

Electronic Supplementary Information

Deamidation analysis of Therapeutic Drugs using Matrix-assisted Laser Desorption Ionization Mass Spectrometry and A Novel Algorithm QuanDA

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1	EVQLVESGGG	LVOPGGSLRL	SCAASGYTFT	NYGMNWVRQA	PGKGLEWVGW
51	INTYTGEPTY	AADFKRRFTF	SLDTSKSTAY	LQMNSLRAED	TAVYYCAKYP
101	HYYGSSHWFY	DVWGQGTLVT	VSSASTKGPS	VFPLAPSSKS	TSGGTAALGC
151	LVKDYFPEPV	TVSWNSGALT	SGVHTFPAVL	QSSGLYSLSS	VVTVPSSSLG
201	TQTYICNVNH	KPSNTKVDKK	VEPKSCDKTH	TCPPCPAPEL	LGGPSVFLFP
251	PKPKDTLMIS	RTPEVTCVVV	DVSHEDPEVK	FNWYVDGVEV	HNAKTKPREE
301	QYNSTYRVVS	VLTVLHQDWL	NGKEYKCKVS	NKALPAPIEK	TISKAKGQPR
351	EPQVYTLPPS	REEMTKNQVS	LTCLVKGFYP	SDIAVEWESN	GQPENNYKTT
401	PPVLDSGDSF	FLYSKLTVDK	SRWQQGNVFS	CSVMHEALHN	HYTQKSLSLS
451	PGK				

Bevacizumab heavy chain

1	DIQMTQSPSS	LSASVGDRVT	ITCSASQDIS	NYLNWYQQKP	GKAPKVLIIYF
51	TSSLHSGVPS	RFSGSGSGTD	FTLTISLQP	EDFATYYCQQ	YSTVPWTFGQ
101	GTKVEIKRTV	AAPSVFIFPP	SDEQLKSGTA	SVVCLLNNFY	PREAKVQWKV
151	DNALQSGNSQ	ESVTEQDSKD	STYLSSTLT	LSKADYEKHK	VYACEVTHQG
201	LSSPVTKSFN	RGEC			

Bevacizumab light chain

Figure S1.- Amino acid sequence of Bevacizumab.

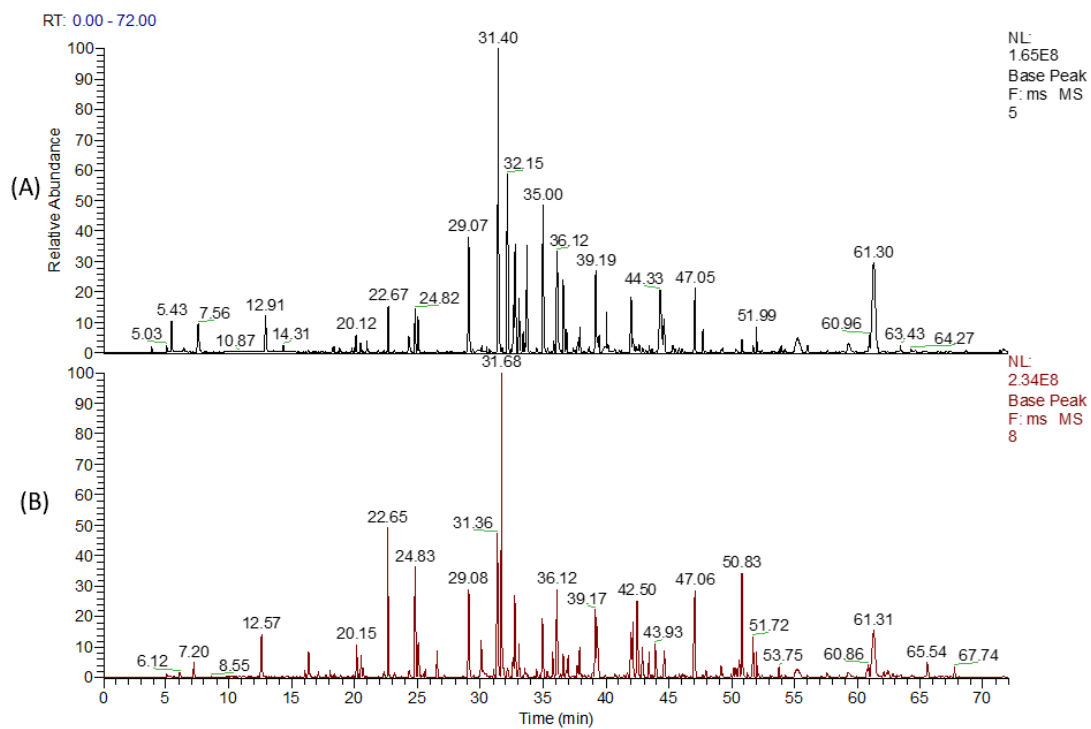


Figure S2.- Liquid chromatogram of Bevacizumab after enzymolysis with Glu-C under
(A) pH=5; (B) pH=8.

Table S1.- Peptide segments and sites where deamidation may occur.

No.	Sequence	Modifications
1	KHKVYACEVTHQGLS- SPVTKSFNRGEC	2xCarbamidomethyl [C7; C27]; 1xDeamidated[N23]
2	NALQSGNSQESVTE	1xDeamidated [N7]
3	WESNGQPE	1xDeamidated [N4]
4	VKFNWYVDGVE	1xDeamidated [N4]
5	VHNAKTKPREE	1xDeamidated [N3]
6	SNGQPE	1xDeamidated [N2]
7	VTHQGLSSPVTKSFNRGE	1xDeamidated[N15]
8	VTHQGLSSPVTKSFNRGEC	1xDeamidated[N15]; 1xCarbamidomethyl[C19]
9	TSKSTAYLQMNSLRAE	1xDeamidated[N11]
10	AKVQWKVDNALQ- SGNSQESVTE	1xDeamidated [N9]
11	NNYKTPPVLDSD	1xDeamidated [N2]
12	YKCKVSNKALPAPIE	1xCarbamidomethyl[C3]; 1xDeamidated [N7]
13	SDGSFFLYSKLTVDKSR- WQQGNVFSCSVMHE	1xCarbamidomethyl[C26]; 1xDeamidated[N22]
14	SGGGLVQPGGSLRLSCA- ASGYTFTNYGMNWVR- QAPGKGLE	1xCarbamidomethyl[C16]; 2xDeamidated [N25; N29]; 1xOxidation [M28]
15	QLKSGTASVVCL- LNNFYPRE	1xCarbamidomethyl[C11]; 2xDeamidated [N14; N15]
16	MTKNQVSLTCLV- KGFYPSDIAVE	1xCarbamidomethyl[C10]; 1xDeamidated [N4]

Abbreviations: QuanDA, Quantification Deamidation