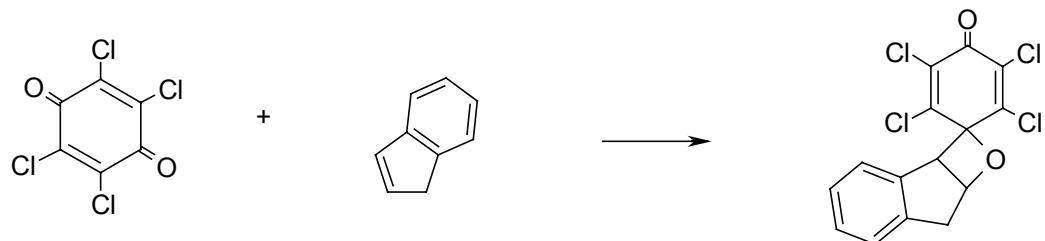


Supporting Information (Q.-Y. Zhang and J. Aires-de-Sousa)

Construction of a reaction MOLMAP

a. Scheme of the reaction.



b. Neurons of the SOM of dimension 12×12 activated by the bonds of the second reactant.

	C-H		C-H		C-H						
						C-H					
									C=C		
									C(Ar)		
					C-C	C(Ar)			C(Ar)		
		H-C	H-C			C(Ar)	C(Ar)				
		H-C				C(Ar)					
		H-C									
			C-C								
				C-C							
					C-H						H-C

**c. Numerical representation of the neurons activated by the bonds of the second reactant
(MOLMAP of the second reactant).**

0.3	1.0	0.6	1.6	1.5	2.6	0.6	0	0	0	0	0
0.3	0.3	0.6	0.3	0.9	1.2	1.2	0.6	0	0	0	0
0	0	0	0	0	0.6	2.0	0.6	1.8	1.8	1.8	0
0	0	0	0	0	0.9	1.5	1.5	2.7	6.3	2.1	0
0	0.3	0.6	0.6	0.3	0.3	2.2	3.5	3.9	3.4	2.1	0
0	0.6	1.6	1.6	0.3	0.3	1.8	3.8	3.8	0.9	0.3	0
0	1.5	2.5	1.8	0.3	0	0.9	2.2	1.5	0.6	0	0
0	1.2	3.6	1.5	0.3	0	0.3	0.3	0.3	0	0	0
0	0.9	1.2	1.9	0.3	0	0	0.6	0.6	0.6	0	0
0.6	0	0.3	0.9	0.9	0.6	0	0.6	2.0	0.6	0.6	0.6
0.6	0	0	1.2	2.6	1.2	0	0.6	0.6	0.6	0.6	2.0
0.9	0.3	0.6	1.5	3.5	1.8	0.6	0	0	0	0.6	0.6

d. Neurons of the SOM activated by the bonds of the two reactants represented in the same map.

	C-H		C-H		C-H			Cl-C			
						C-H					
									C=C C(Ar)		
						C-C	C(Ar)		C(Ar)		C-Cl
		H-C	H-C			C(Ar) C-C	C(Ar) C-C	C-C			
		H-C				C(Ar)					
C=O		H-C									
			C-C			C-C					
							C(Ar)				
				C-C	O=C					H-C	
				C-H							

e. Sum of the MOLMAPs for the two reactants (the MOLMAP of the first reactant is represented in Figure 3.b and the MOLMAP of the second reactant is represented in c. of this Supporting Information section).

0.3	1.0	0.6	1.6	1.5	2.6	0.6	1.2	4.0	1.2	0	0
0.3	0.3	0.6	0.3	0.9	1.2	1.2	1.8	1.2	1.2	0	0
0	0	0	0	0	0.6	2.0	0.6	1.8	1.8	1.8	0
1.2	0	0	0	0	0.9	1.5	1.5	2.7	6.3	3.3	1.2
1.2	0.3	0.6	0.6	0.3	0.3	2.2	3.5	5.1	4.6	4.5	4.0
1.2	0.6	1.6	1.6	0.3	0.3	1.8	3.8	5.0	4.9	2.7	1.2
0.6	2.1	2.5	1.8	0.3	0	0.9	2.2	2.7	1.8	1.2	0.6
2.0	1.8	3.6	1.5	0.3	0	1.5	1.5	1.5	0	0	0.6
0.6	1.5	1.2	1.9	0.3	0	1.2	5.8	3.0	1.8	0	0.6
0.6	0	0.3	0.9	0.9	1.2	1.8	3.6	7.2	1.8	0.6	0.6
0.6	0	0	1.2	2.6	1.8	2.0	2.4	1.8	1.8	0.6	2.0
0.9	0.3	0.6	1.5	3.5	2.4	1.2	1.8	1.2	1.2	0.6	0.6

f. Neurons of the SOM activated by the bonds of the product.

C-H					C-H			Cl-C			
									C-C		
								C(Ar)			
C-Cl							C(Ar)		C(Ar)		C-Cl
		H-C				C(Ar)	C-C	C(Ar)			
		H-C		H-C		C(Ar)	C(Ar)	C-C	C-C	C-O	
C=O							C=C		C-C		
			H-C	H-C		C-C	C=C	C-C			
C-O			C-C						C-C		
C-C	C-C				O=C						
	O-C			C-H		O-C	Cl-C				C-H C-C

**g. Numerical representation of the neurons activated by the bonds of the product
(MOLMAP of the product).**

3.9	1.2	0.3	0.9	1.2	1.9	0.6	1.5	2.9	1.2	0.6	1.5
0.9	0.9	0	0	0.3	0.3	0.3	0.6	1.2	1.2	0.6	0.9
0	0	0	0	0	0	0	0.6	1.2	2.6	0.6	0
1.2	0.6	0	0	0	0	0.6	1.2	3.8	1.8	1.8	1.2
2.6	0.9	0.3	0.3	0	0	1.2	3.5	3.0	3.2	1.5	2.6
1.5	1.8	1.9	1.5	0.3	0.3	1.5	3.8	4.3	3.1	2.4	1.8
0.6	1.5	3.3	1.5	1.0	0.3	0.9	3.1	4.4	3.4	2.2	1.9
1.3	1.2	1.5	2.1	1.2	0.6	0.9	2.7	4.7	3.0	2.2	1.2
0.6	0.6	0.9	2.6	1.9	0.3	0.6	3.2	3.8	2.8	0.9	0.9
2.8	2.1	2.4	1.9	1.2	0.6	0.9	1.5	1.8	1.9	0.6	0.6
3.7	5.9	2.1	1.2	1.2	1.2	1.3	1.2	1.2	0.9	0.9	1.2
3.6	3.7	1.8	0.9	3.3	1.5	0.9	2.5	2.9	1.2	0.6	3.2

h. The difference between the MOLMAPs of the product and the reactants (MOLMAP of the reaction).

3.6	0.2	-0.3	-0.7	-0.3	-0.7	0	0.3	-1.1	0	0.6	1.5
0.6	0.6	-0.6	-0.3	-0.6	-0.9	-0.9	-1.2	0	0	0.6	0.9
0	0	0	0	0	-0.6	-2.0	0	-0.6	0.8	-1.2	0
0	0.6	0	0	0	-0.9	-0.9	-0.3	1.1	-4.5	-1.5	0
1.4	0.6	-0.3	-0.3	-0.3	-0.3	-1.0	0	-2.1	-1.4	-3.0	-1.4
0.3	1.2	0.3	-0.1	0	0	-0.3	0	-0.7	-1.8	-0.3	0.6
0	-0.6	0.8	-0.3	0.7	0.3	0	0.9	1.7	1.6	1.0	1.3
-0.7	-0.6	-2.1	0.6	0.9	0.6	-0.6	1.2	3.2	3.0	2.2	0.6
0	-0.9	-0.3	0.7	1.6	0.3	-0.6	-2.6	0.8	1.0	0.9	0.3
2.2	2.1	2.1	1.0	0.3	-0.6	-0.9	-2.1	-5.4	0.1	0	0
3.1	5.9	2.1	0	-1.4	-0.6	-0.7	-1.2	-0.6	-0.9	0.3	-0.8
2.7	3.4	1.2	-0.6	-0.2	-0.9	-0.3	0.7	1.7	0	0	2.6