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Supporting Information

Analogues of the Epoxy Resin Monomer Diglycidyl Ether of Bisphenol F: Effects on Contact Allergenic Potency and Cytotoxicity

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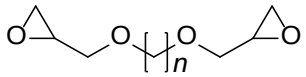
Table S1. Inter-atomic distances for linear epoxides and DGEBF [a]

	**Distance between epoxide oxygens (Å)**
n=4	12.94
n=5	14.47
n=6	15.42
n=7	16.63
n=8	17.95
n=9	19.15
DGEBF	*14.75*

[a] Measured with Avogadro v.1.0.3. Structures were energy minimized.

Table S2. Detailed results from the LLNA[a]

Compound Test Concentration		[^{3}H]thymidine incorporation	SI	EC3 value	
(% w/v)	(M)	(dpm/lymph node)		(% w/v)	(M)
1					
Control		253			
1	0.032	261	1.03		
5	0.16	1777	7.03	2.3	0.074
10	0.32	2248	8.89		
20	0.64	1004	3.97		
30	0.96	1268	5.01		
2					
Control		195			
1	0.032	298	1.53		
5	0.16	148	0.76	---	---
10	0.32	320	1.64		
20	0.63	247	1.27		
30	0.95	234	1.20		

[a]Groups of mice were treated with the test substance in five different concentrations, on the dorsum of both ears for three consecutive days. Sham treated control animals received the vehicle alone. On day five, all mice were injected intravenously with PBS (250 μL) containing 20 μCi of [methyl-^{3}H]thymidine. After 5 h the mice were sacrificed, the draining lymph nodes were excised and pooled for each group, single cell suspensions of lymph-node cells were prepared, and the thymidine incorporation into DNA was measured by β-scintillation counting. The increase in thymidine incorporation relative to vehicle-treated controls was derived for each experimental group and recorded as stimulation index (SI). The EC3 values (the estimated concentration required to induce an SI of 3) were calculated using linear interpolation

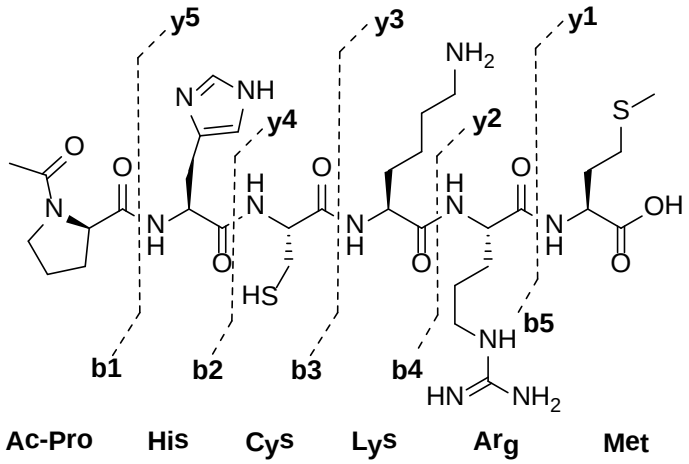
Table S3. Percentage peptide depletion with DGEBF, compound 1 and PGE[a]

Time (min)	Percentage of free peptide left (DGEBF)	Percentage of free peptide left (**1**)	Percentage of free peptide left (PGE)
0	100	100	100
20	37	60	41
40	15	37	25
60	8.3	22	15
80	7.8	18	10
100	6.8	13	7.9
120	7.1	12	7.1
1160	5.1	8.0	5.3

[a]N-terminal acylated hexapeptide AcPHCKRM was incubated with the relevant compound (1: 10) in a mixture of 1:1 DMSO: potassium phosphate buffer (100 mM, pH 7.4). The reaction mixture was kept under argon at room temperature and was monitored by UV/ESI-MS.

Figure S1. Fragment assignments for Ac-Pro-His-Cys-Lys-Arg-Met (AcPHCKRM)

The haptenated positions on the peptide were determined by analysis of the fragmentation pattern of the mass spectra of conjugates formed between compound and peptide. Peptides are known to form specific fragments by collision-induced decomposition (CID).[1] The most common fragments observed in the mass spectra of AcPHCKRM conjugates were b- and y-fragments.[2]



Molecular ion mass:
MH^+: 813.2
b- and y- fragment masses:

b1: 140.1	y1: 150.1
b2: 277.1	y2: 306.2
b3: 380.1	y3: 434.2
b4: 508.2	y4: 537.3
b5: 664.3	y5: 674.3

References

(1) Johnson, R. S., Martin, S. A., Biemann, K., Stults, J. T. and Watson, J. T. (1987) Novel fragmentation process of peptides by collision-induced decomposition in a tandem mass spectrometer: differentiation of leucine and isoleucine. *Anal. Chem. 59*, 2621-2625.

(2) Biemann, K. (1988) Contributions of mass spectrometry to peptide and protein structure. *Biological Mass Spectrometry 16*, 99-111.