

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
 Data File : BF084096.D
 Acq On : 24 Dec 2015 23:20
 Operator : UM/SJ
 Sample : G4927-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-19

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-BF122415.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	4.967	249	252	259	rBB	113166	141345	7.88%	1.311%
2	5.413	289	291	301	rVB	359028	356995	19.90%	3.312%
3	6.453	380	382	390	rBB	167739	230625	12.86%	2.139%
4	6.567	390	392	394	rBV	854370	738970	41.20%	6.855%
5	6.613	394	396	397	rVV	34055	35869	2.00%	0.333%
6	6.636	397	398	404	rVB	44371	45592	2.54%	0.423%
7	6.727	405	406	410	rBV	36664	47213	2.63%	0.438%
8	6.796	410	412	414	rBV	360060	295035	16.45%	2.737%
9	6.876	416	419	421	rBV	33055	42066	2.35%	0.390%
10	6.956	423	426	428	rVB	1130235	1122824	62.60%	10.416%
11	7.367	459	462	464	rBV	794680	888923	49.56%	8.246%
12	7.996	515	517	522	rBV	17929	24608	1.37%	0.228%
13	8.088	522	525	526	rBV	290608	379190	21.14%	3.518%
14	8.362	548	549	551	rVB	37713	31332	1.75%	0.291%
15	8.408	551	553	555	rVB	24927	27082	1.51%	0.251%
16	8.590	565	569	572	rBV3	14466	18283	1.02%	0.170%
17	9.162	616	619	620	rBV	1898476	1793721	100.00%	16.639%
18	9.185	620	621	624	rVV	78818	69030	3.85%	0.640%
19	9.288	628	630	631	rVB	28643	24848	1.39%	0.231%
20	9.516	647	650	652	rBV	199057	314094	17.51%	2.914%
21	9.551	652	653	655	rVB	34560	40641	2.27%	0.377%
22	9.768	670	672	675	rVV	29390	29328	1.64%	0.272%
23	9.836	675	678	680	rVB	499469	451570	25.18%	4.189%
24	10.111	699	702	706	rVB5	6592	19845	1.11%	0.184%
25	10.271	710	716	718	rBV2	21742	31593	1.76%	0.293%
26	10.488	732	735	739	rVB2	31479	48833	2.72%	0.453%
27	10.625	744	747	749	rVV	689148	687828	38.35%	6.381%
28	10.682	751	752	756	rBV	74089	69926	3.90%	0.649%
29	10.739	756	757	760	rBV2	24116	37183	2.07%	0.345%
30	11.185	794	796	800	rBV3	19530	29107	1.62%	0.270%
31	11.322	805	808	810	rBV	343014	413647	23.06%	3.837%
32	11.505	820	824	827	rBV3	14402	26853	1.50%	0.249%
33	11.688	838	840	844	rVB	20619	22573	1.26%	0.209%
34	11.859	853	855	856	rBV	68908	73263	4.08%	0.680%

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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

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35	12.534	912	914	917	rBV2	9477	20692	1.15%	0.192%
36	12.637	921	923	926	rBV	25616	34191	1.91%	0.317%
37	12.785	935	936	942	rVB2	35749	39590	2.21%	0.367%
38	12.899	944	946	949	rBV	1462030	1374728	76.64%	12.753%
39	13.437	990	993	995	rBV4	9461	19081	1.06%	0.177%
40	13.802	1022	1025	1030	rVB3	34155	67273	3.75%	0.624%
41	13.951	1036	1038	1041	rBV	303239	332453	18.53%	3.084%
42	14.785	1109	1111	1113	rBV	25716	25676	1.43%	0.238%
43	15.380	1161	1163	1167	rBV	169418	256395	14.29%	2.378%

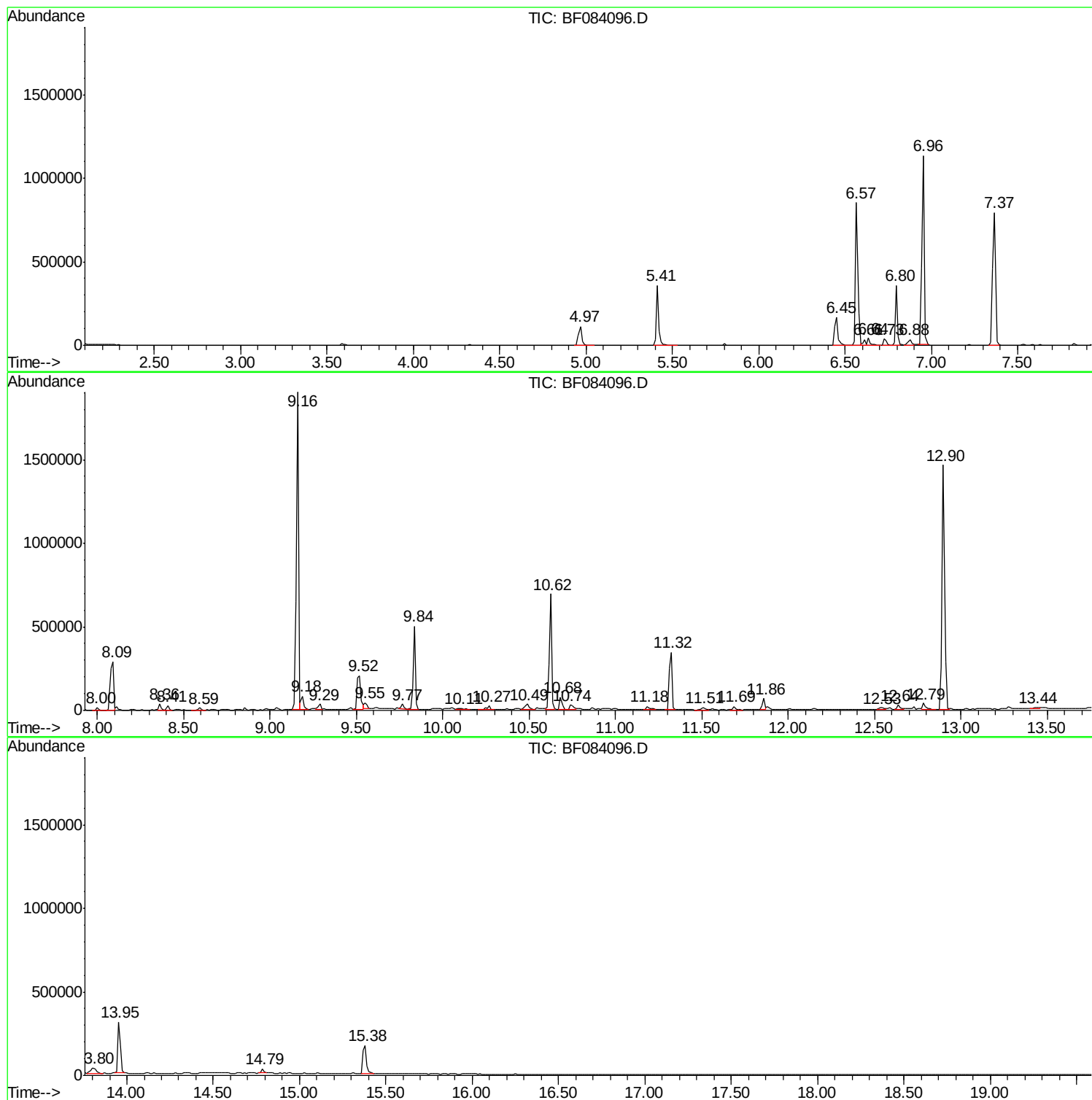
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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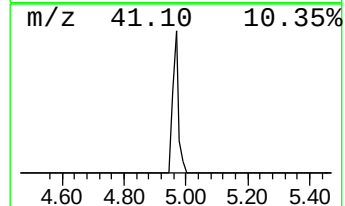
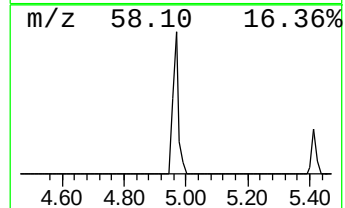
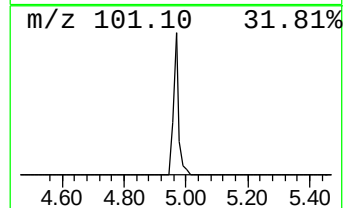
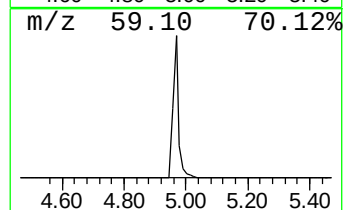
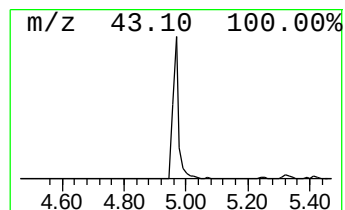
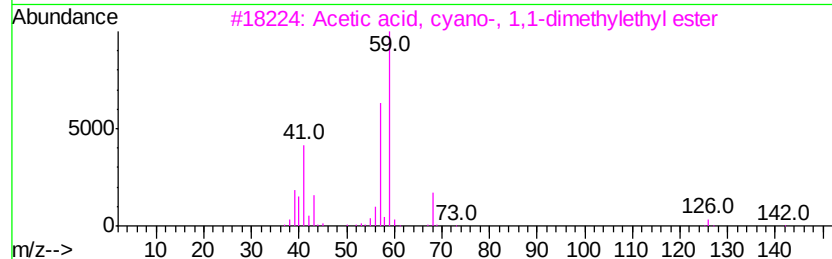
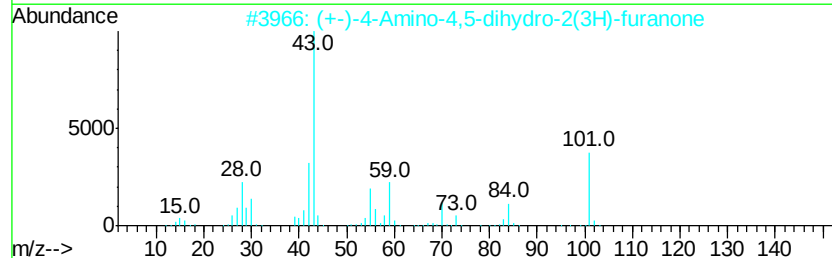
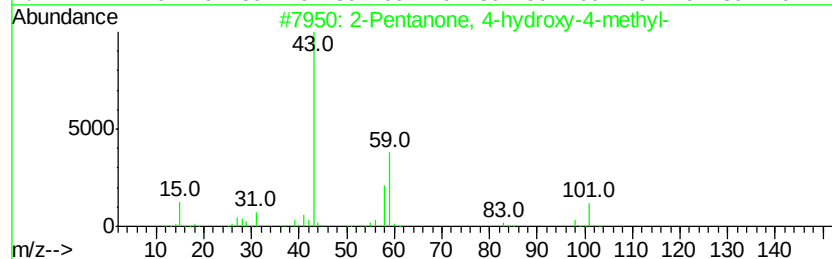
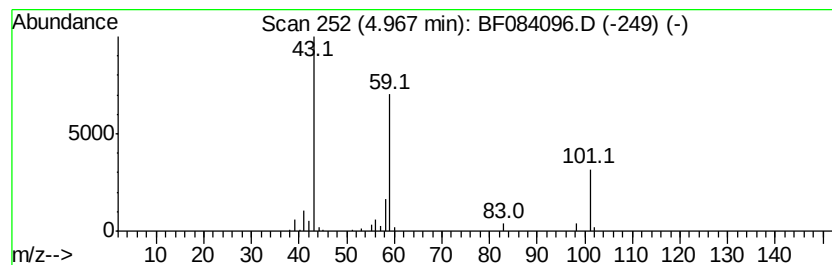
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	9.58 ng	141345	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	47
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	10
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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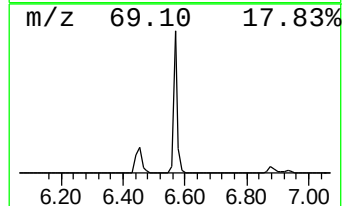
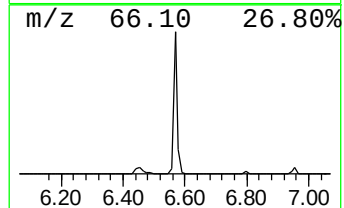
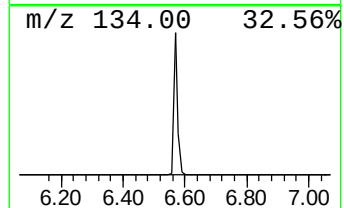
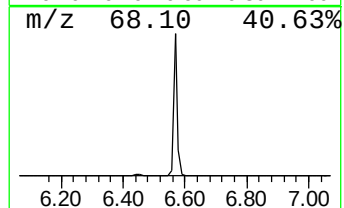
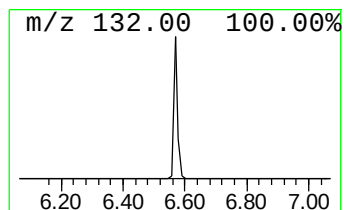
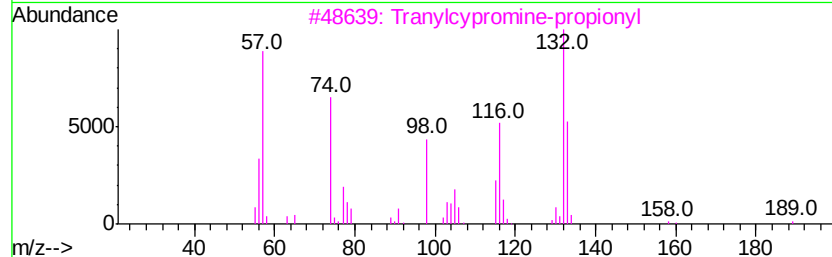
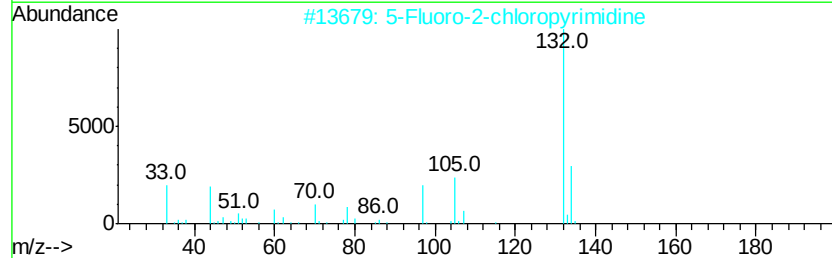
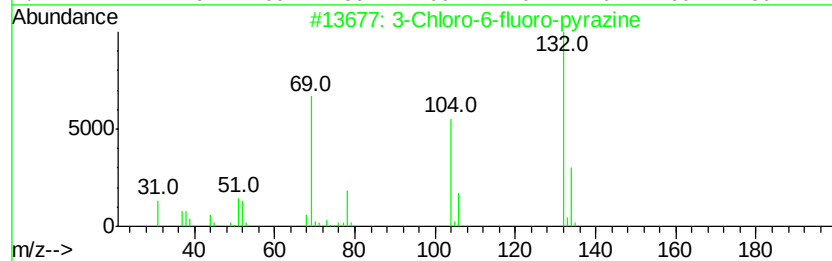
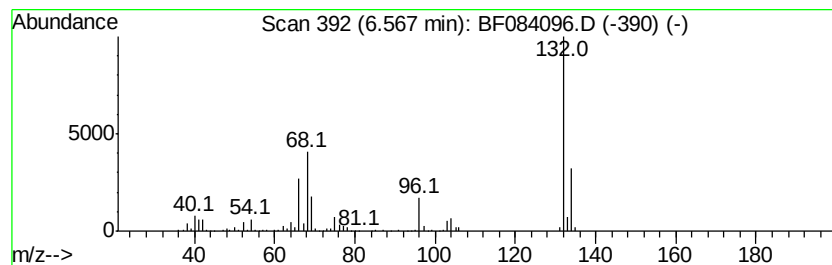
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	50.09 ng	738970	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TEC-19

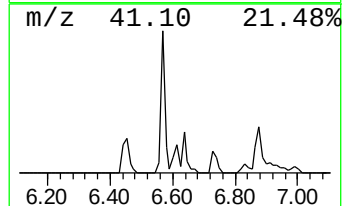
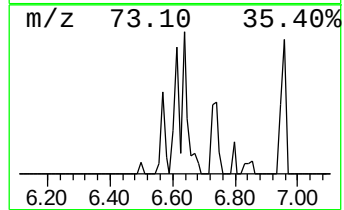
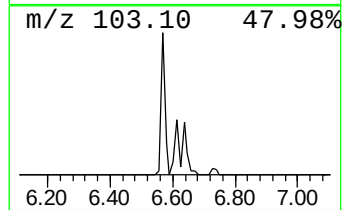
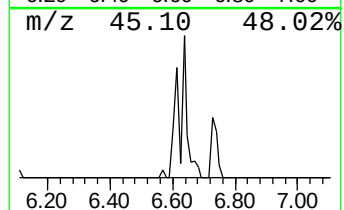
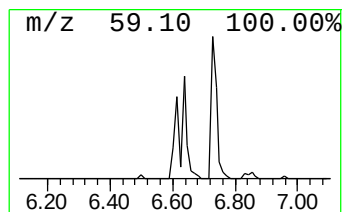
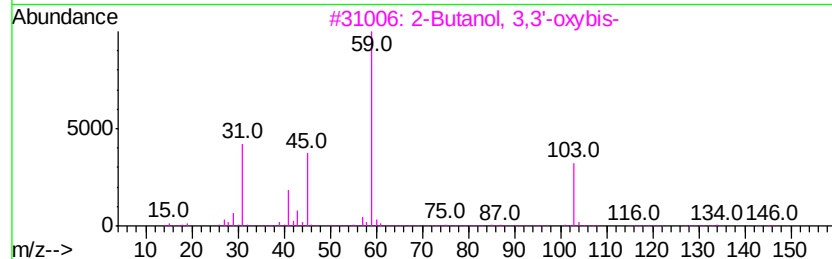
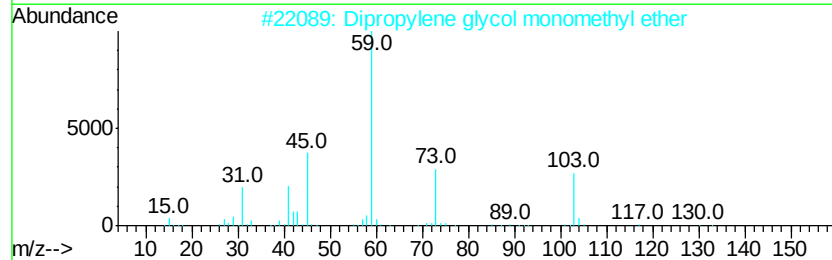
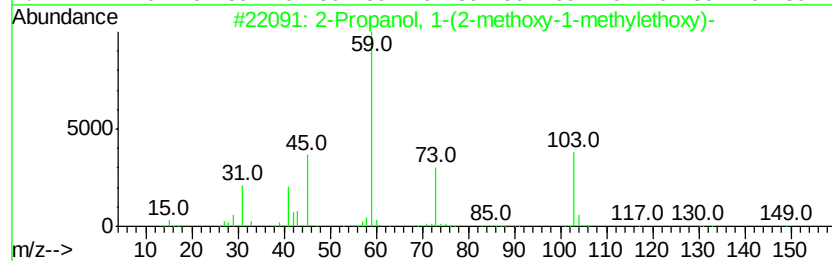
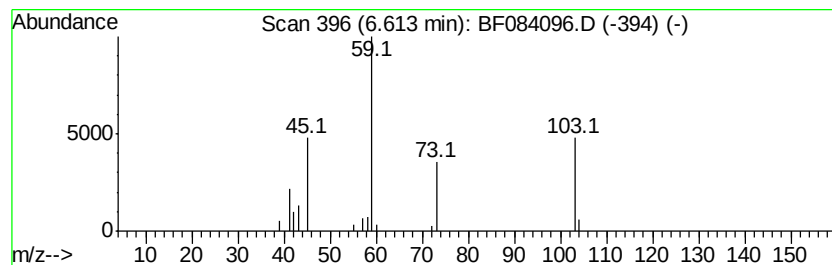
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	2.43 ng	35869	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2			Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	64
3			2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	50
4			2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	45
5			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	38



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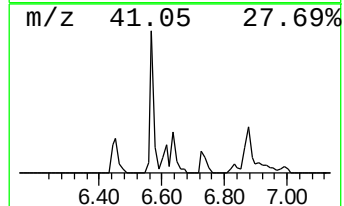
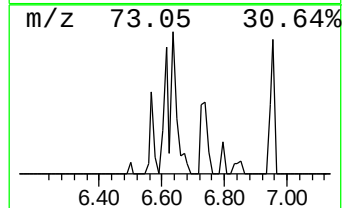
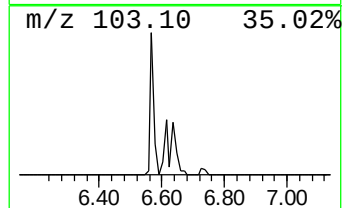
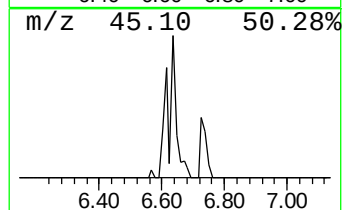
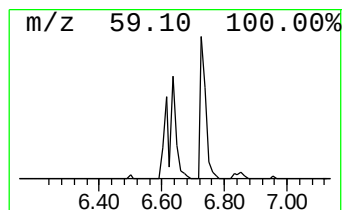
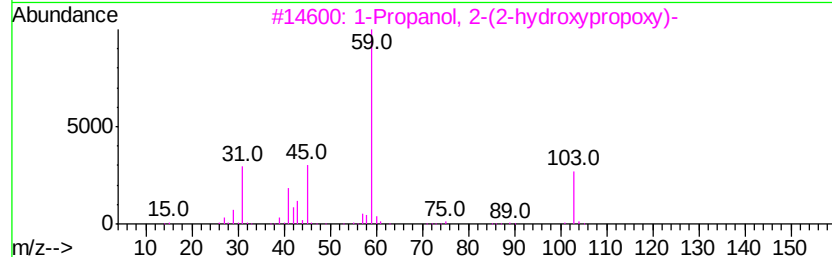
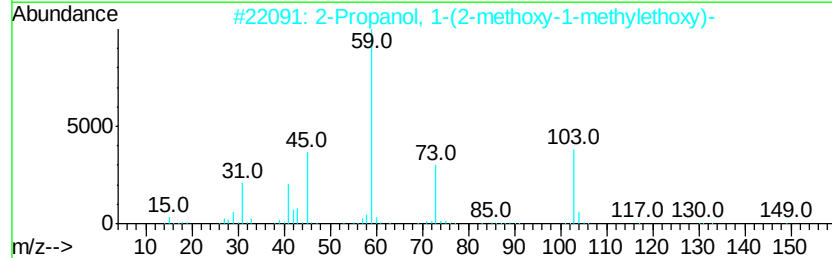
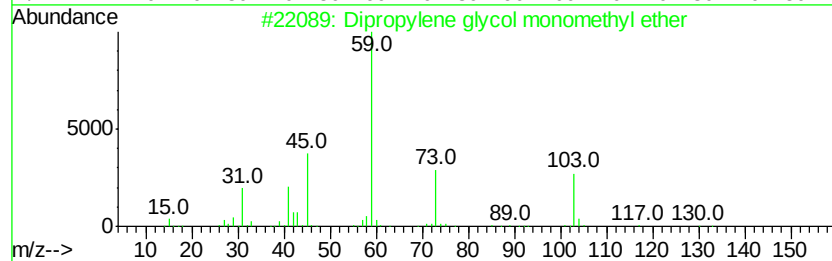
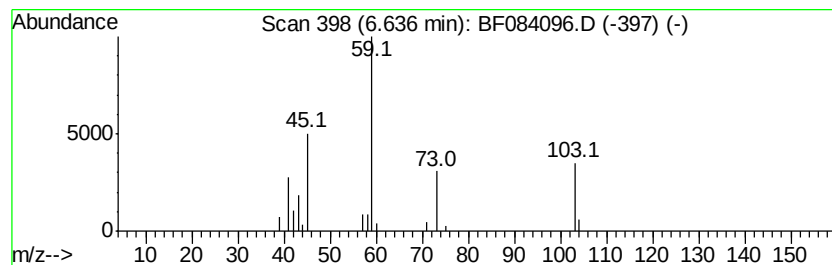
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dipropylene glycol monometh... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	3.09 ng	45592	1,4-Dichlorobenzene-d4	6.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	83	
2	2-Propanol, 1-(2-methoxy-1-methyl-...	148	C7H16O3	020324-32-7	83	
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59	
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53	
5	Dipropylene glycol	134	C6H14O3	025265-71-8	53	



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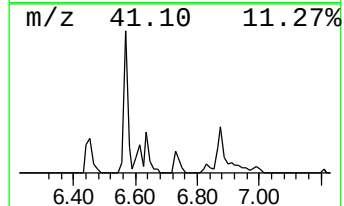
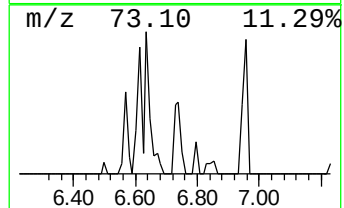
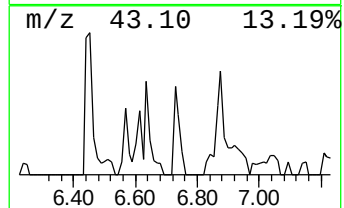
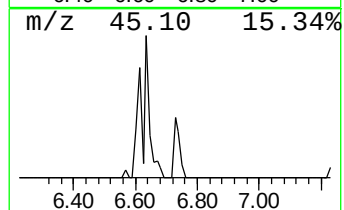
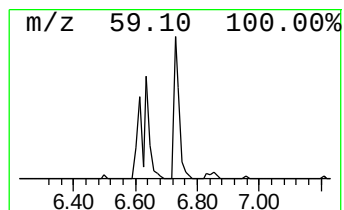
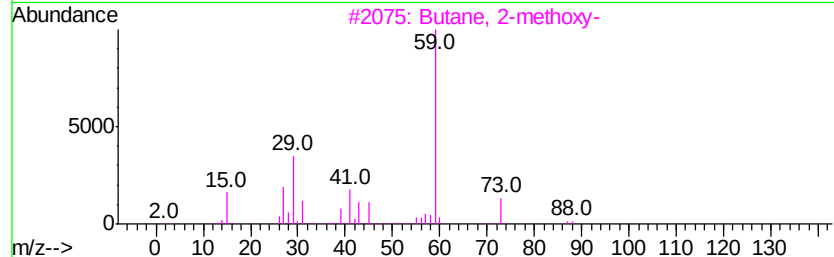
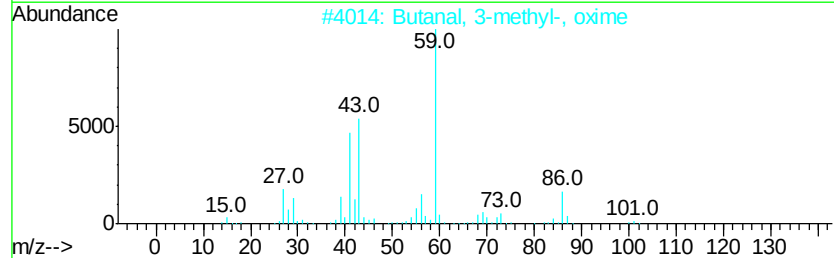
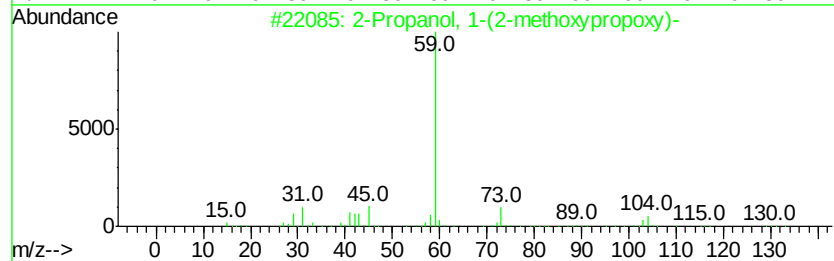
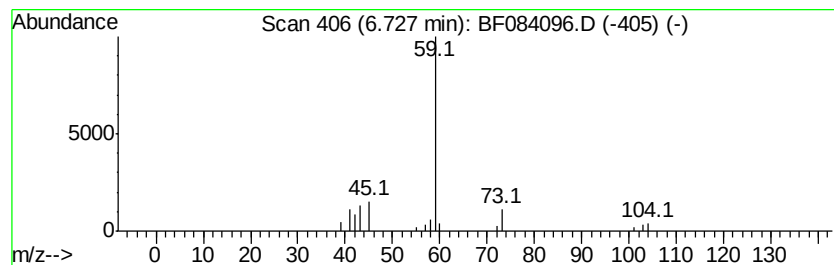
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	3.20 ng	47213	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2		Butanal, 3-methyl-, oxime	101	C5H11NO	000626-90-4	59
3		Butane, 2-methoxy-	88	C5H12O	006795-87-5	43
4		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	40
5		2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084096.D
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Operator : UM/SJ
Sample : G4927-02
Misc :
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Instrument :
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ClientSampleId :
TEC-19

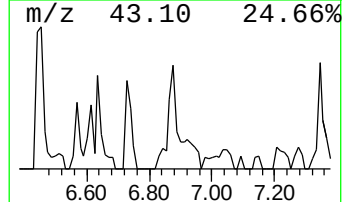
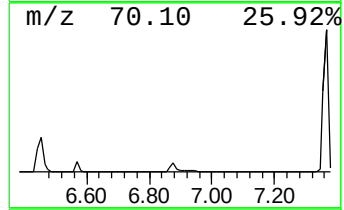
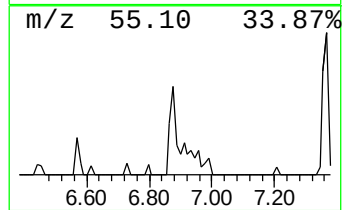
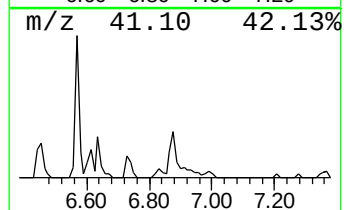
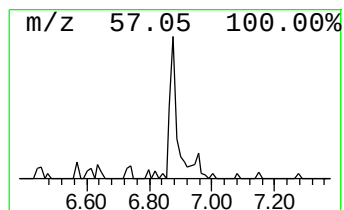
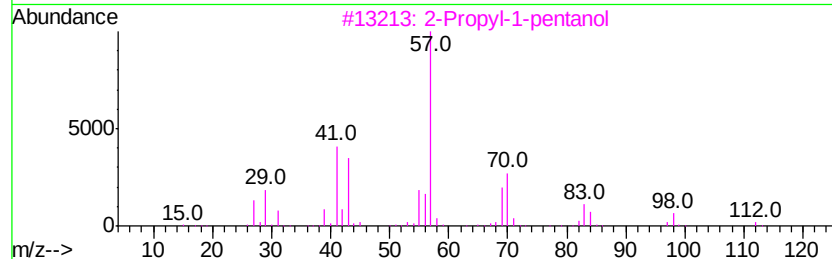
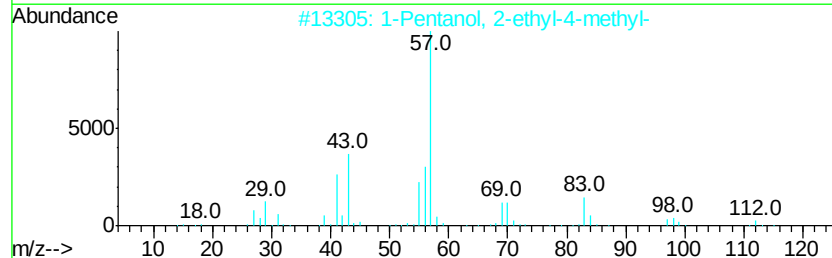
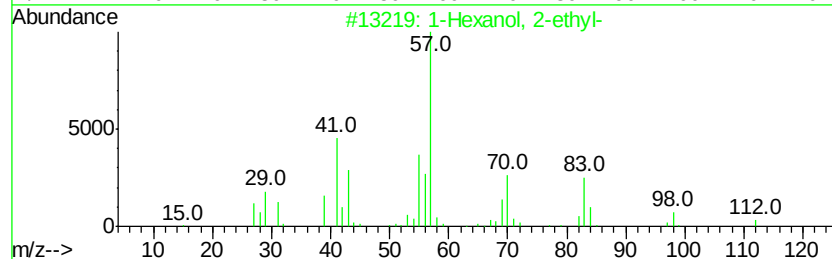
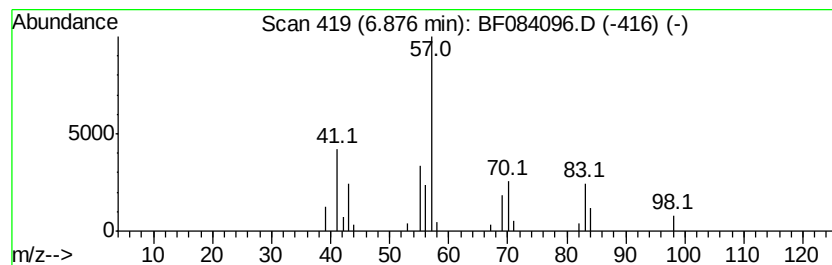
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	2.85 ng	42066	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	45
4		Sulfone, 2-hydroxyhexyl t-butyl	222	C10H22O3S	1000161-82-5	23
5		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084096.D
Acq On : 24 Dec 2015 23:20
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Sample : G4927-02
Misc :
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ClientSampleId :
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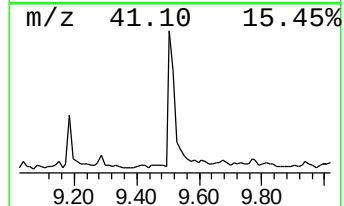
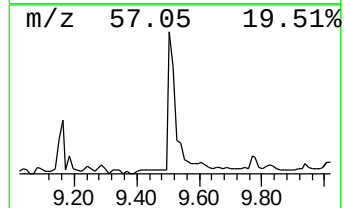
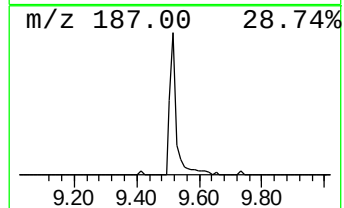
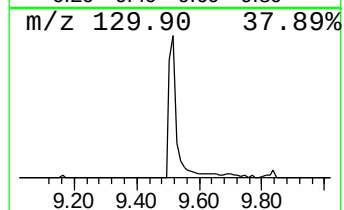
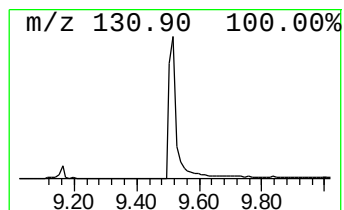
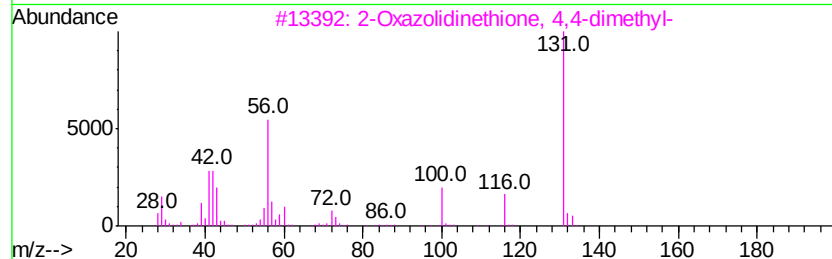
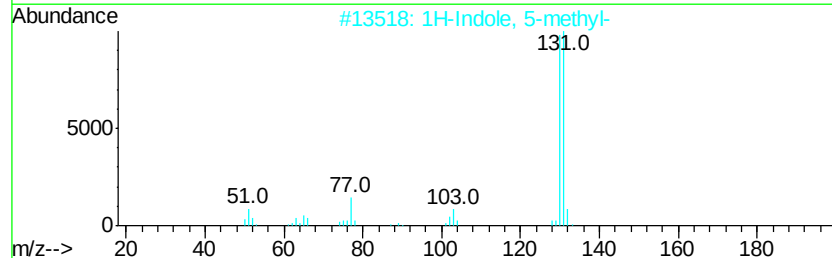
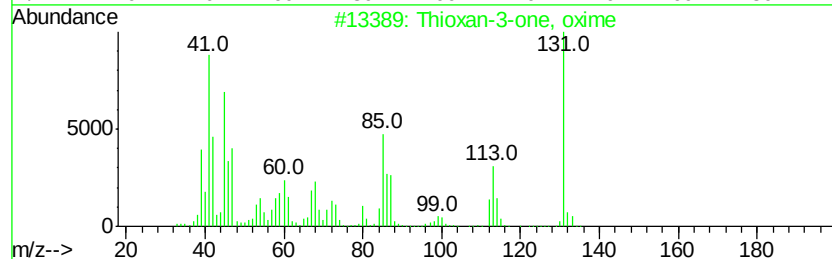
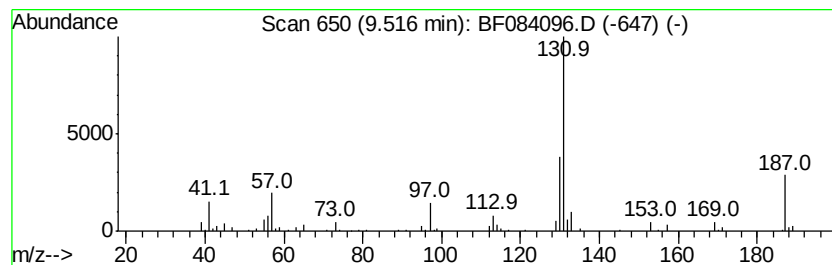
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	13.91 ng	314094	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thioxan-3-one, oxime	131	C5H9NOS	058230-51-6	38
2		1H-Indole, 5-methyl-	131	C9H9N	000614-96-0	9
3		2-Oxazolidinethione, 4,4-dimethyl-	131	C5H9NOS	054013-55-7	9
4		1H-Indole-3-ethanamine, .alpha.-...	174	C11H14N2	000299-26-3	9
5		Butane-1,3-diol, 1-methylene-3-m...	260	C12H28O2Si2	117201-96-4	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084096.D
Acq On : 24 Dec 2015 23:20
Operator : UM/SJ
Sample : G4927-02
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ClientSampleId :
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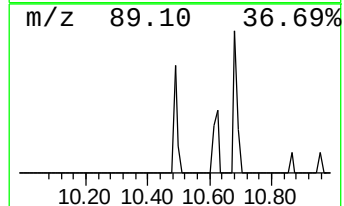
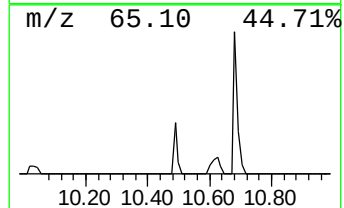
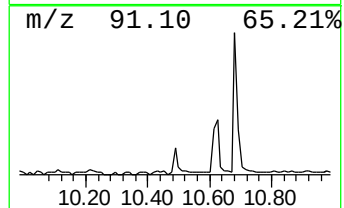
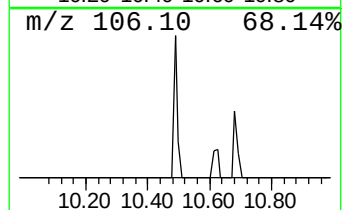
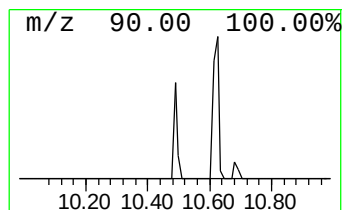
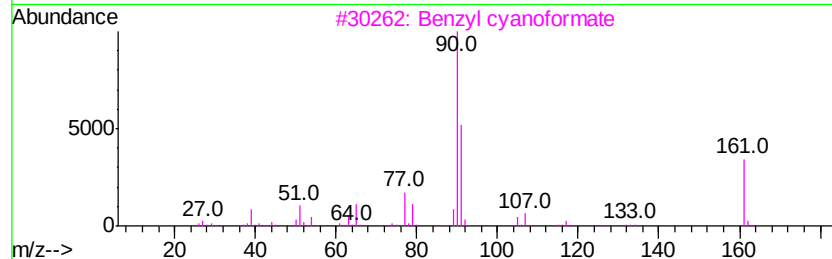
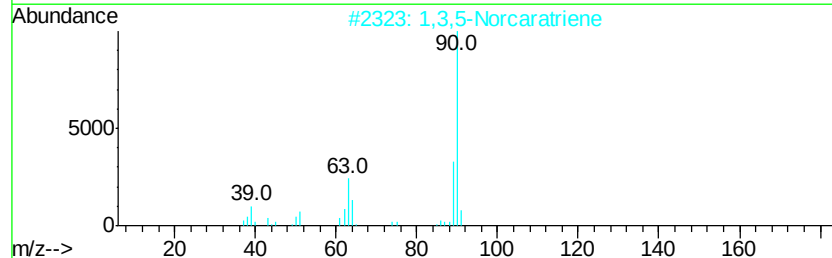
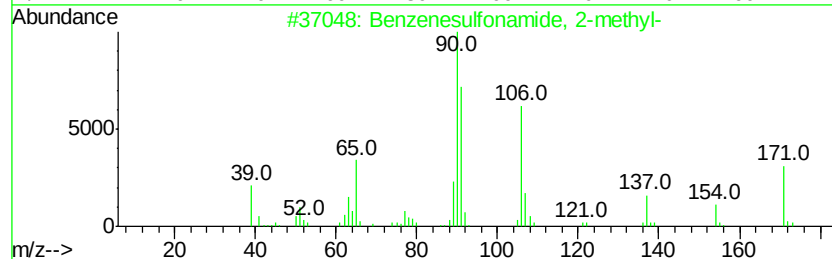
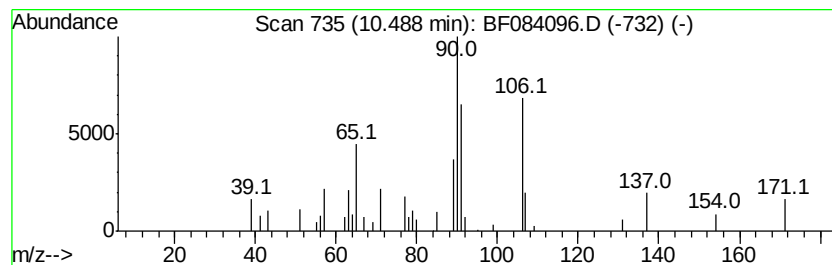
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzenesulfonamide, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	2.16 ng	48833	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	94
2		1,3,5-Norcaratriene	90	C7H6	004646-69-9	43
3		Benzyl cyanoformate	161	C9H7NO2	005532-86-5	32
4		Benzeneacetonitrile, .alpha.-ethyl-	145	C10H11N	000769-68-6	23
5		Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084096.D
Acq On : 24 Dec 2015 23:20
Operator : UM/SJ
Sample : G4927-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

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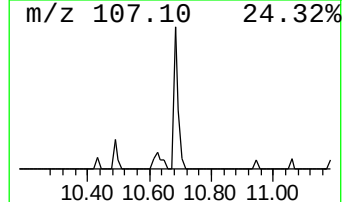
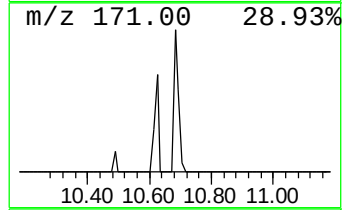
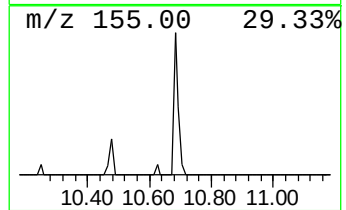
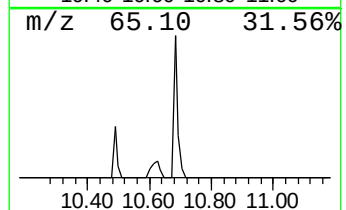
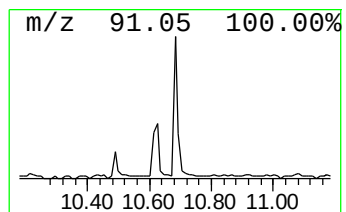
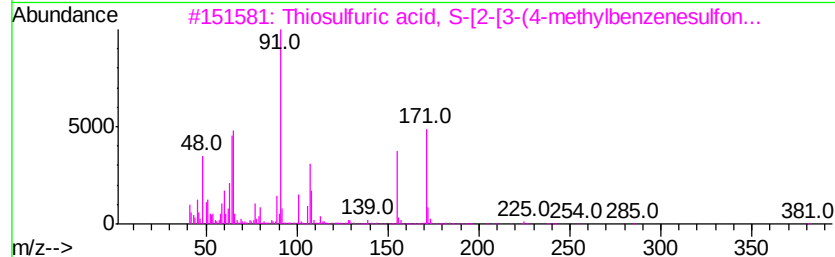
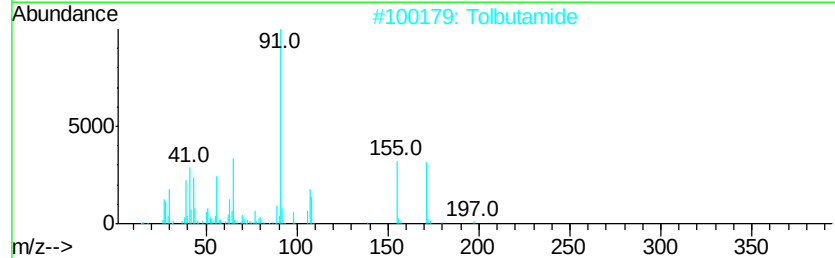
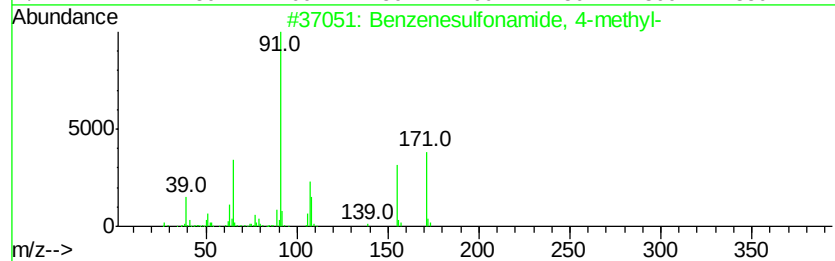
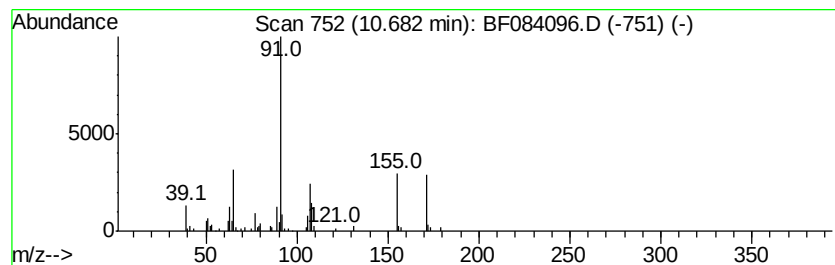
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzenesulfonamide, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	3.38 ng	69926	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2		Tolbutamide	270	C12H18N2O3S	000064-77-7	87
3		Thiosulfuric acid, S-[2-[3-(4-methyl-...]	381	C12H19N3O5S3	1000255-60-3	86
4		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	83
5		O-p-toluenesulfonyl-L-N-acetylser...	315	C13H17NO6S	1000126-44-8	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084096.D
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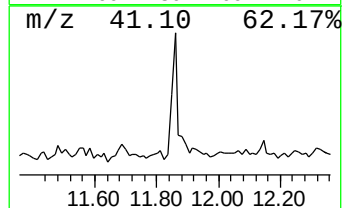
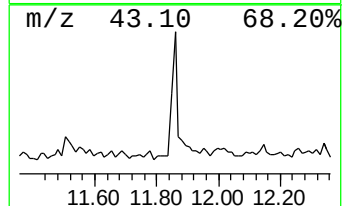
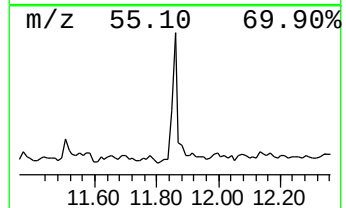
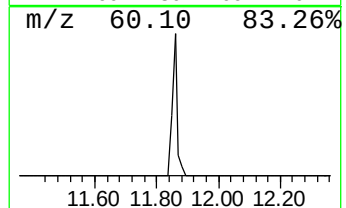
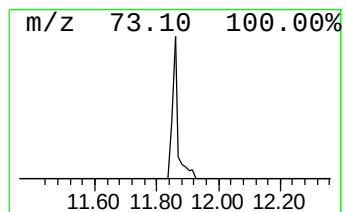
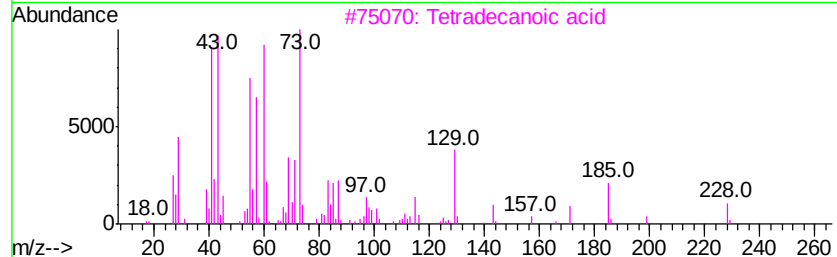
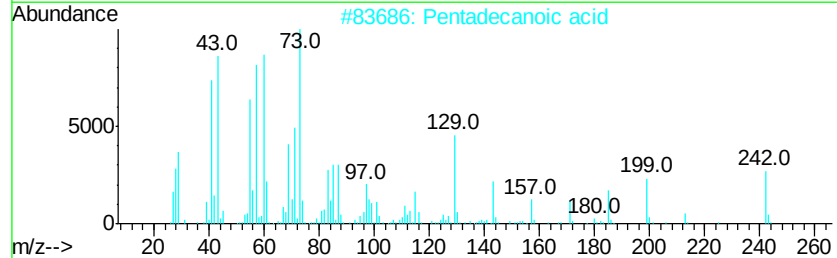
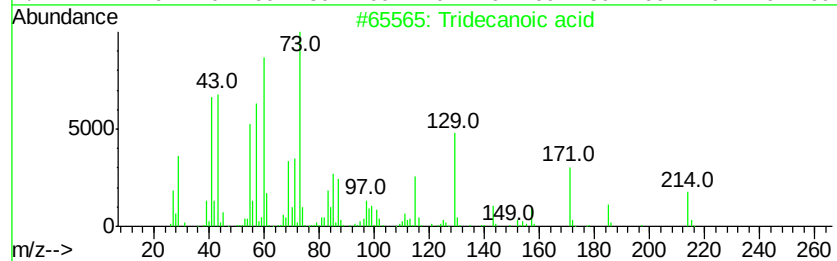
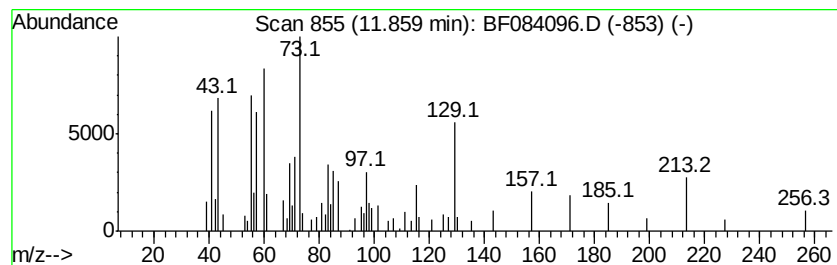
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	3.54 ng	73263	Phenanthrene-d10	11.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	81
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084096.D
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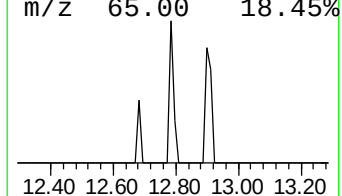
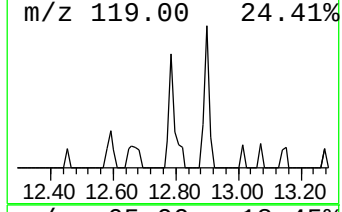
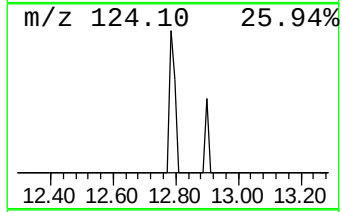
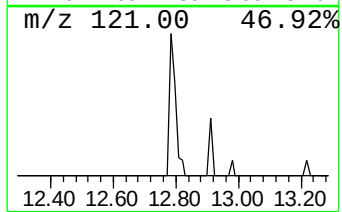
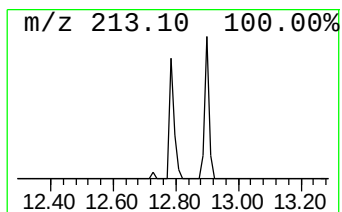
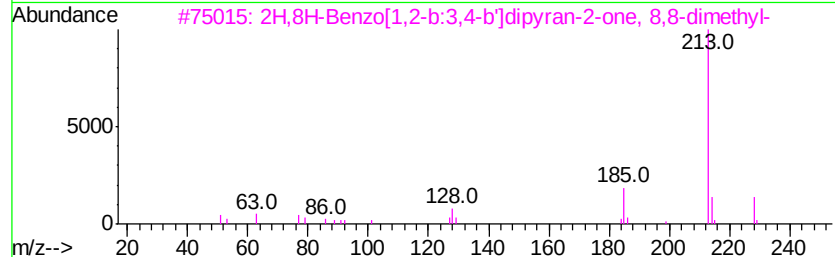
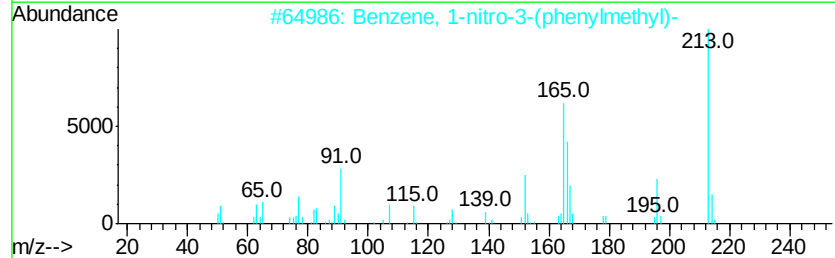
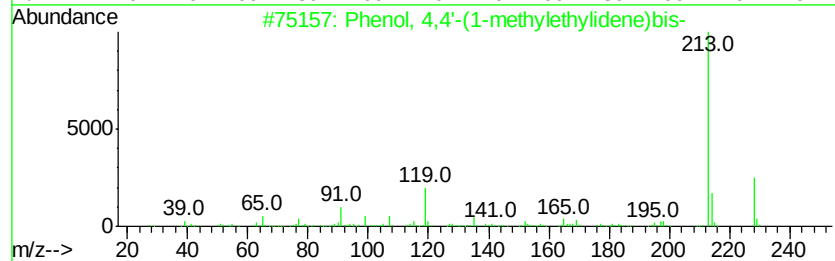
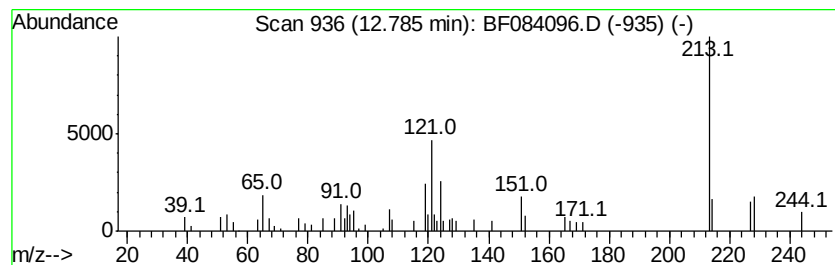
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phenol, 4,4'-(1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.38 ng	39590	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	52
2		Benzene, 1-nitro-3-(phenylmethyl)-	213	C13H11NO2	005840-41-5	43
3		2H,8H-Benzo[1,2-b:3,4-b']dipyrans...	228	C14H12O3	000523-59-1	43
4		Acridine, 9-chloro-	213	C13H8ClN	001207-69-8	38
5		2H,8H-Benzo[1,2-b:5,4-b']dipyrans...	228	C14H12O3	000553-19-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
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Misc :
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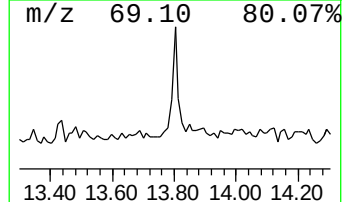
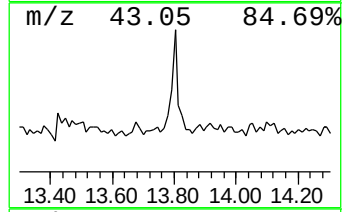
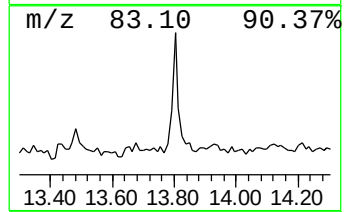
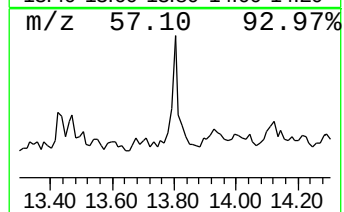
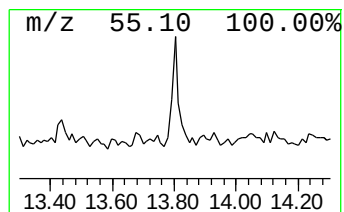
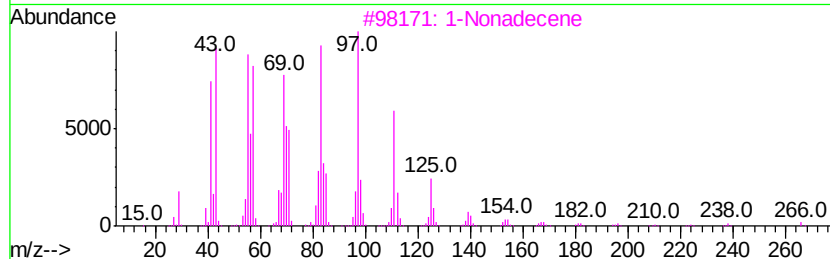
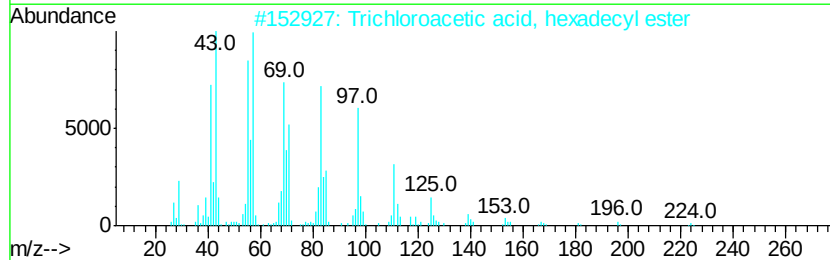
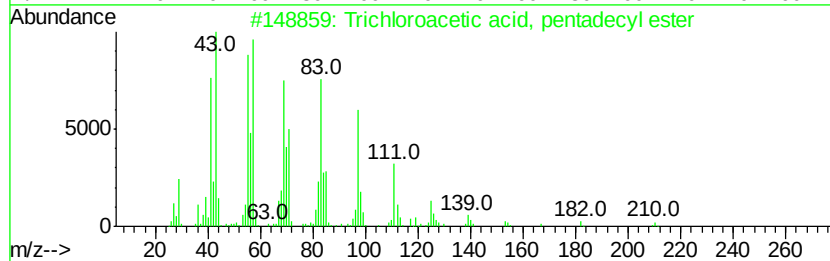
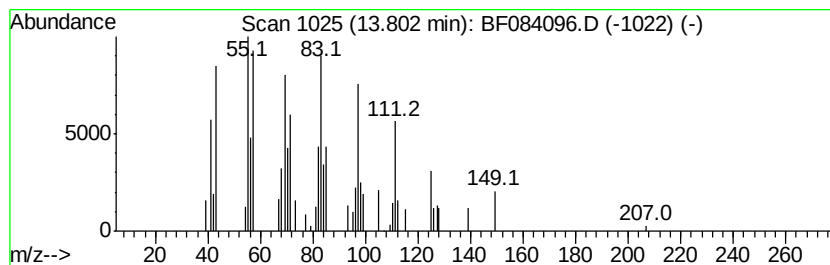
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	4.05 ng	67273	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3		1-Nonadecene	266	C19H38	018435-45-5	81
4		11-Tricosene	322	C23H46	052078-56-5	81
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084096.D
Acq On : 24 Dec 2015 23:20
Operator : UM/SJ
Sample : G4927-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-19

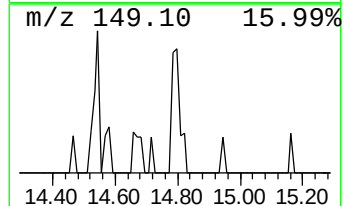
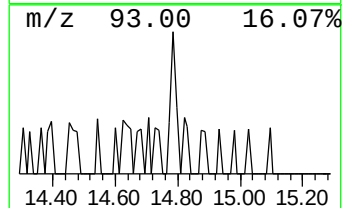
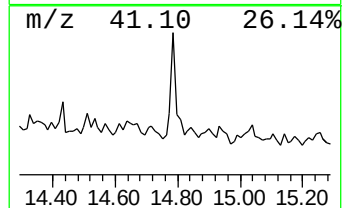
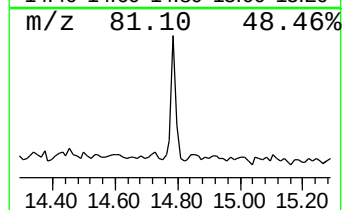
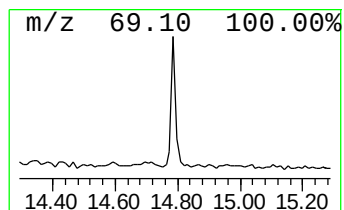
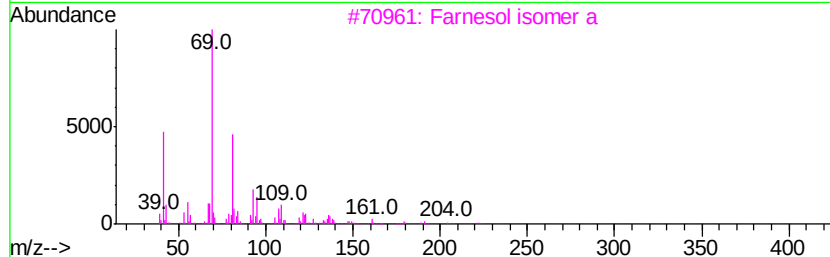
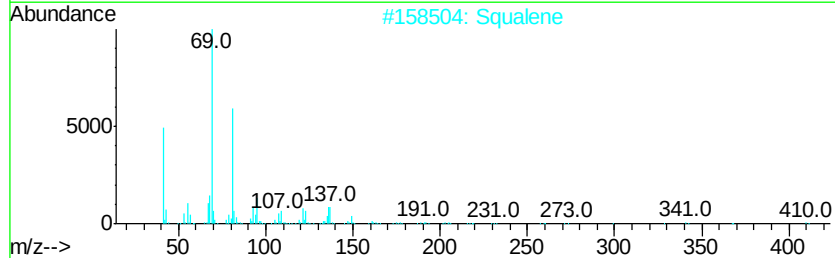
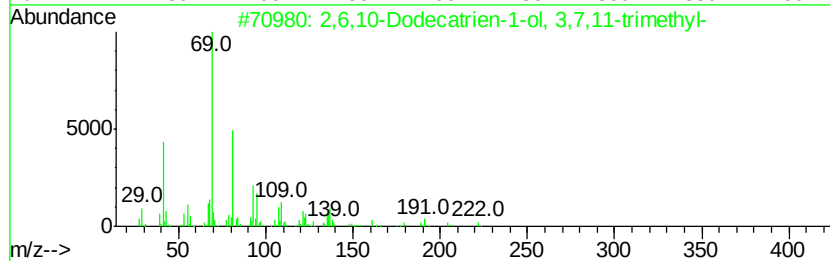
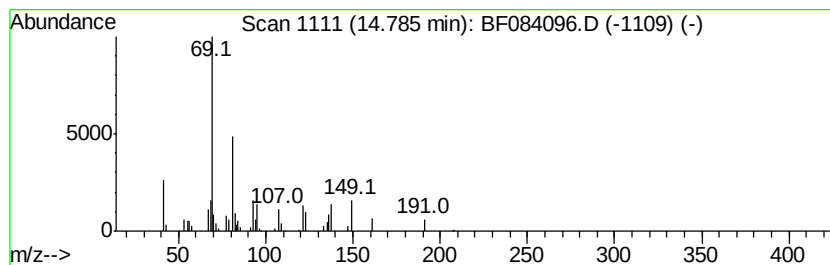
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.00 ng	25676	Perylene-d12	15.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	80
2			Squalene	410	C30H50	007683-64-9	78
3			Farnesol isomer a	222	C15H26O	1000108-92-4	72
4			2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
5			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
 Data File : BF084096.D
 Acq On : 24 Dec 2015 23:20
 Operator : UM/SJ
 Sample : G4927-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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
2-Pentanone, 4-hy...	4.97	9.6 ng		141345	1	6.80	295035	20.0
unknown6.57	6.57	50.1 ng		738970	1	6.80	295035	20.0
2-Propanol, 1-(2-...	6.61	2.4 ng		35869	1	6.80	295035	20.0
Dipropylene glyco...	6.64	3.1 ng		45592	1	6.80	295035	20.0
2-Propanol, 1-(2-...	6.73	3.2 ng		47213	1	6.80	295035	20.0
1-Hexanol, 2-ethyl-	6.88	2.9 ng		42066	1	6.80	295035	20.0
unknown9.52	9.52	13.9 ng		314094	3	9.84	451570	20.0
Benzenesulfonamid...	10.49	2.2 ng		48833	3	9.84	451570	20.0
Benzenesulfonamid...	10.68	3.4 ng		69926	4	11.32	413647	20.0
Tridecanoic acid	11.86	3.5 ng		73263	4	11.32	413647	20.0
Phenol, 4,4'-(1-m...	12.79	2.4 ng		39590	5	13.95	332453	20.0
Trichloroacetic a...	13.80	4.0 ng		67273	5	13.95	332453	20.0
2,6,10-Dodecatric...	14.79	2.0 ng		25676	6	15.38	256395	20.0