

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052015\
 Data File : BF079399.D
 Acq On : 21 May 2015 1:14
 Operator : TP/IZ
 Sample : G2305-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KM-SP-002-150518

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-BF043015.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	1.233	3	4	7	rVB	3172822	4262493	100.00%	17.046%
2	1.358	12	15	27	rVB2	95463	236013	5.54%	0.944%
3	1.518	27	29	32	rVB	210659	230153	5.40%	0.920%
4	1.621	36	38	46	rVB	149964	267657	6.28%	1.070%
5	1.736	46	48	85	rVB	1251770	2262362	53.08%	9.048%
6	4.833	317	319	325	rBV	355019	456350	10.71%	1.825%
7	5.370	364	366	369	rBV	1305202	1526668	35.82%	6.105%
8	5.873	408	410	413	rBV	37792	54262	1.27%	0.217%
9	6.673	477	480	482	rBV	1344037	1742642	40.88%	6.969%
10	6.799	489	491	494	rBV	1474925	1685109	39.53%	6.739%
11	7.085	514	516	519	rBV	326862	439810	10.32%	1.759%
12	7.279	530	533	535	rBV	1127981	1178876	27.66%	4.714%
13	7.782	575	577	580	rBV	781067	874915	20.53%	3.499%
14	8.662	652	654	657	rBV	450894	598694	14.05%	2.394%
15	10.011	770	772	775	rBV	1409660	1663999	39.04%	6.655%
16	10.525	814	817	819	rBV	142726	128406	3.01%	0.514%
17	10.834	842	844	847	rVB	605796	687677	16.13%	2.750%
18	11.817	927	930	933	rBV	1200382	1250515	29.34%	5.001%
19	12.674	1003	1005	1008	rBV	709410	736651	17.28%	2.946%
20	14.674	1177	1180	1183	rBV	2160697	2158713	50.64%	8.633%
21	15.851	1280	1283	1290	rBV	208678	393835	9.24%	1.575%
22	15.954	1290	1292	1295	rBV	593129	822956	19.31%	3.291%
23	16.126	1304	1307	1310	rBV	93996	121350	2.85%	0.485%
24	17.680	1440	1443	1445	rBV	663107	810426	19.01%	3.241%
25	18.389	1503	1505	1509	rVB2	129718	206840	4.85%	0.827%
26	19.200	1573	1576	1579	rBV3	104066	207953	4.88%	0.832%

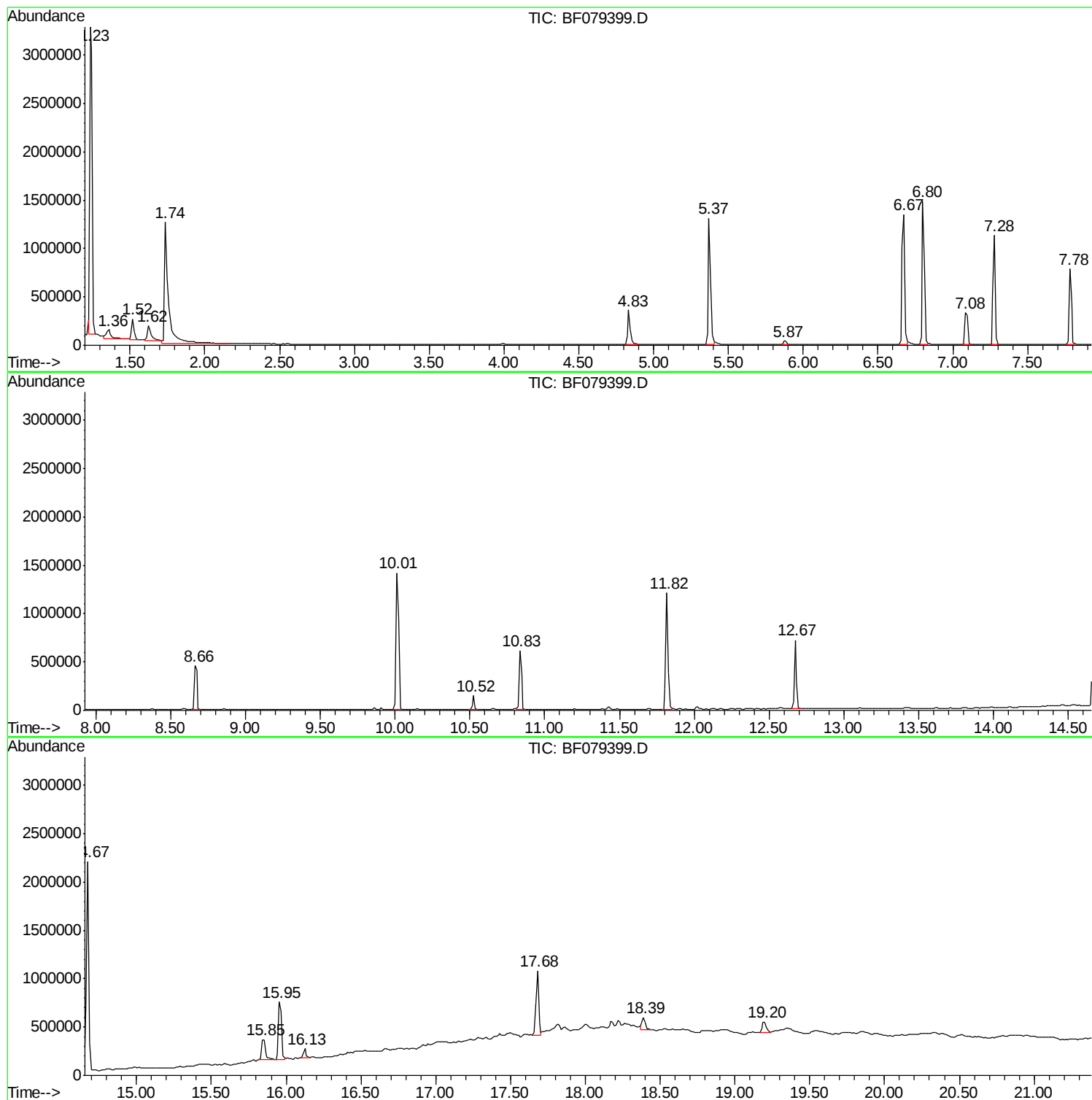
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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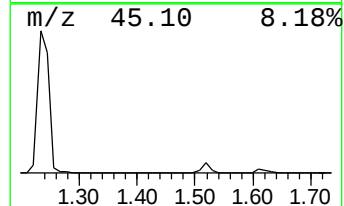
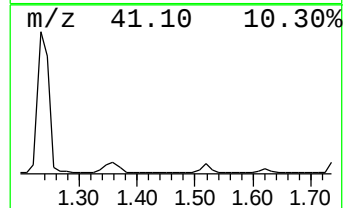
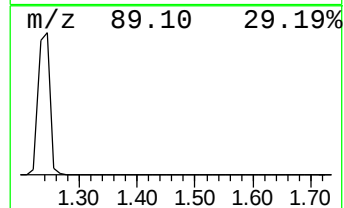
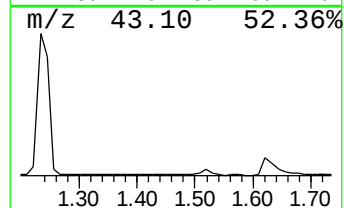
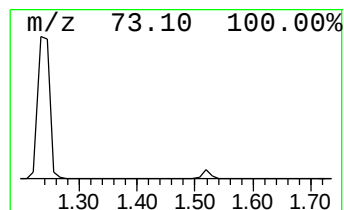
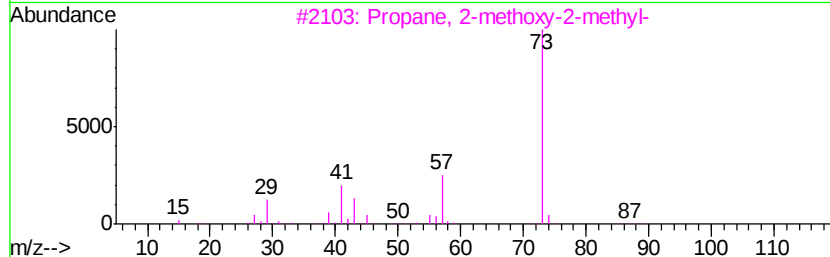
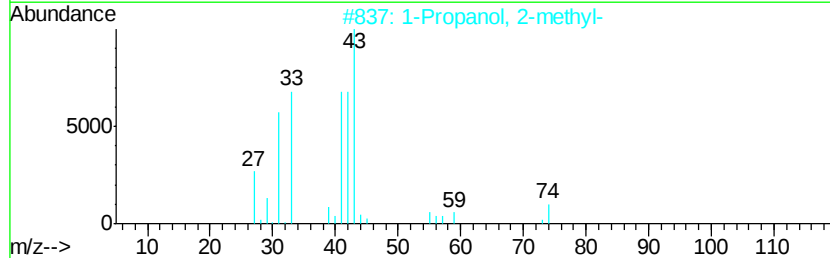
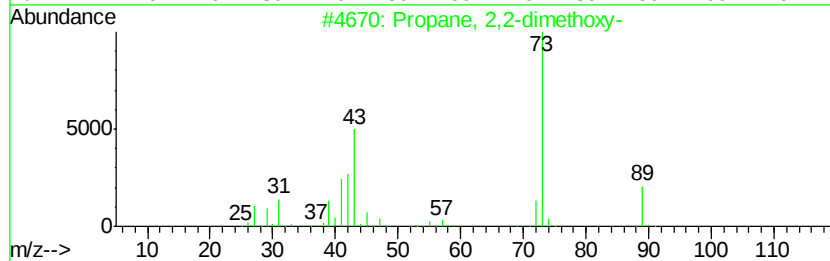
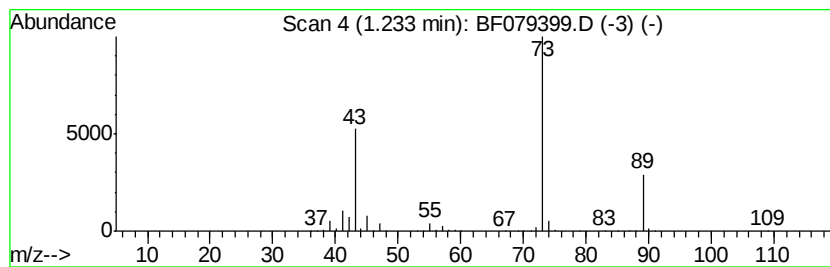
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.23	193.83 ng	4262490	1,4-Dichlorobenzene-d4	7.10

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		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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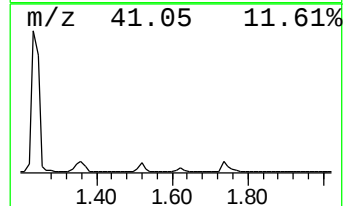
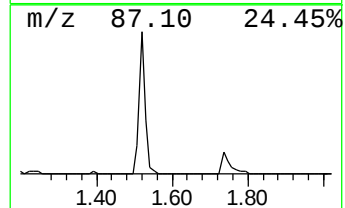
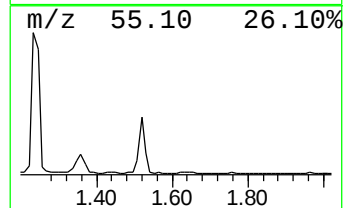
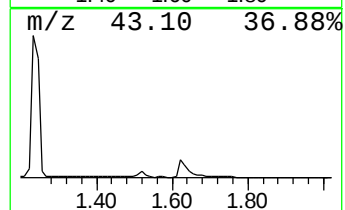
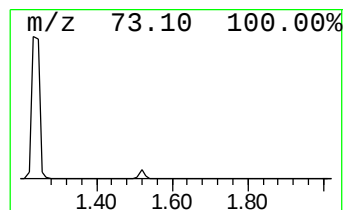
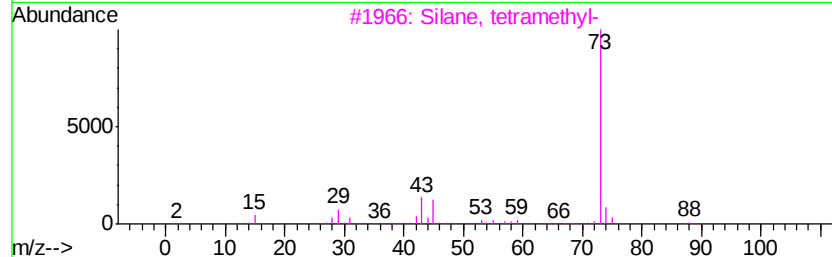
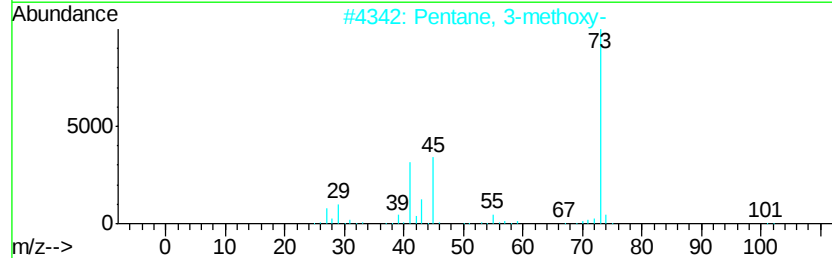
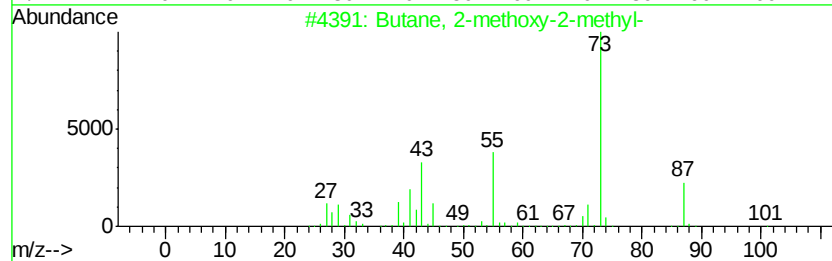
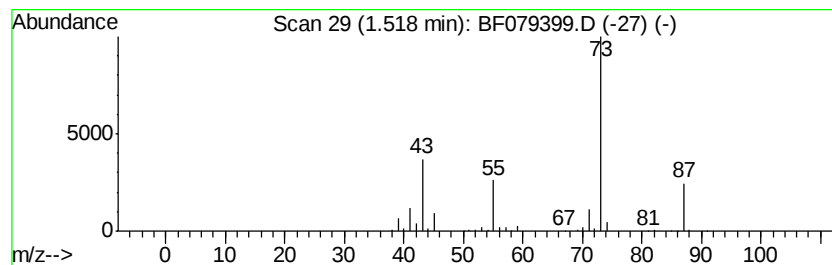
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.52	10.47 ng	230153	1,4-Dichlorobenzene-d4	7.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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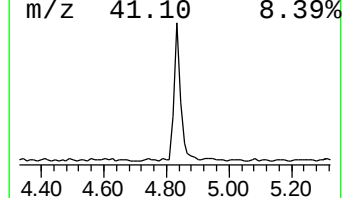
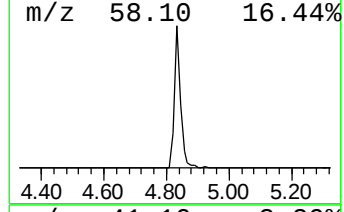
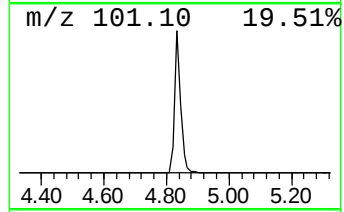
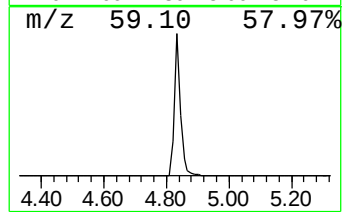
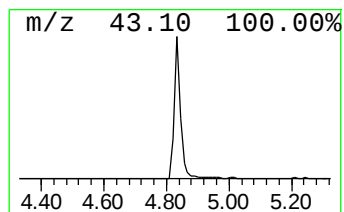
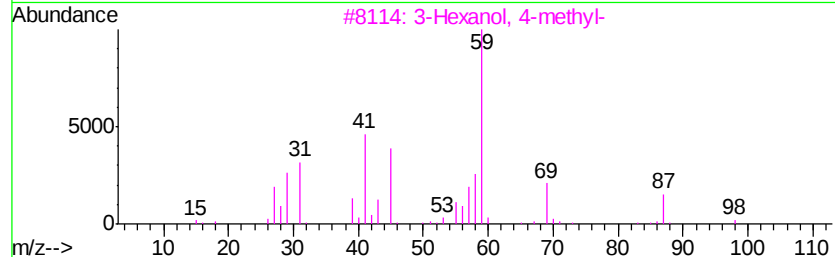
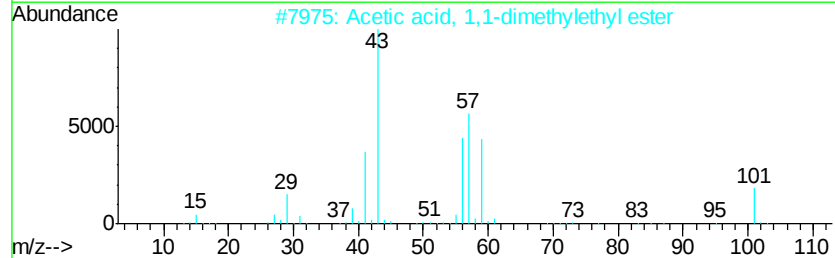
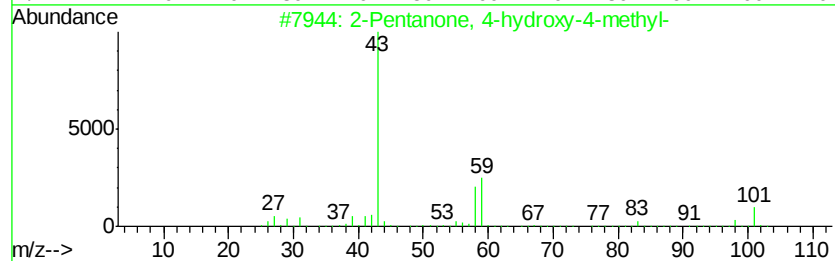
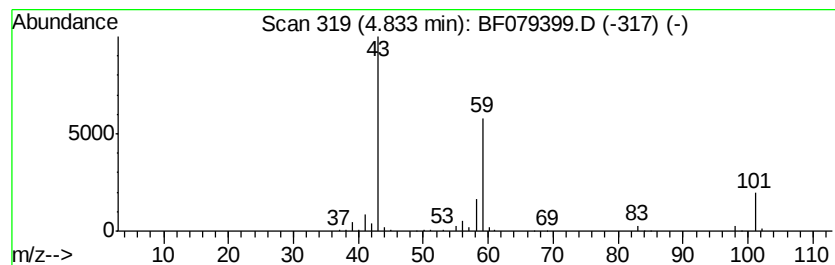
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	20.75 ng	456350	1,4-Dichlorobenzene-d4	7.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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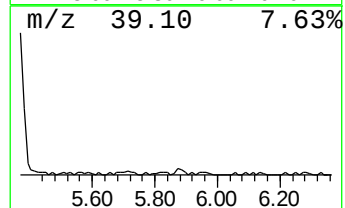
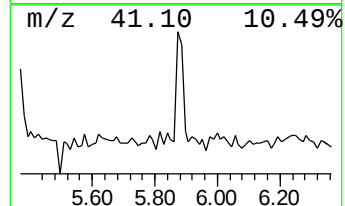
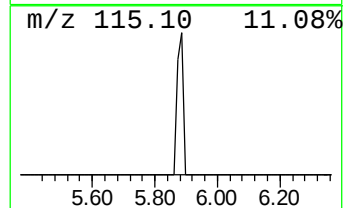
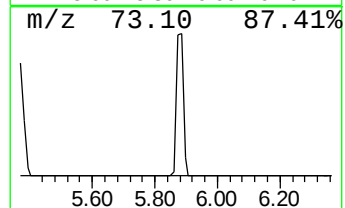
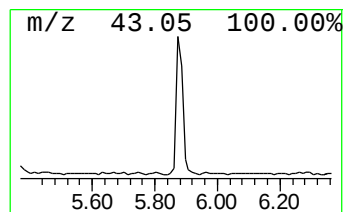
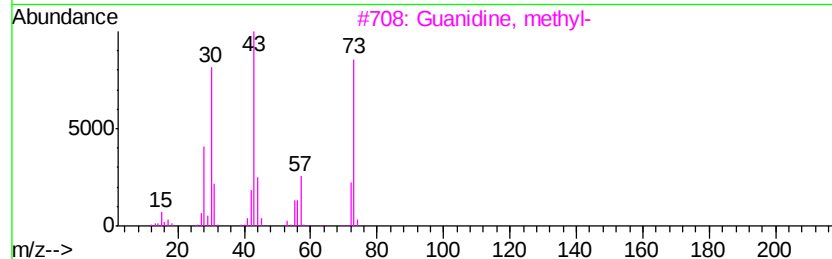
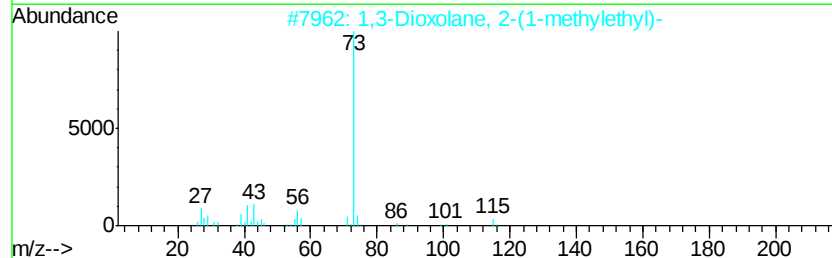
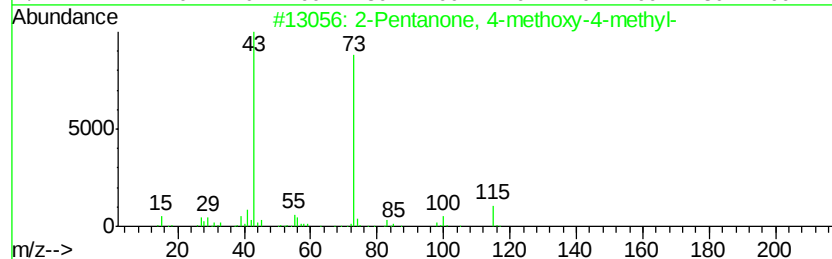
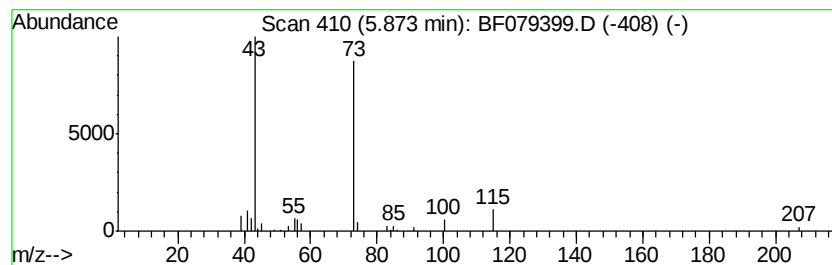
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Peak Number 7 2-Pentanone, 4-methoxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	2.47 ng	54262	1,4-Dichlorobenzene-d4	7.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	28
3		Guanidine, methyl-	73	C2H7N3	000471-29-4	9
4		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5		3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	9



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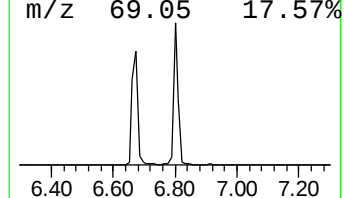
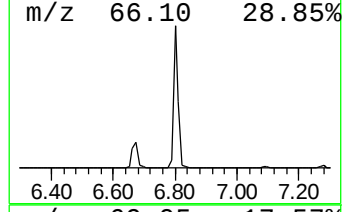
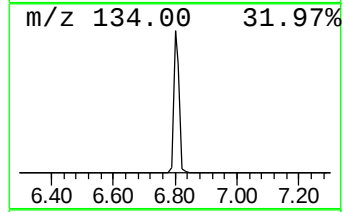
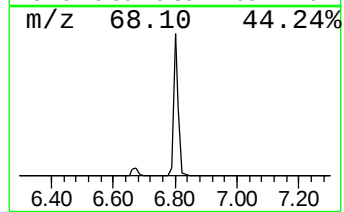
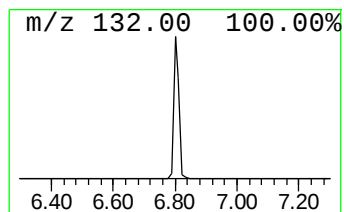
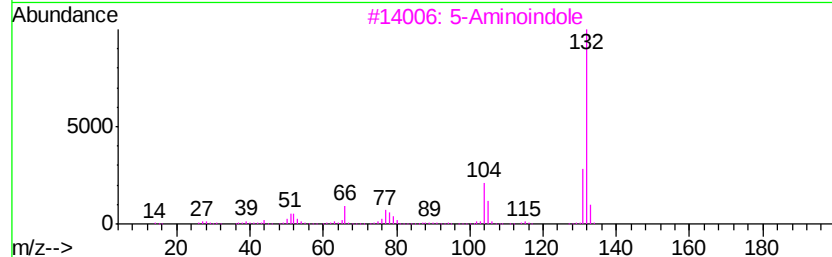
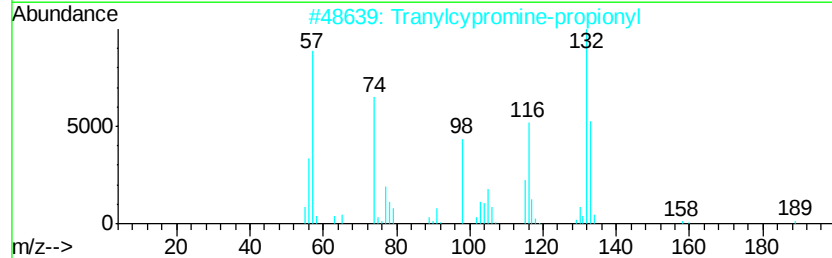
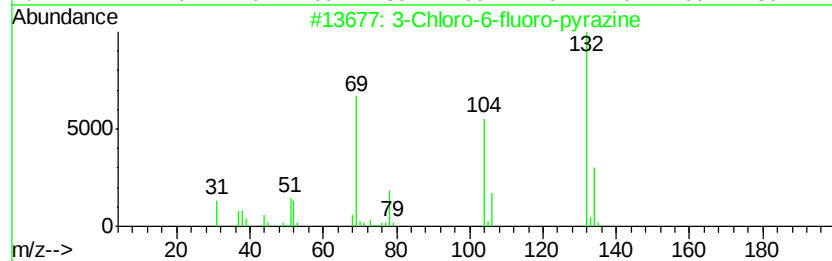
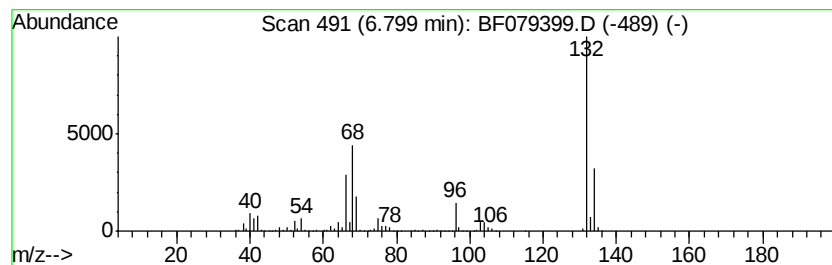
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Peak Number 8 unknown6.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	76.63 ng	1685110	1,4-Dichlorobenzene-d4	7.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			5-Aminoindole	132	C8H8N2	005192-03-0	10
4			Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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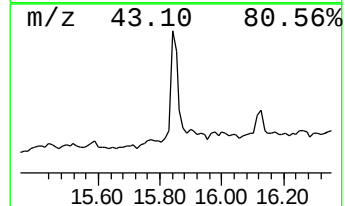
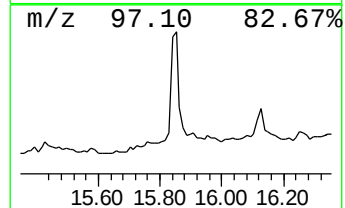
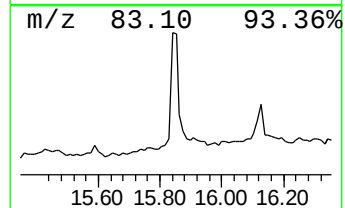
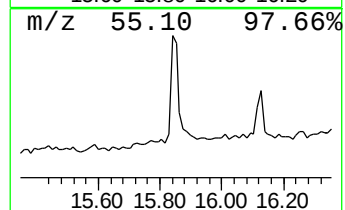
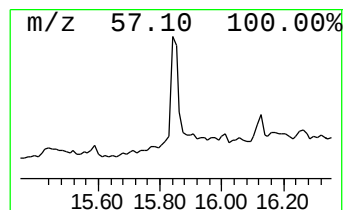
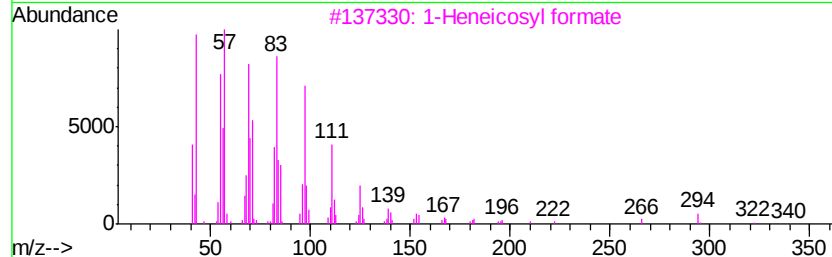
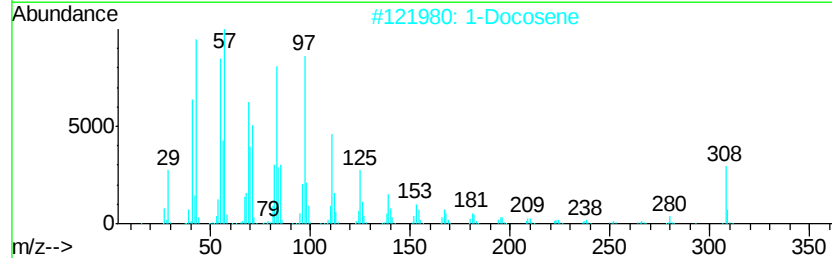
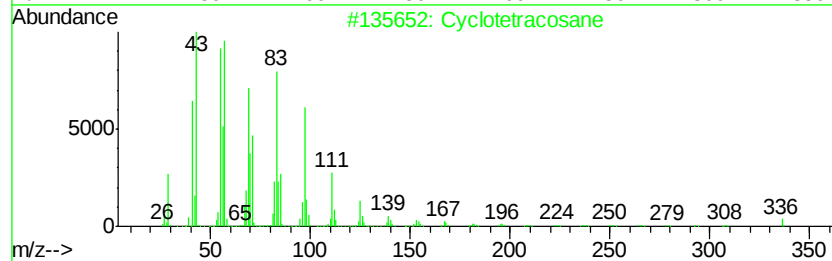
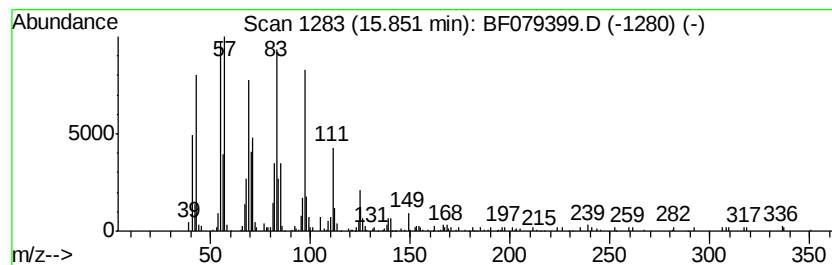
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclotetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	9.57 ng	393835	Chrysene-d12	15.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetracosane	336	C24H48	000297-03-0	99
2		1-Docosene	308	C22H44	001599-67-3	95
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		1-Octadecene	252	C18H36	000112-88-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052015\
Data File : BF079399.D
Acq On : 21 May 2015 1:14
Operator : TP/IZ
Sample : G2305-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

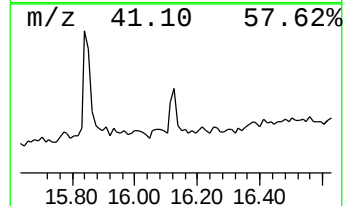
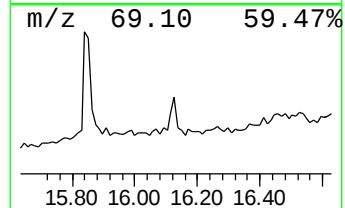
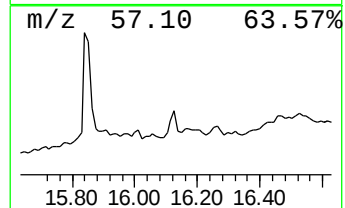
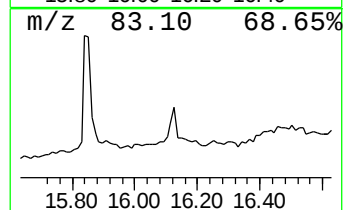
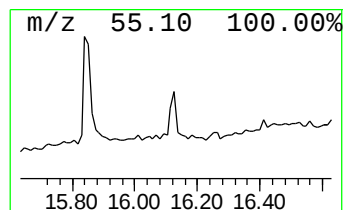
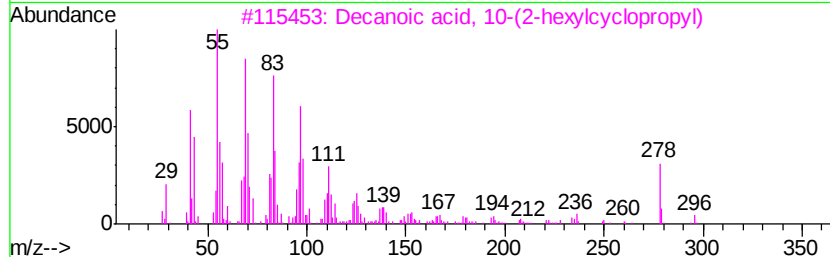
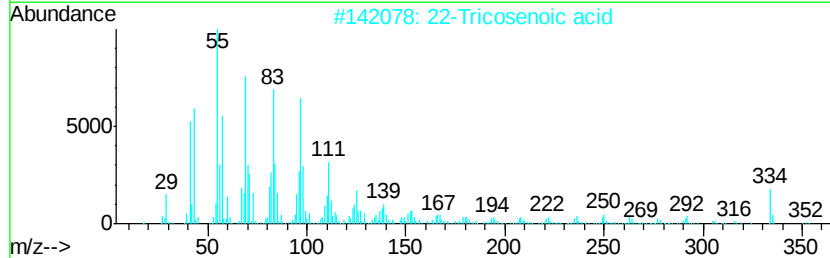
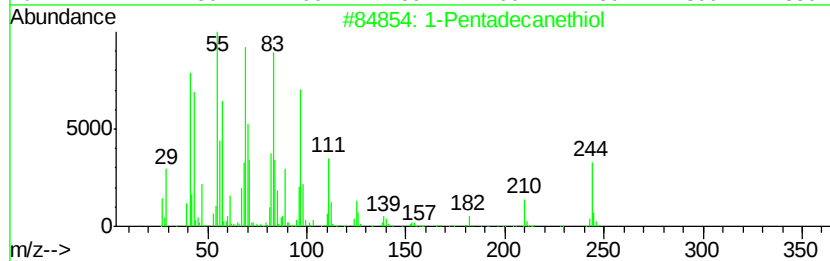
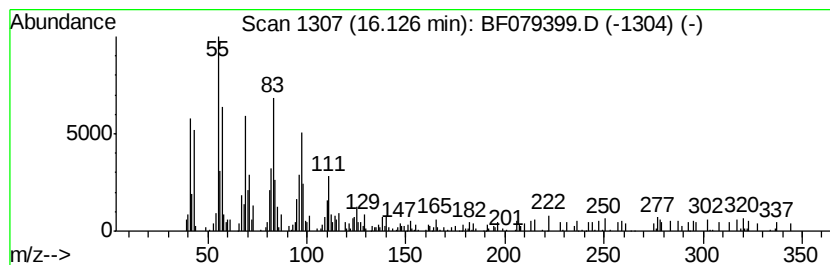
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ClientSampleId :
KM-SP-002-150518

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Pentadecanethiol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.13	2.95 ng	121350	Chrysene-d12	15.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	93
2		22-Tricosenoic acid	352	C23H44O2	065119-95-1	91
3		Decanoic acid, 10-(2-hexylcyclop...	296	C19H36O2	1000197-99-5	83
4		1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	78
5		Cyclopentadecane	210	C15H30	000295-48-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052015\
Data File : BF079399.D
Acq On : 21 May 2015 1:14
Operator : TP/IZ
Sample : G2305-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KM-SP-002-150518

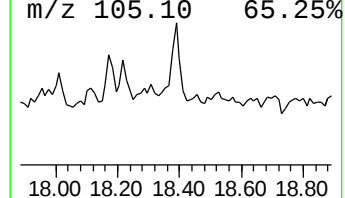
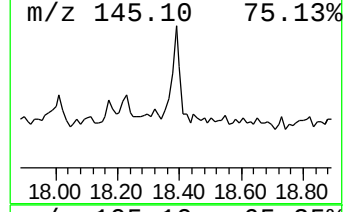
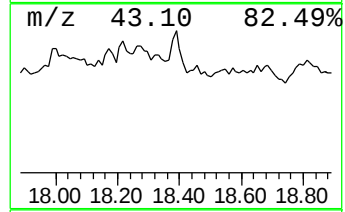
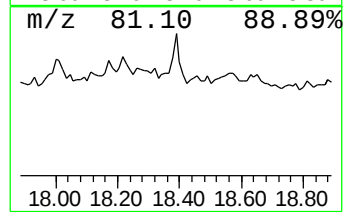
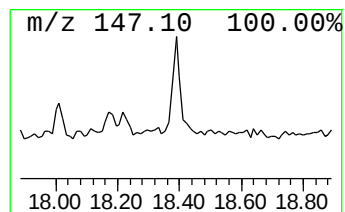
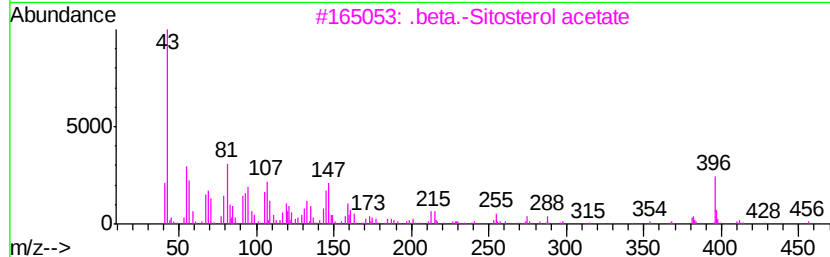
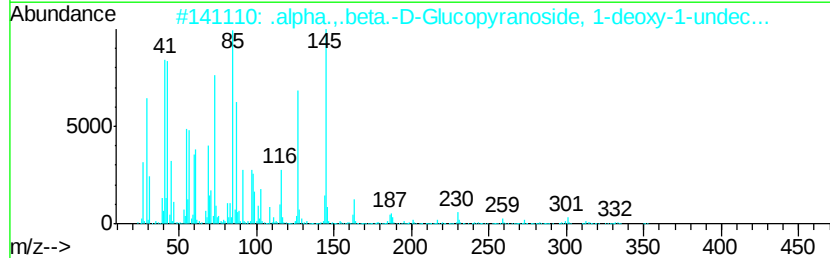
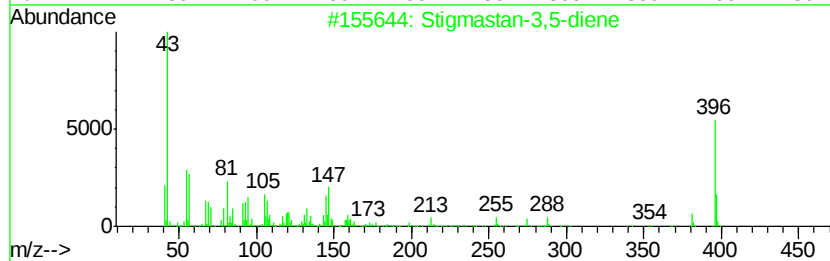
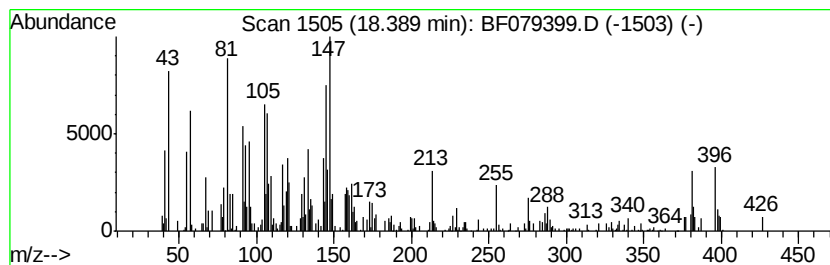
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Stigmastan-3,5-diene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	5.10 ng	206840	Perylene-d12	17.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	86
2		.alpha.,.beta.-D-Glucopyranoside...	350	C17H34O5S	1000160-71-9	25
3		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	22
4		Naphthalene, 5-(1-decylundecyl)-...	426	C31H54	056282-45-2	11
5		1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052015\
Data File : BF079399.D
Acq On : 21 May 2015 1:14
Operator : TP/IZ
Sample : G2305-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KM-SP-002-150518

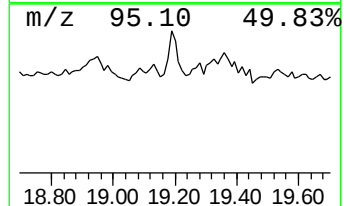
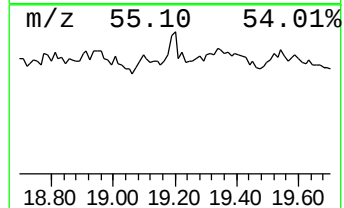
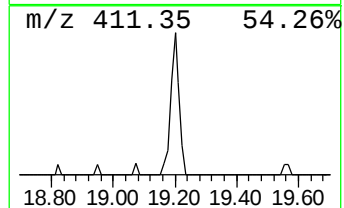
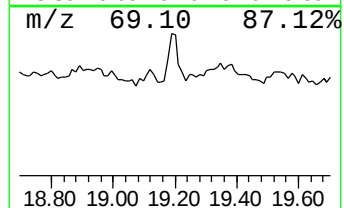
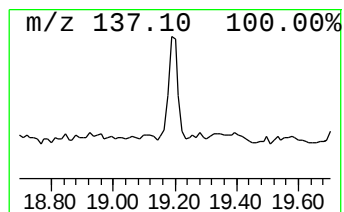
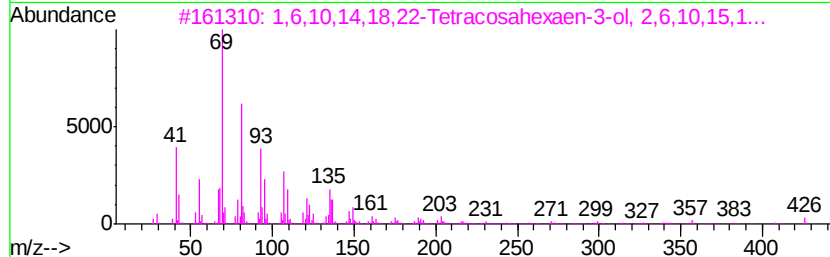
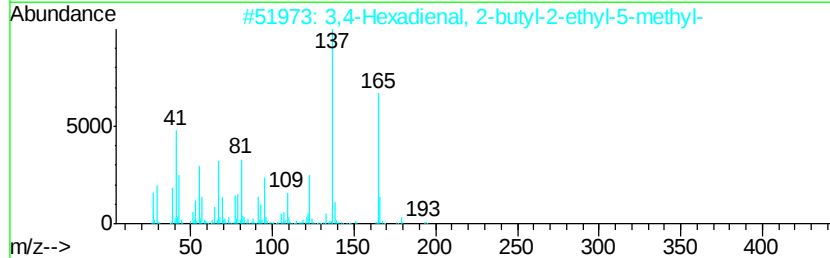
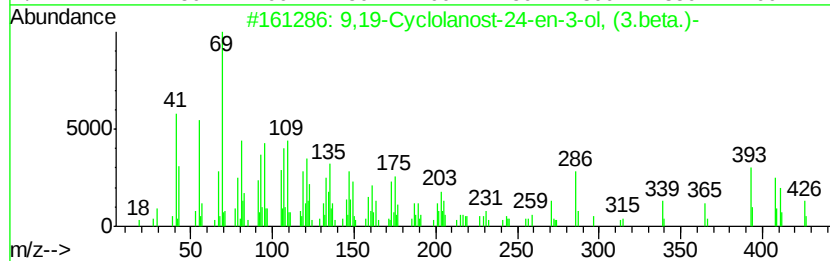
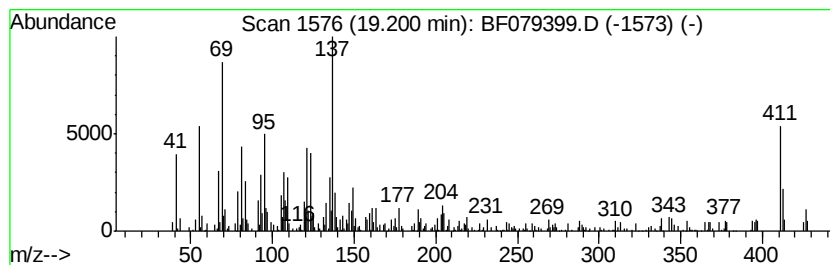
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown19.20 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	5.13 ng	207953	Perylene-d12	17.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, (3...	426	C30H500	000469-38-5	42		
2	3,4-Hexadienal, 2-butyl-2-ethyl-...	194	C13H220	023739-80-2	32		
3	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H500	054159-46-5	30		
4	Naphthalene, 1,1'-methylenebis[d...	288	C21H36	055125-02-5	22		
5	Naphthalene, decahydro-1-pentade...	348	C25H48	066359-82-8	22		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052015\
Data File : BF079399.D
Acq On : 21 May 2015 1:14
Operator : TP/IZ
Sample : G2305-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KM-SP-002-150518

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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
Propane, 2,2-dime...	1.23	193.8	ng	4262490	1	7.10	439810	20.0
Butane, 2-methoxy...	1.52	10.5	ng	230153	1	7.10	439810	20.0
2-Pentanone, 4-hy...	4.83	20.8	ng	456350	1	7.10	439810	20.0
2-Pentanone, 4-me...	5.87	2.5	ng	54262	1	7.10	439810	20.0
unknown6.80	6.80	76.6	ng	1685110	1	7.10	439810	20.0
Cyclotetracosane	15.85	9.6	ng	393835	5	15.97	822956	20.0
1-Pentadecanethiol	16.13	3.0	ng	121350	5	15.97	822956	20.0
Stigmastan-3,5-diene	18.39	5.1	ng	206840	6	17.68	810426	20.0
unknown19.20	19.20	5.1	ng	207953	6	17.68	810426	20.0