Supplemental Information

Therapeutic efficacy of stable analogues of Vasoactive Intestinal Peptide against pathogens

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Files in this Data Supplement: Supplemental figure 1 and Tables S1 to S6

Supplemental Figures

Figure S1. Structural properties of native VIP, VIP51 and VIP51$_{(6-30)}$. For each peptide, top images: ribbon schemes with side chains of amino acids; bottom images: predicted molecular surface model showing theoretical distribution of charges in the surface. The molecular modelling of VIP and VIP derivatives was resolved in the I-TASSER server. Distribution of charged amino acids in ribbon models and in 3D surfaces was visualized using the Pisson-Boltzman algorithm of Swiss Protein Data Bank viewer v4.0.4 (http://spdbv.vital-it.ch/refs.html). Negative residues (red), positive residues (dark-blue), polar residues (pink), and apolar residues (light-blue).

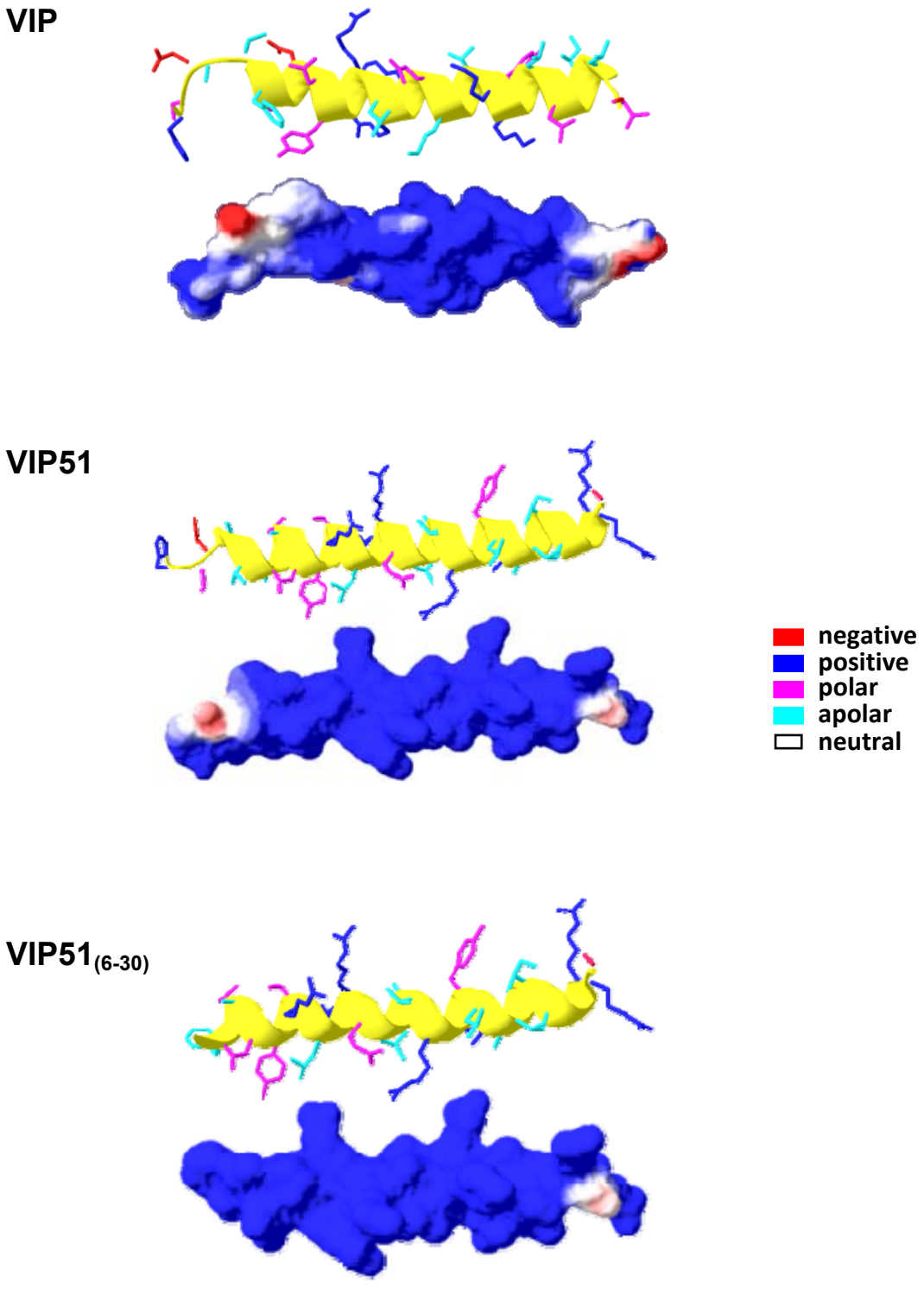

Table S1. Specific hydrogen-bonding contacts between VIP and D21"Ra"

Position[a]	VIP	FTT	PO4	DPO	PA1	GCN	KDO	GMH	GLC	GLA	∑Aa[b]	%Aa[c]
1	H											
2	S											
3	D								2	1	3	10.3
4	A											
5	V											
6	F											
7	T					1	2				3	10.3
8	D						1				1	3.4
9	N											
10	Y											
11	T			1			2		1		4	13.8
12	R			2					1		3	10.3
13	L											
14	R	3	3	1				1			8	27.6
15	K	1	1		2				2		6	20.7
16	Q	1									1	3.4
17	M											
18	A											
19	V											
20	K											
21	K											
22	Y											
23	L											
24	N											
25	S											
26	I											
27	L											
28	N											
	∑Ch[d]	5	4	4	2	1	5	1	6	1		
	%Ch[e]	17	14	14	7	3	17	3	21	3		

[a] Position of each amino acid in the sequence of the VIP molecule.
[b] Summation of hydrogen-bonding contacts between specific amino acids of VIP and D21"Ra".
[c] % of total hydrogen-bonding amino acid implicated in the interaction between VIP and D21"Ra".
[d] Summation of the total of hydrogen-bonding implicated in the interaction between each carbohydrate residue with VIP.
[e] % of total hydrogen-bonding carbohydrate residue implicated in the interaction with VIP.

Table S2. Specific hydrogen-bonding contacts between VIP51 and D21"Ra".

Position[a]	VIP51	FTT	PO4	DPO	PA1	GCN	KDO	GMH	GLC	GLA	∑Aa[b]	%Aa[c]
1	H								1		1	2.6
2	S								4	2	6	15.8
3	D											
4	A											
5	V									1	1	2.6
6	F											
7	T											
8	A	1									1	2.6
9	N			6							6	15.8
10	Y											
11	T				1						1	2.6
12	R	7	2	1	1		3				14	36.8
13	L											
14	R		2								2	5.3
15	R			1			3		1		5	13.2
16	Q	1									1	2.6
17	L											
18	A											
19	V											
20	R											
21	R											
22	Y											
23	L											
24	A											
25	A											
26	I											
27	L											
28	G											
29	R											
30	R											
	∑Ch[d]	9	4	8	2	0	6	0	6	3		
	%Ch[e]	24	11	21	5	0	16	0	16	8		

[a] Position of each amino acid in the sequence of the VIP51 molecule.
[b] Summation of hydrogen-bonding contacts between specific amino acids of VIP51 and D21"Ra".
[c] % of total hydrogen-bonding amino acid implicated in the interaction between VIP51 and D21"Ra".
[d] Summation of the total of hydrogen-bonding implicated in the interaction between each carbohydrate residue with VIP51.
[e] % of total hydrogen-bonding carbohydrate residue implicated in the interaction with VIP51.

Table S3. Specific hydrogen-bonding contacts between VIP51$_{(6-30)}$ and D21"Ra".

Position[a]	VIP51$_{(6-30)}$	FTT	PO4	DPO	PA1	GCN	KDO	GMH	GLC	GLA	∑Aa[b]	%Aa[c]
6	F											
7	T											
8	A								1		1	2
9	N									1	1	2
10	Y									1	1	2
11	T						1		1		2	4
12	R	1		2	2		3				8	16
13	L											
14	R				1		2		1	2	6	12
15	R	1	2	1		1	10		5		20	40
16	Q	1					1				2	4
17	L											
18	A											
19	V											
20	R			1			2	1			4	8
21	R	1					2				3	6
22	Y											
23	L											
24	A											
25	A											
26	I											
27	L											
28	G											
29	R	1							1		2	4
30	R											
	∑Ch[d]	5	2	4	3	1	21	1	9	4		
	%Ch[e]	10	4	8	6	2	42	2	18	8		

[a] Position of each amino acid in the sequence of the VIP51$_{(6-30)}$ molecule.
[b] Summation of hydrogen-bonding contacts between specific amino acids of VIP51$_{(6-30)}$ and D21"Ra".
[c] % of total hydrogen-bonding amino acid implicated in the interaction between VIP51$_{(6-30)}$ and D21"Ra".
[d] Summation of the total of hydrogen-bonding implicated in the interaction between each carbohydrate residue with VIP51$_{(6-30)}$.
[e] % of total hydrogen-bonding carbohydrate residue implicated in the interaction with VIP51$_{(6-30)}$.

Table S4. Specific hydrogen-bonding contacts between VIP and D21f2"Rd"

Position[a]	VIP	FTT	PO4	DPO	PA1	GCN	KDO	∑Aa[b]	%Aa[c]
1	H								
2	S								
3	D						2	2	5.6
4	A								
5	V								
6	F								
7	T	1						1	2.8
8	D	2						2	5.6
9	N								
10	Y								
11	T	5				1		6	16.7
12	R	4					7	11	30.6
13	L								
14	R	1	1	2	2		5	11	30.6
15	K			1			1	2	5.6
16	Q								
17	M								
18	A								
19	V								
20	K								
21	K			1				1	2.8
22	Y								
23	L								
24	N								
25	S								
26	I								
27	L								
28	N								
	∑Ch[d]	13	1	4	2	1	15		
	%Ch[e]	36	3	11	6	3	42		

[a] Position of each amino acid in the sequence of the VIP molecule.
[b] Summation of hydrogen-bonding contacts between specific amino acids of VIP and D21F2"Rd".
[c] % of total hydrogen-bonding amino acid implicated in the interaction between VIP and D21f2"Rd".
[d] Summation of the total of hydrogen-bonding implicated in the interaction between each carbohydrate residue with VIP.
[e] % of total hydrogen-bonding carbohydrate residue implicated in the interaction with VIP.

Table S5. Specific hydrogen-bonding contacts between VIP51 and D21f2"Rd"

Position[a]	VIP51	FTT	PO4	DPO	PA1	GCN	KDO	∑Aa[b]	%Aa[c]
1	H	2					3	5	11.4
2	S	1					1	2	4.5
3	D					1	1	2	4.5
4	A								
5	V						1	1	2.3
6	F								
7	T								
8	A						1	1	2.3
9	N			4	1		3	8	18.2
10	Y								
11	T	1						1	2.3
12	R	3					1	4	9.1
13	L								
14	R	3						3	6.8
15	R				1	1	1	3	6.8
16	Q								
17	L								
18	A								
19	V								
20	R								
21	R			1	1	1	7	10	22.7
22	Y	1						1	2.3
23	L								
24	A								
25	A								
26	I								
27	L								
28	G								
29	R	2	1					3	6.8
30	R								
	∑Ch[d]	13	1	5	3	3	19		
	%Ch[e]	31	2	11	7	7	43		

[a] Position of each amino acid in the sequence of the VIP51 molecule.
[b] Summation of hydrogen-bonding contacts between specific amino acids of VIP51 and D21f2"Rd".
[c] % of total hydrogen-bonding amino acid implicated in the interaction between VIP51 and D21f2"Rd".
[d] Summation of the total of hydrogen-bonding implicated in the interaction between each carbohydrate residue with VIP51.
[e] % of total hydrogen-bonding carbohydrate residue implicated in the interaction with VIP51.

Table S6. Specific hydrogen-bonding contacts between VIP51$_{(6-30)}$ and D21f2"Rd"

Position[a]	VIP51f	FTT	PO4	DPO	PA1	GCN	KDO	∑Aa[b]	%Aa[c]
6	F								
7	T								
8	A								
9	N			2			1	3	9.4
10	Y								
11	T								
12	R	1						1	3.1
13	L								
14	R	2		1	1			4	12.5
15	R						1	1	3.1
16	Q								
17	L								
18	A								
19	V								
20	R								
21	R			1	1	2	8	12	37.5
22	Y								
23	L								
24	A								
25	A								
26	I								
27	L								
28	G								
29	R	2	1					3	9.4
30	R				1		7	8	25.0
	∑Ch[d]	5	1	4	3	2	17		
	%Ch[e]	15	3	12	9	6	53		

[a] Position of each amino acid in the sequence of the VIP51$_{(6-30)}$ molecule.
[b] Summation of hydrogen-bonding contacts between specific amino acids of VIP51$_{(6-30)}$ and D21"Ra".
[c] % of total hydrogen-bonding amino acid implicated in the interaction between VIP51$_{(6-30)}$ and D21"Ra".
[d] Summation of the total of hydrogen-bonding implicated in the interaction between each carbohydrate residue with VIP51$_{(6-30)}$.
[e] % of total hydrogen-bonding carbohydrate residue implicated in the interaction with VIP51$_{(6-30)}$.