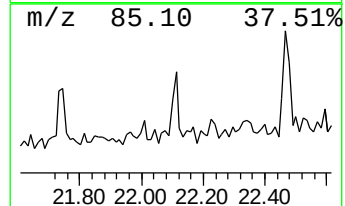
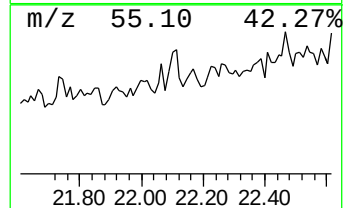
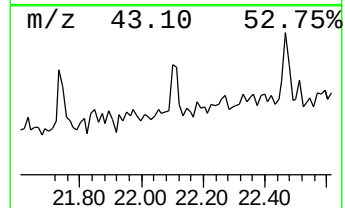
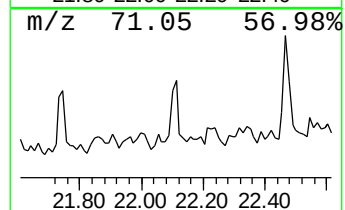
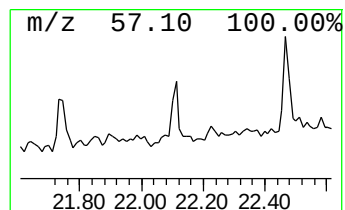
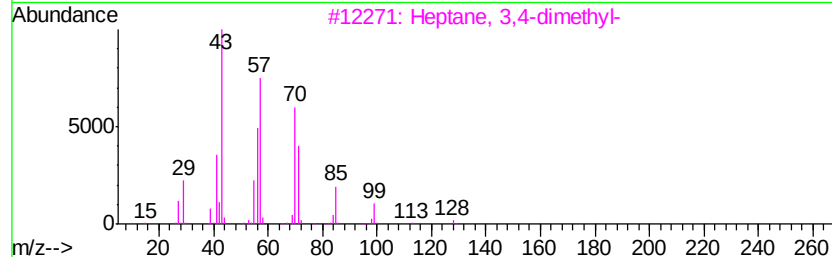
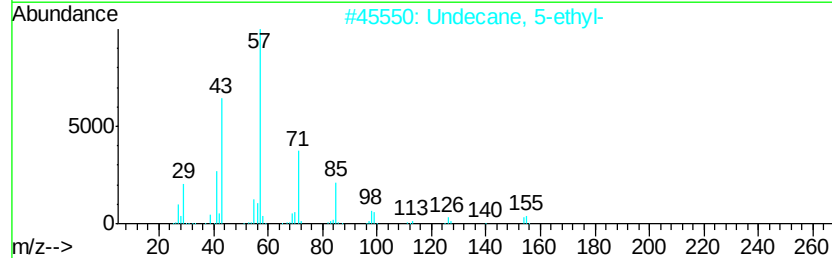
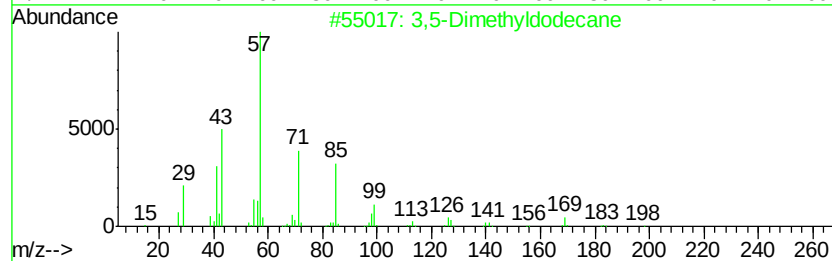
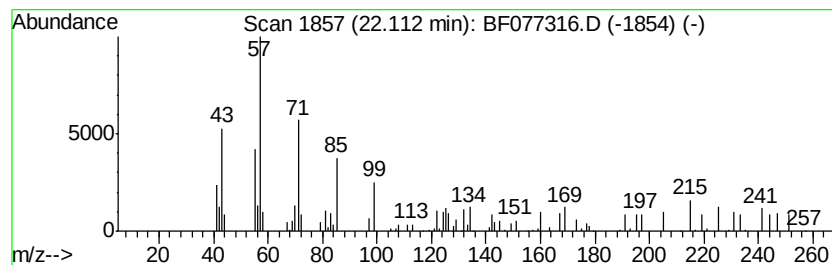
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown22.11 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	2.65 ng	33832	Perylene-d12	22.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Dimethyldodecane	198	C14H30	107770-99-0	38
2		Undecane, 5-ethyl-	184	C13H28	017453-94-0	38
3		Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	38
4		Dodecane, 5,8-diethyl-	226	C16H34	024251-86-3	38
5		Dodecane, 2-methyl-	184	C13H28	001560-97-0	35



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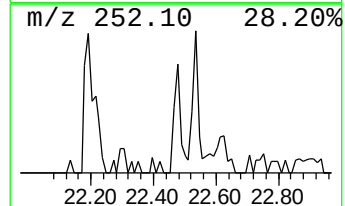
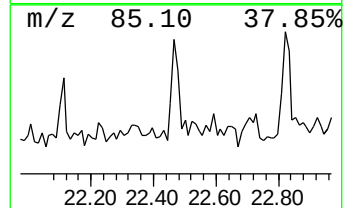
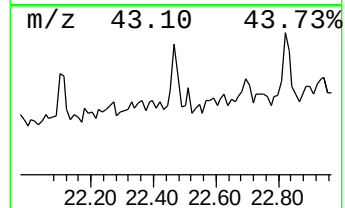
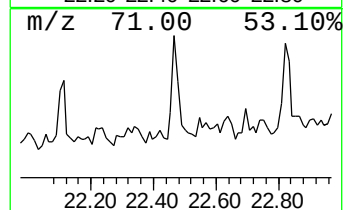
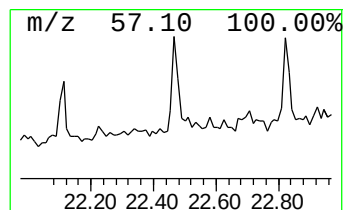
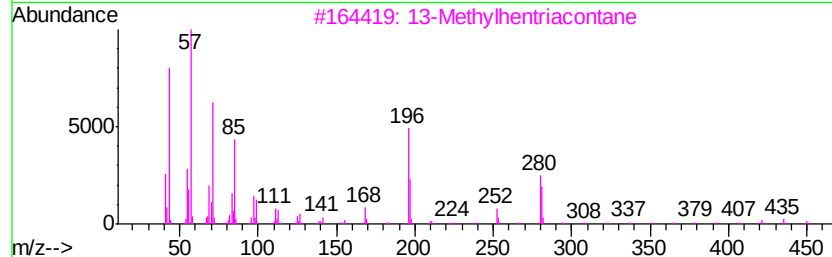
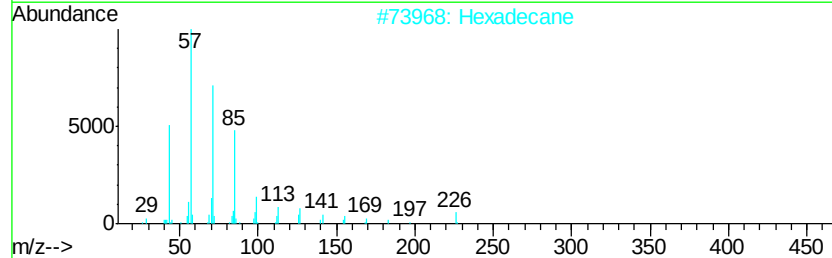
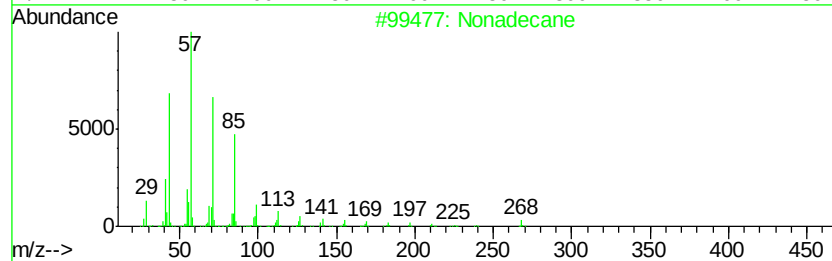
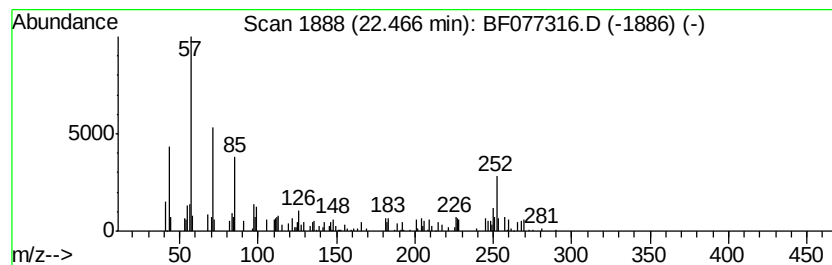
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BNA_F
ClientSampleId :
1003-20(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	3.50 ng	44807	Perylene-d12	22.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268 C19H40	000629-92-5	55
2	Hexadecane	226 C16H34	000544-76-3	43
3	13-Methylhentriacontane	451 C32H66	1000131-19-4	43
4	Eicosane	282 C20H42	000112-95-8	43
5	Pentadecane	212 C15H32	000629-62-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021315\
Data File : BF077316.D
Acq On : 13 Feb 2015 19:41
Operator : TP/IZ
Sample : G1294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

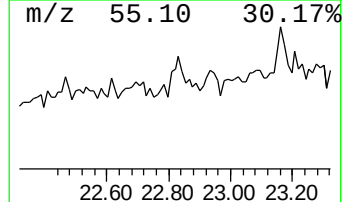
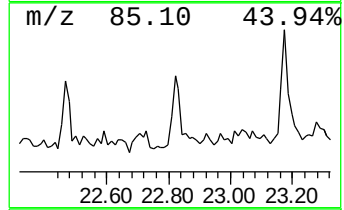
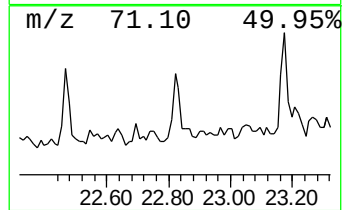
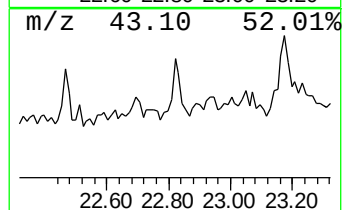
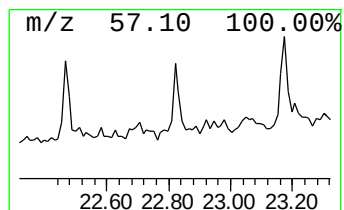
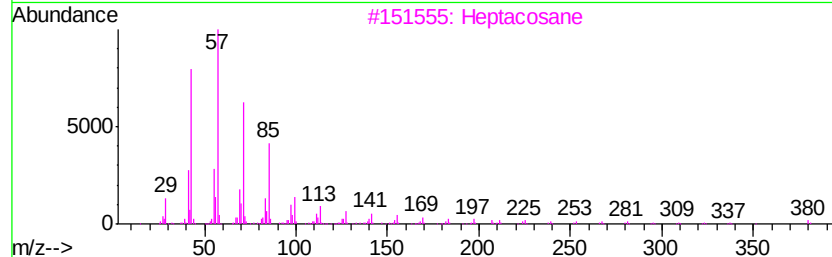
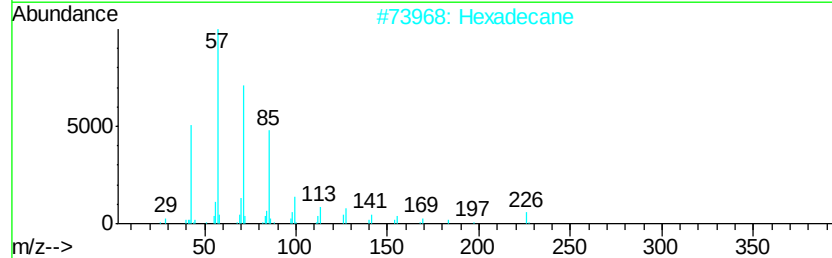
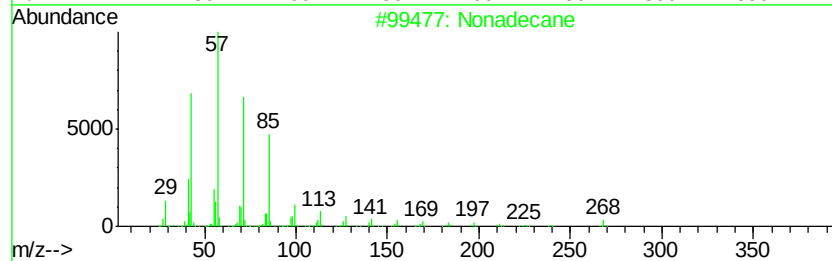
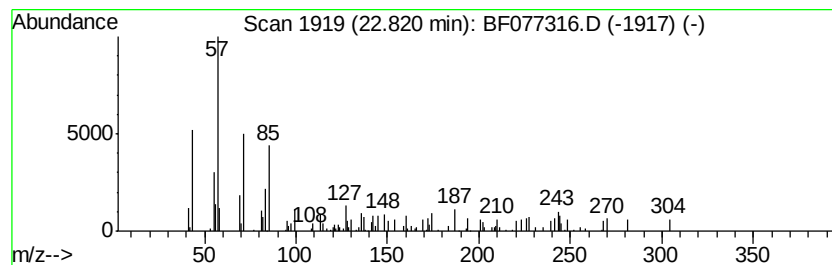
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
22.82	4.52 ng	57799	Perylene-d12		22.58
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	58
2	Hexadecane	226	C16H34	000544-76-3	53
3	Heptacosane	380	C27H56	000593-49-7	50
4	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	47
5	Docosane	310	C22H46	000629-97-0	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF021315\
Data File : BF077316.D
Acq On : 13 Feb 2015 19:41
Operator : TP/IZ
Sample : G1294-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
1003-20(0-2)

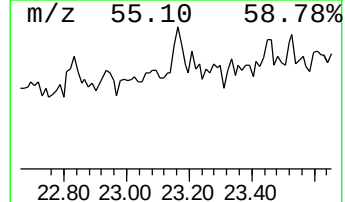
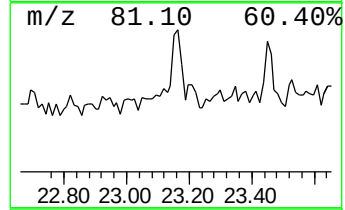
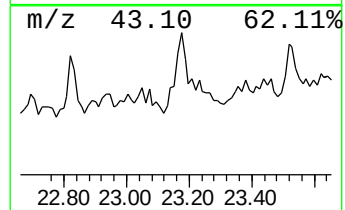
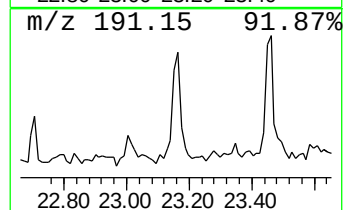
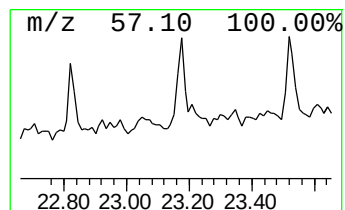
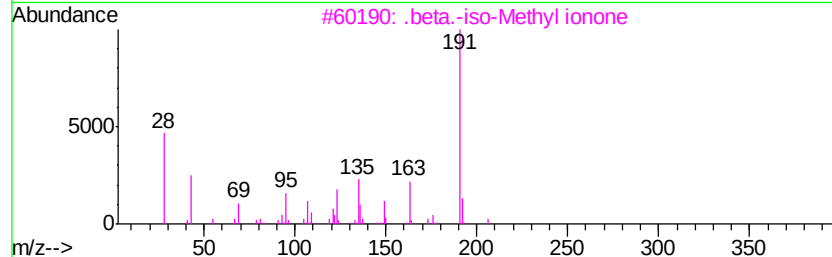
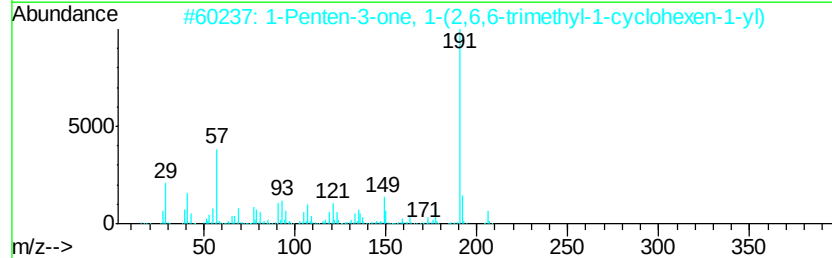
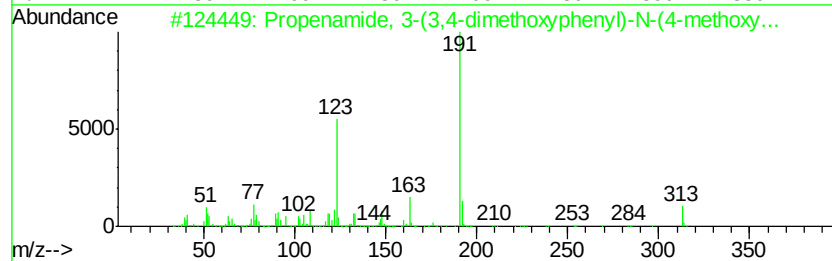
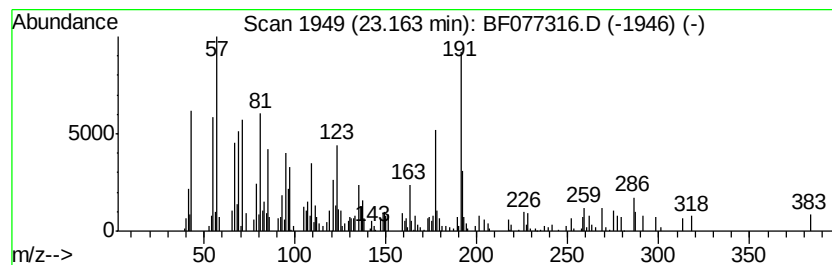
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown23.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	11.48 ng	146863	Perylene-d12	22.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19N04	339165-72-9	41
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
3		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	30
4		2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	041436-42-4	25
5		2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021315\
Data File : BF077316.D
Acq On : 13 Feb 2015 19:41
Operator : TP/IZ
Sample : G1294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1003-20(0-2)

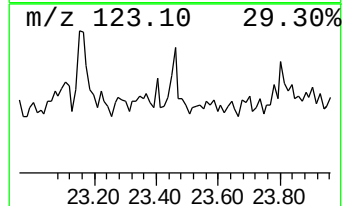
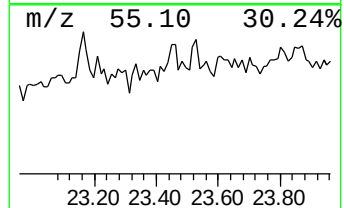
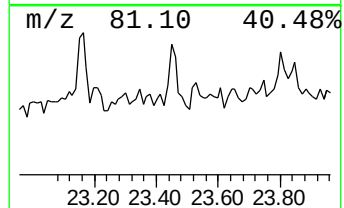
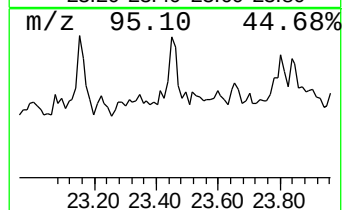
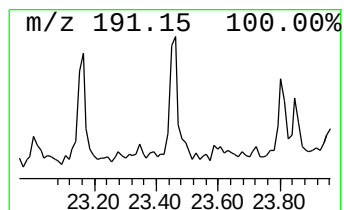
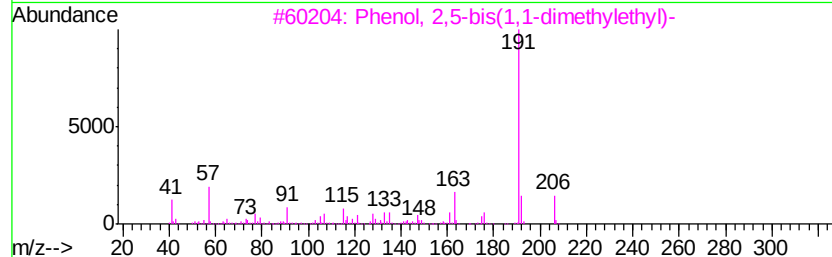
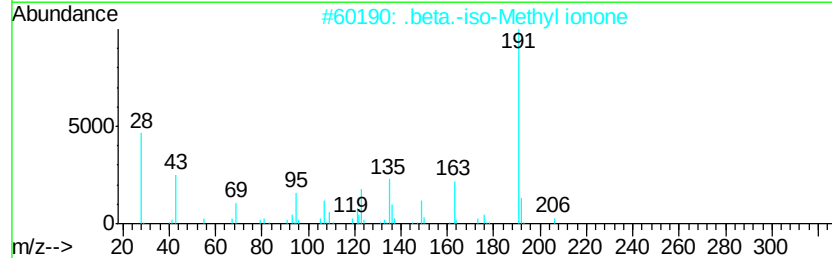
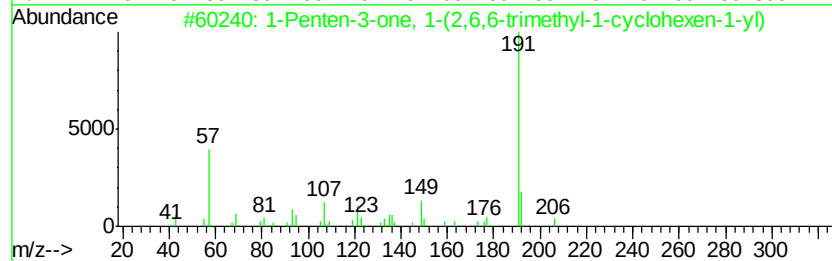
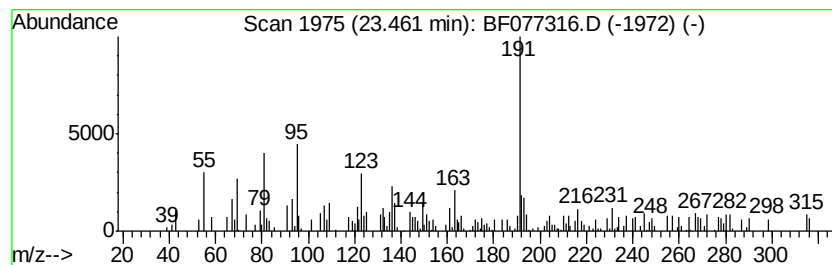
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Penten-3-one, 1-(2,6,6-tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.46	7.42 ng	94863	Perylene-d12	22.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	83
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
3		Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	38
4		3-Indolethanamine, N-acetyl-5-fl...	250	C13H15FN2O2	1000116-27-1	38
5		2-Phenyliminoperhydro-1,3-thiazine	192	C10H12N2S	1000138-91-3	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021315\
Data File : BF077316.D
Acq On : 13 Feb 2015 19:41
Operator : TP/IZ
Sample : G1294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1003-20(0-2)

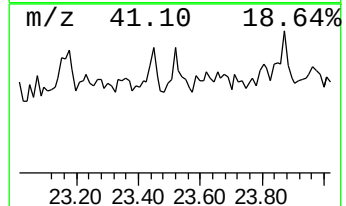
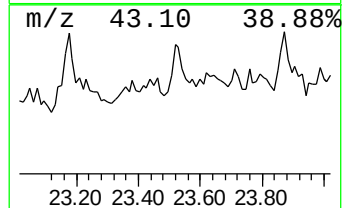
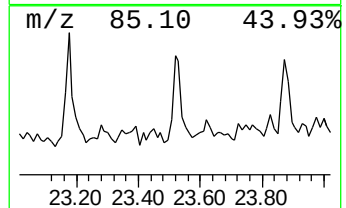
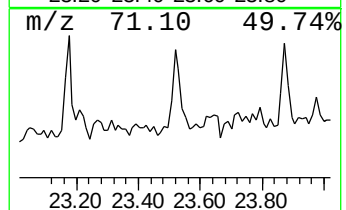
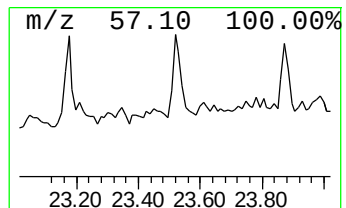
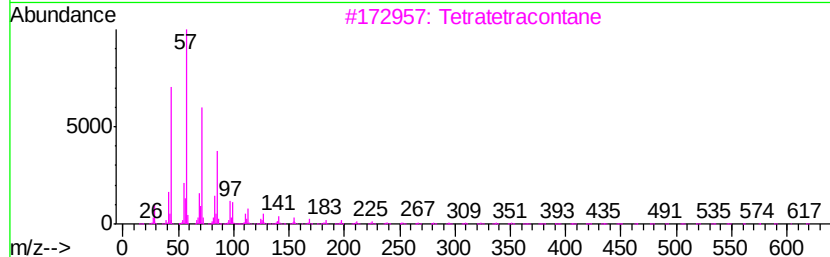
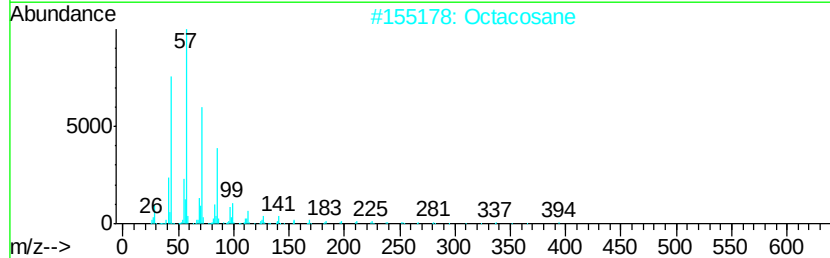
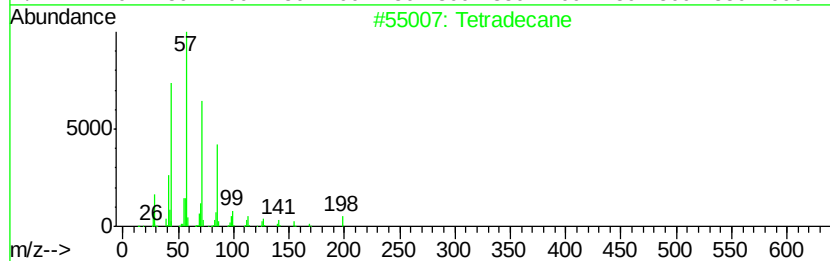
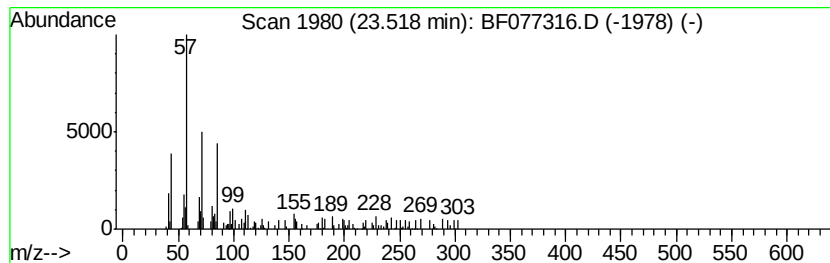
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.52	6.24 ng	79827	Perylene-d12	22.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	52
2		Octacosane	394	C28H58	000630-02-4	52
3		Tetratetracontane	619	C44H90	007098-22-8	50
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	50
5		Nonadecane	268	C19H40	000629-92-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021315\
Data File : BF077316.D
Acq On : 13 Feb 2015 19:41
Operator : TP/IZ
Sample : G1294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1003-20(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021215.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
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unknown6.99	6.99	105.6	ng	878266	1	7.50	166416	20.0
unknown21.75	21.75	2.2	ng	47005	5	20.95	428168	20.0
unknown22.11	22.11	2.6	ng	33832	6	22.58	255813	20.0
Nonadecane	22.47	3.5	ng	44807	6	22.58	255813	20.0
Hexadecane	22.82	4.5	ng	57799	6	22.58	255813	20.0
unknown23.16	23.16	11.5	ng	146863	6	22.58	255813	20.0
1-Penten-3-one, 1...	23.46	7.4	ng	94863	6	22.58	255813	20.0
Tetradecane	23.52	6.2	ng	79827	6	22.58	255813	20.0