



Figure 1. Schematic representation of method.

Table 1 summarizes the obtained distribution of the distance, which is divided into several classes according to both the size of compounds, that is, the number of atoms of each chemical compound and the distance of reaction centers. In Table 1, the observed frequencies are shown in boldface when they are more than the 15% of total observations classified in each compound class.

	Size of compounds									
	1-5	6-10	11-15	16-20	21-25	26-30	31-35	36-50	51-	
Distance of reaction centers	0	107	374	263	77	52	25	26	30	206
	1	20	170	177	86	51	14	17	38	111
	2	1	75	74	54	32	5	3	17	23
	3	1	41	54	67	43	5	6	24	10
	4	-	37	38	41	34	9	3	5	11
	5	-	16	49	39	43	6	6	3	11
	6	-	5	9	18	15	4	5	17	13
	7	-	-	7	11	23	8	2	7	3
	8	-	-	1	5	6	11	2	-	1
	9	-	1	-	5	4	3	2	1	-
	10	-	-	-	6	2	1	3	5	-
	10-	-	-	-	-	5	9	4	38	8
Total		129	719	672	409	310	100	79	185	397

Table 1. Distribution of observed distances between reaction centers.

3 Discussions

We found the strong and global tendency that the successive enzymatic reactions occur nearby the former reactive site in the target chemical compounds. Interestingly, even for very large size of chemical compounds the reaction may prefer to act on around the proximity of pre-acted atoms. These findings will help us to decrease the computational complexity when reconstructing metabolic pathways and to improve the accuracy of enzymatic reaction predictions. In addition, we will be able to consider the relationship between such meaningful chemical continuities and the genomic information.

References

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