

## Supporting Information

# Identification of Antioxidant Peptides using Radical Directed Dissociation

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Supporting information includes A $\beta$  1-40 RDD from Tyrosine radical, RDD of PHCKRM and SLHTLFGDK peptides, and comparison of CID of even and odd electron species of antioxidant peptides. Lipid peroxidation assay for peptides not identified as antioxidants is also included. All peptides examined with RDD from HSA digest.

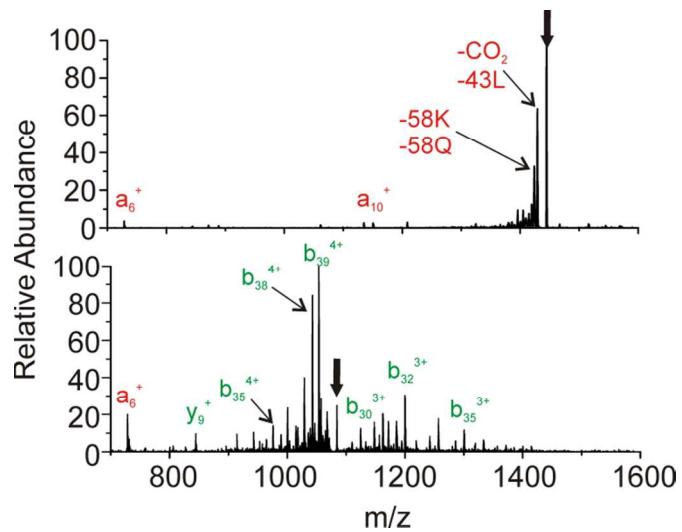


Figure S1: CID of radical A $\beta$  1-40 from iodotyrosine, +3 (top) and +4 (bottom)

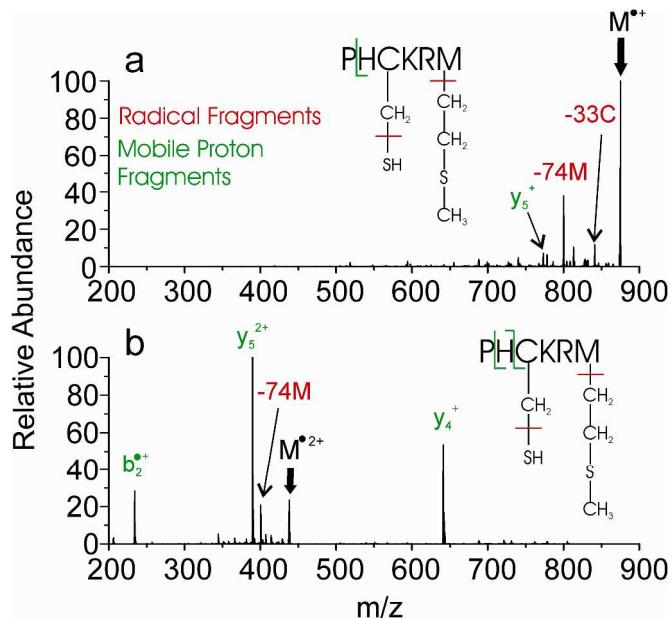


Figure S2: CID of PHCKRM radical in a) +1 and b) +2 charge states

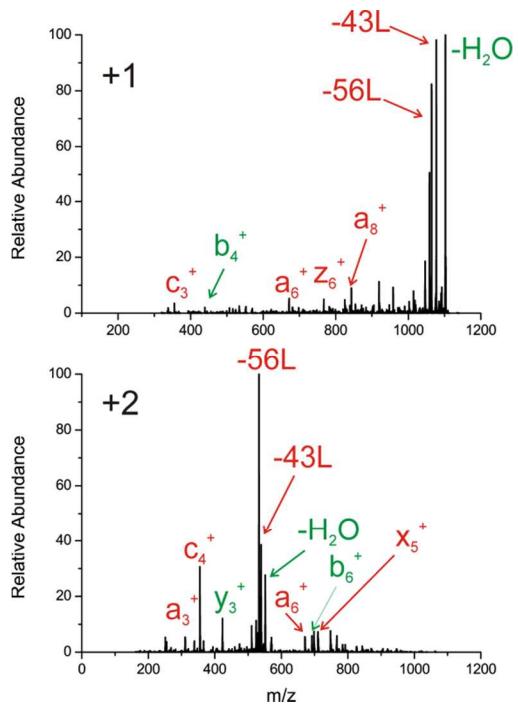


Figure S3: CID of  $SLHTLFKGDK^{4IB}$  radical in +1 and +2 charge states.

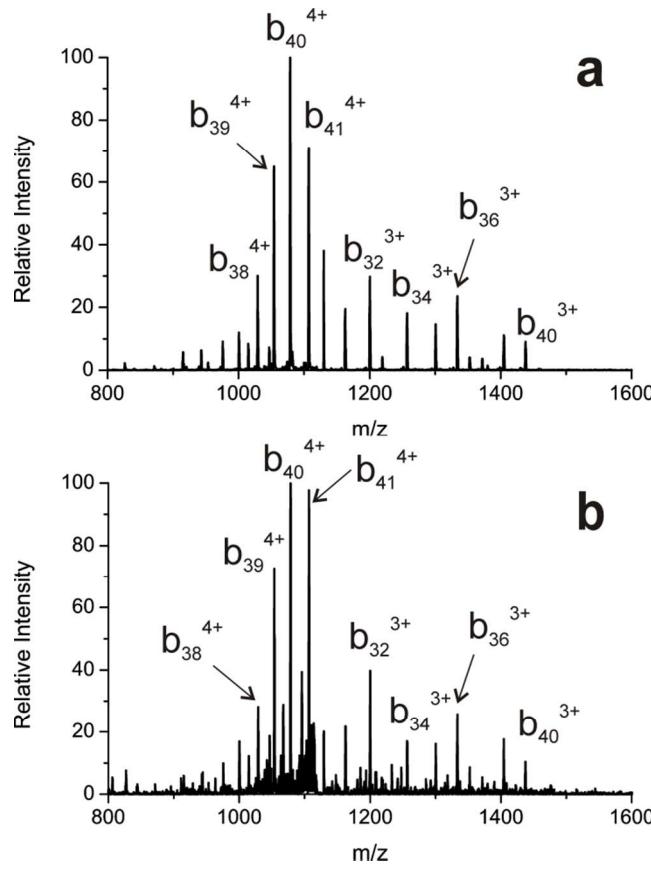


Figure S4: Comparison of CID fragmentation of a)  $\text{A}\beta$  1-42 and b)  $\text{A}\beta$  1-42 radical for +4.

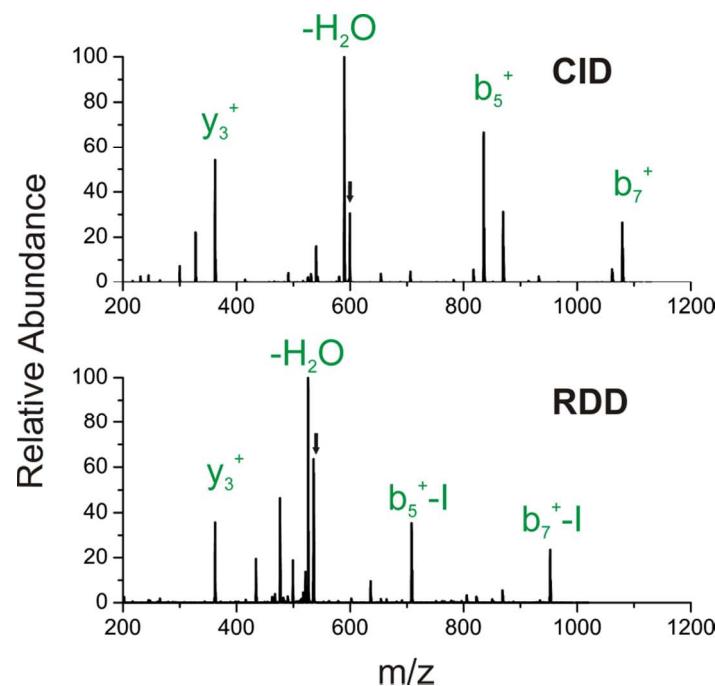


Figure S5: CID of even electron and radical species of PSK<sup>4<sup>1</sup>B</sup>YEPFV

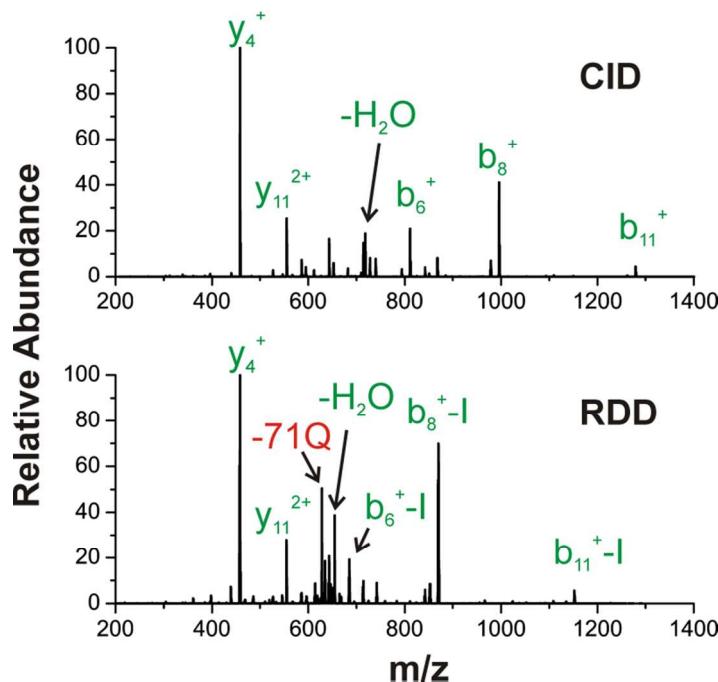


Figure S6: CID of even electron and radical species of <sup>4<sup>1</sup>B</sup>NGPLQAGQPGER

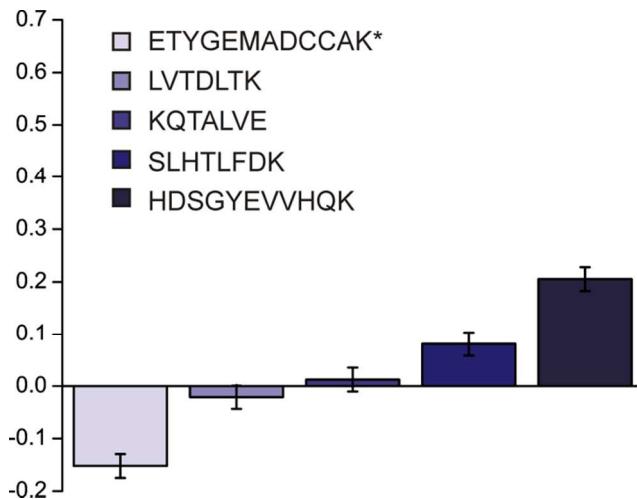


Figure S7: Lipid Peroxidation inhibition in the presence of peptides with RSS<1. \*Cysteines blocked using iodoacetamide.

Table S1: RSS values for all HSA peptides

<b>TFLK</b>	<b>14.67</b>
<b>VAHRFK</b>	<b>5.21</b>
<b>VPQVSTPTLVEVSR</b>	<b>4.21</b>
<b>DVFLGMFLYEYAR</b>	<b>3.79</b>
<b>DDNPNLPR</b>	<b>2.83</b>
<b>LYYEIAR</b>	<b>1.30</b>
SEVAHR	0.89
NYEAK	0.79
TPVSDRVTK	0.68
LVTDLTK	0.57
LVNEVTEFAK	0.55
KQTALVE	0.53
EQLK	0.52
KYLYE	0.51
FQNALLVR	0.51
DAHKSE	0.49
AWAVAR	0.48
SLHTLFGDKLCTVATLR	0.46
SLHTLFGDK	0.46
VSKLVTDLTK	0.43
AACLLPK	0.41
LDELRDEGK	0.39
CASLQK	0.36
KSLHTLFGD	0.35
TYETTLEK	0.35
SEVAHRFK	0.34
QEPPERNE	0.33

AEFAEVSK	0.32
ADDKETCFAEEGK	0.31
HPDYSVVLRLR	0.29
RPCFSALEVDETYVPK	0.27
KVPQVSTPTLVEVSR	0.25
FAKTCVADE	0.24
DLGEENFK	0.24
AEFAEVSKLVTDLTK	0.21
TCVADESAENCDK	0.20
ETYGEMADCCAK	0.20
QEPERNECFLQHK	0.17
VSRNLGK	0.16
SISSKLK	0.15
NYAEAKD	0.14
ETCFAEEGK	0.14
YKAAFTECCQAADK	0.14
AAFTECCQAADK	0.12
CAAADPHECYAK	0.11
KPLLEK	0.10
CFLQHKD	0.08
LVRPEVDVMCTAFHDNEETFLK	0.08
TCFAEEGKK	0.06
AVMDDFAAFVEK	0.06
TPVSDRVTKCCTE	0.05
FQNALLVRYTK	0.05
NECFLQHK	0.05
ICTLSEKE	0.04
VPQVSTPTLVE	0.04
VMCTAFHDNEE	0.03
VHTECCHGDLLECADDR	0.03
PLEKSHCIAE	0.02
CCQAADK	0.01

**Peptides Identified and examined for antioxidant activity from Trypsin HSA digest:**

HPEAK, SEVAHR, TCVADESAENCDK, CCAAADPHECYAK, TPVSDR, DDNPNLPR, NYEAK, AEFAEVSKLVTDLTK, LDELRDEGK, VHTECCHGDLLECADDR, AAFTECCQAADK, QEPERNECFLQHK, ETYGEMADCCAK, ADDKETCFAEEGK, EQLK, CASLQK, ETCFAEEGK, KVPQVSTPTLVEVSR, NECFLQHK, YKAAFTECCQAADK, SLHTLFGDKLCTVATLR, TYETTLEK, AEFAEVSK, DLGEENFK, VPQVSTPTLVEVSR, LVTDLTK, FQNALLVR, RPCFSALEVDETYVPK, AACLLPK, LVNEVTEFAK,

LVRPEVDVMCTAFHDNEETFLK, YLYEIAR, SLHTLFGDK, HPDYSVVLLR, AWAVAR, AVMDDFAAFVEK, CCKHPEAK, DVFLGMFLYEAR.

**Peptides Identified and examined for antioxidant activity from Glu-C/Lys-C HSA digest:**

DAHKSE, CCQAAD, SISSKLK, VS KLVTDLTK, QEPERNE, P LLEKSHCIAE, CFLQHKD, CCQAADK, TPVSDRVTKCCTE, VSRNLGK, TPVSDRVTK, FAKTCVADE, SEVAHRFK, FQNALLVRYTK, VMCTAFHDNEE, KQTALVE, KYLYE, NYAEAKD, KPLLEK, ICTLSEKE, VPQVSTPTLVE, KSLHTLFGD, VAHRFK, NQDSISSK, AAFTECCQAADK, KQTALVE, KVPQVSTPTLVE, KLVAASQAALGL, TFLK.