Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Gated Electron Transfer Reactions of Truncated Hemoglobin from *Bacillus subtilis* Differently Orientated on SAM-modified Electrodes

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Figures

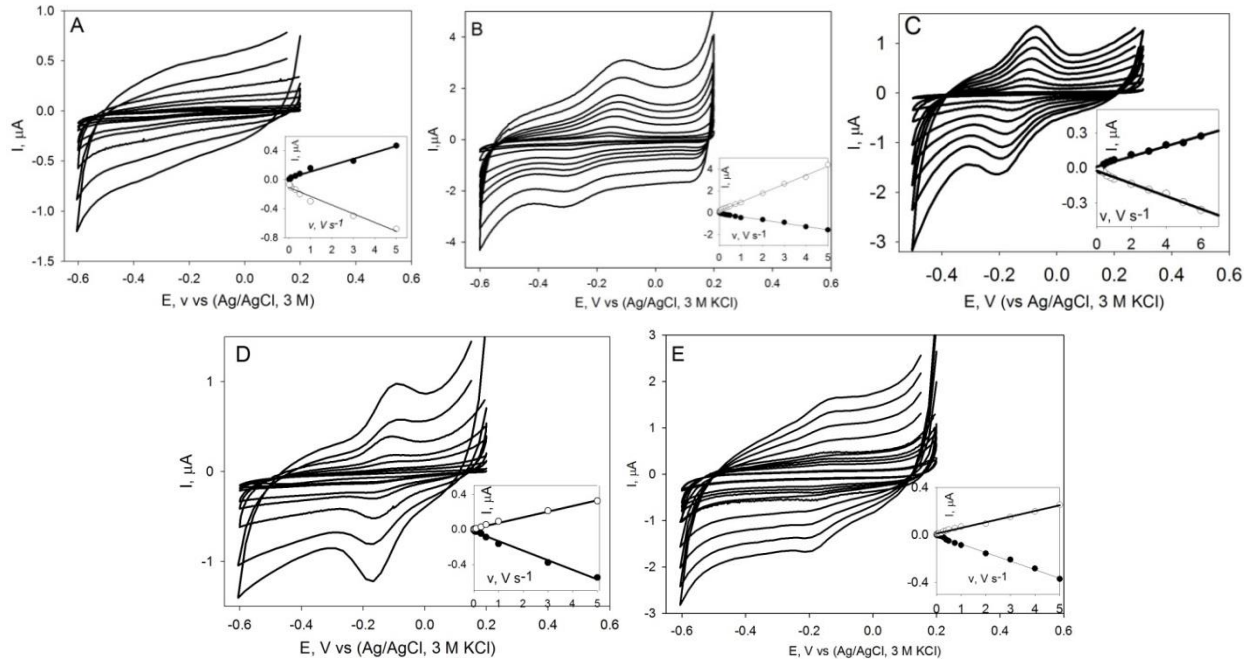

Figure S1. Representative cyclic voltammograms recorded at different scan rates in deaerated 10 mM PBS with *TrHb-Bs* –modified electrodes; *TrHb-Bs* was adsorbed onto (a) $C_{11}OH$-, and covalently attached to (b) C_5COOH-, (c) C_8NH_2-, (d) C_6NH_2-, and (e) C_2NH_2-modified gold electrodes, pH 7.0. Insets: The dependence of anodic and cathodic peaks currents on the potential scan rate.

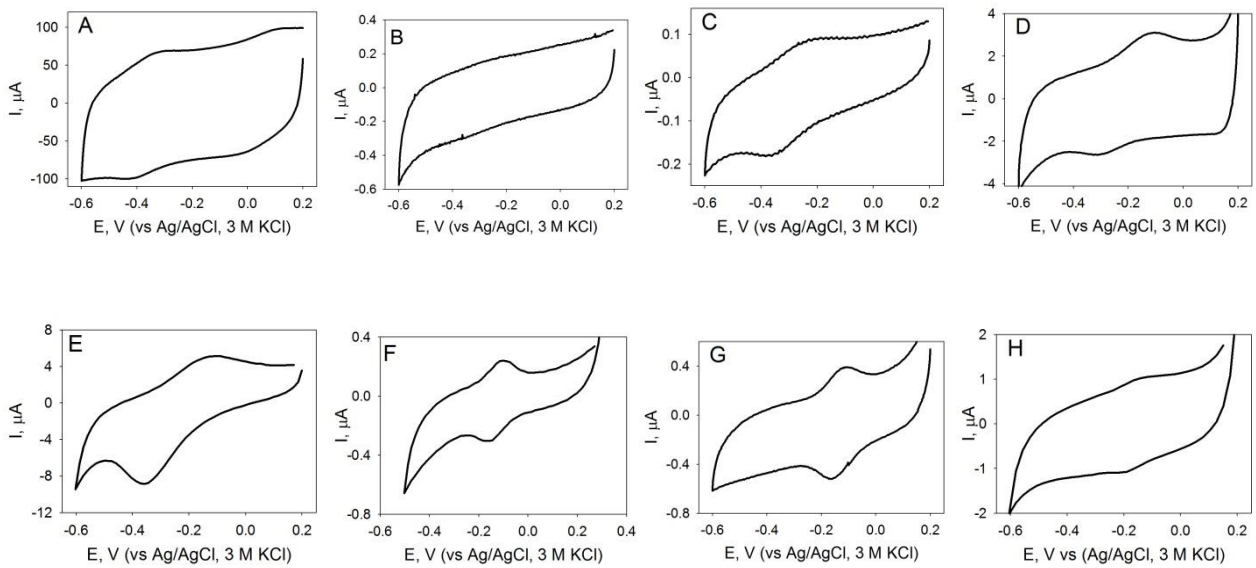

Figure S2. Representative CVs recorded in deaerated 10 mM PBS with *TrHb-Bs* –modified electrodes: (a) graphite, (b) $C_{11}OH$-, (c) $C_{10}COOH$-, (d) C_5COOH-, (e) $C_{11}NH_2$-, (f) C_8NH_2-, (g) C_6NH_2- and (h) C_2NH_2-modified gold electrodes, pH 7.0, potential scan rate 1 V s^{-1}.

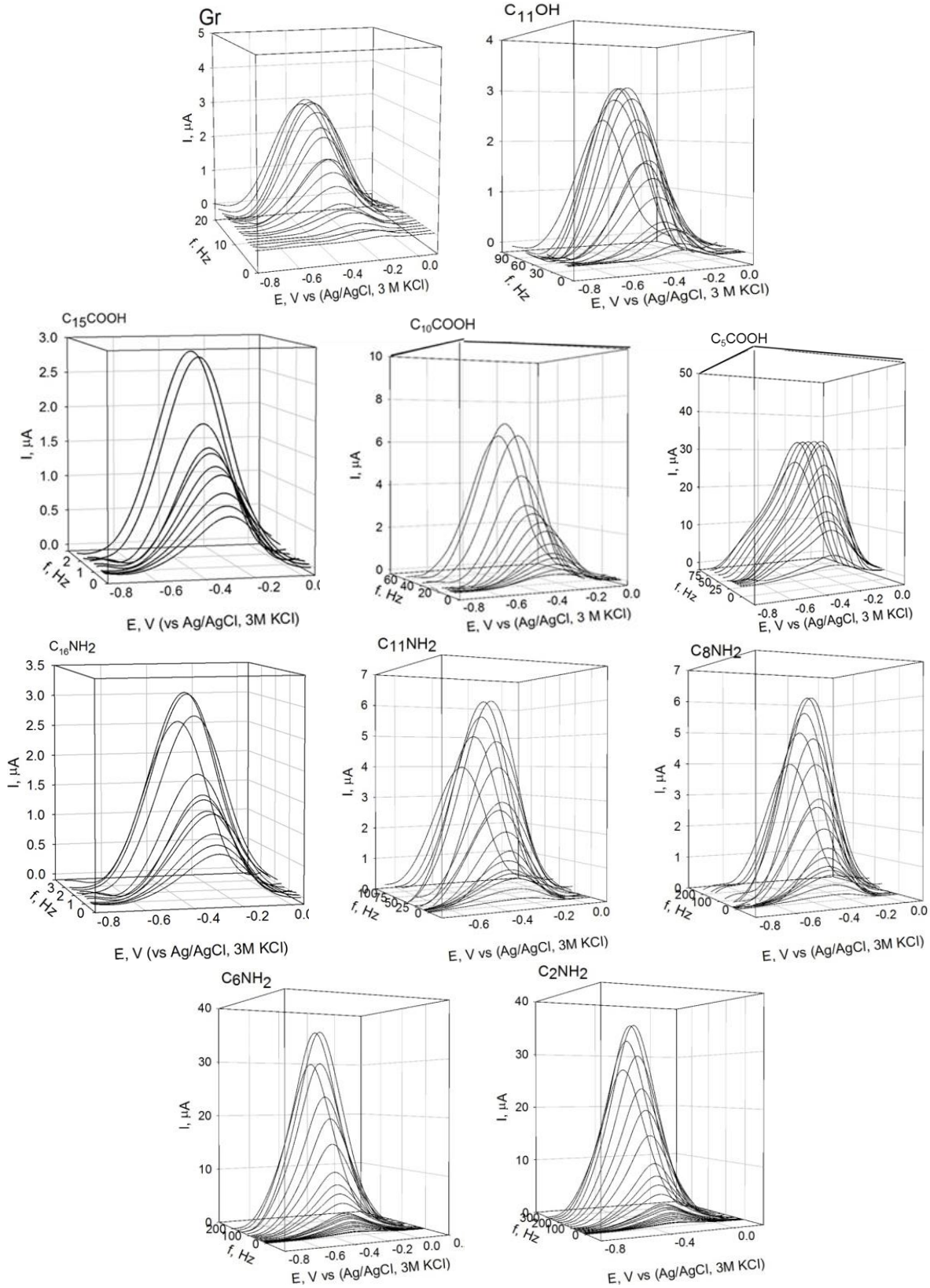

Figure S3. Representative background corrected SWVs recorded in deaerated 10 mM PBS, pH 7, with *TrHb-Bs* –modified electrodes: graphite, OH and COOH terminated- and NH_2- terminated SAMs of different alkane chain lengths.

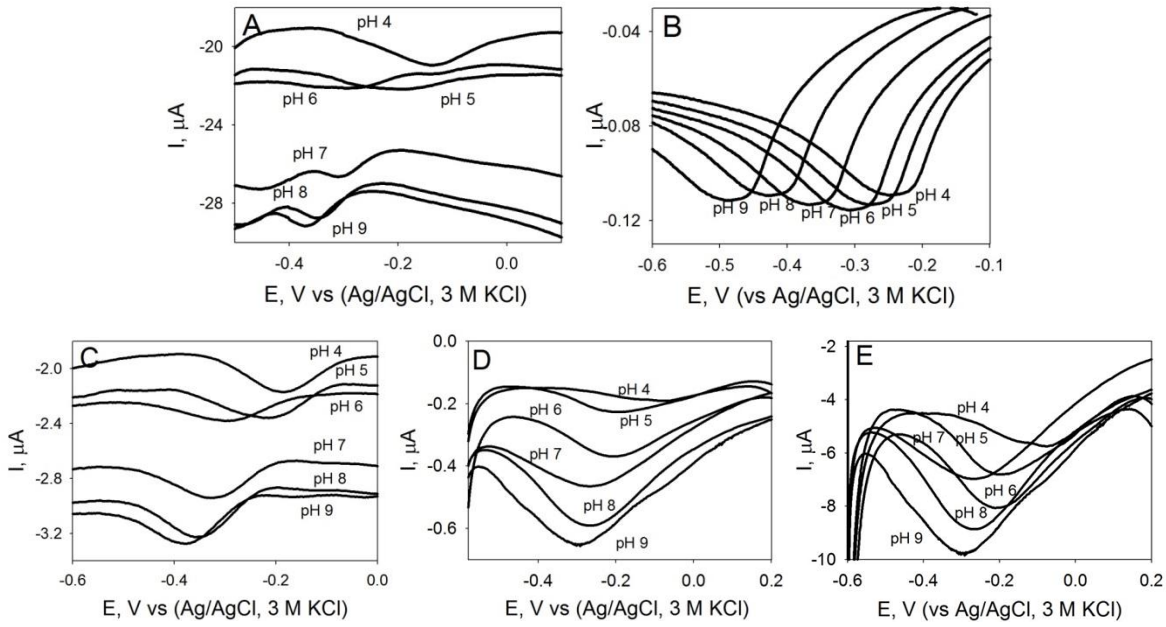

Figure S4. Representative DPVs recorded in deaerated 10 mM PBS with *TrHb-Bs* –modified electrodes: (a) graphite, (b) $C_{16}NH_2$, (c) $C_{11}NH_2$, (d) C_6NH_2 and (e) C_2NH_2 -modified gold electrodes; pH 4.0, 5.0, 6.0, 7.0, 8.0, and 9.0.

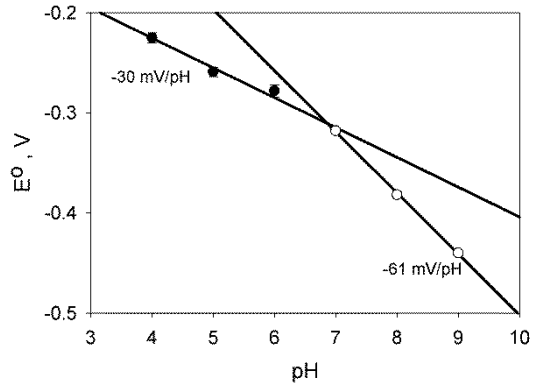

Figure S5. pH dependences of the heme redox potential in trHb-*Bs* immobilized on $C_{16}NH_2$, (modified gold, DPV (Figure S4, ESI) were recorded in deaerated 10 mM PBS of the corresponding pH.

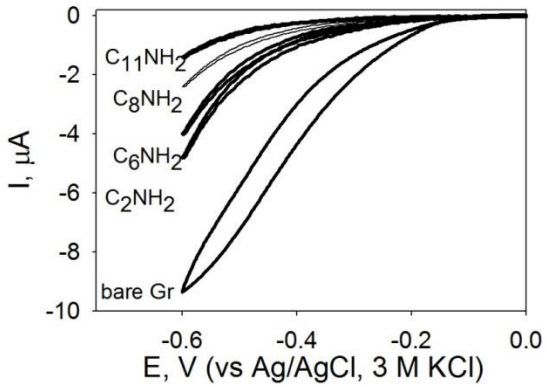

Figure S6. Representative cyclic voltammograms of O_2 reduction at bare graphite electrode and gold electrodes modified with $C_{11}NH_2$, C_8NH_2, C_6NH_2 and C_2NH_2 SAMs recorded in 10 mM PBS, pH 7, potential scan rate 0.05 V s^{-1}.

Tables

Table S1. The atomic packing density ρ (the fraction of the volume between redox centres that is within the united van der Waals radius of intervening atoms), the distance r between the heme iron of trHb-*Bs* and the corresponding surface amino acid residues, and resulting ET rates.

Amino acid	Sequence position	distance, Å	density, ρ	k_{ET}	log k_{ET}
Asp, D	22	13,55	0,93	2,95E+08	8,47
	41	12,69	0,42	1,32E+05	5,12
	87	11,33	0,95	4,79E+09	9,68
	95	15,90	0,94	4,07E+07	7,61
	98	18,83	0,85	1,32E+05	5,12
Glu, E	10	21,72	0,85	3,98E+03	3,60
	14	18,69	0,66	7,94E+02	2,90
	15	19,54	0,82	2,19E+04	4,34
	26	13,43	0,90	2,19E+08	8,34
	44	12,32	0,87	4,27E+08	8,63
	65	17,15	0,96	1,91E+07	7,28
	66	15,94	0,84	3,63E+06	6,56
	84	12,87	0,81	3,47E+08	8,54
	103	22,10	0,64	2,00E+00	0,30
	105	21,52	0,91	5,50E+04	4,74
	108	18,58	0,91	9,55E+05	5,98
	115	11,92	0,85	4,90E+08	8,69
Asn, N	6	24,91	0,85	1,00E+02	2,00
	83	13,00	0,84	1,12E+08	8,05
	123	9,67	0,74	2,00E+09	9,30
Gln, Q	19	16,18	0,68	5,25E+04	4,72
	49	5,04	0,67	1,10E+12	12,04
	51	12,11	0,82	2,69E+08	8,43
	55	13,34	0,82	5,75E+07	7,76
Lys, K	35	11,75	0,85	6,46E+08	8,81
	48	9,13	0,81	9,77E+09	9,99
	50	10,57	0,78	1,07E+09	9,03
	94	13,81	0,86	6,61E+07	7,82
Arg, R	27	13,09	0,69	7,41E+06	6,87
	47	11,52	0,65	3,98E+07	7,60
	73	8,37	0,76	1,55E+10	10,19
	75	7,15	0,74	6,92E+10	10,84
	85	9,16	0,89	2,00E+10	10,30
	107	17,68	0,78	9,12E+04	4,96
	113	12,02	0,78	1,48E+08	8,17
	119	10,25	0,87	5,01E+09	9,70