

Exhaustive conformational search for transition states: the case of catechol *O*-methyltransferase active site

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Cartesian coordinates of all located transition states are bundled within this PDF as an attachment.

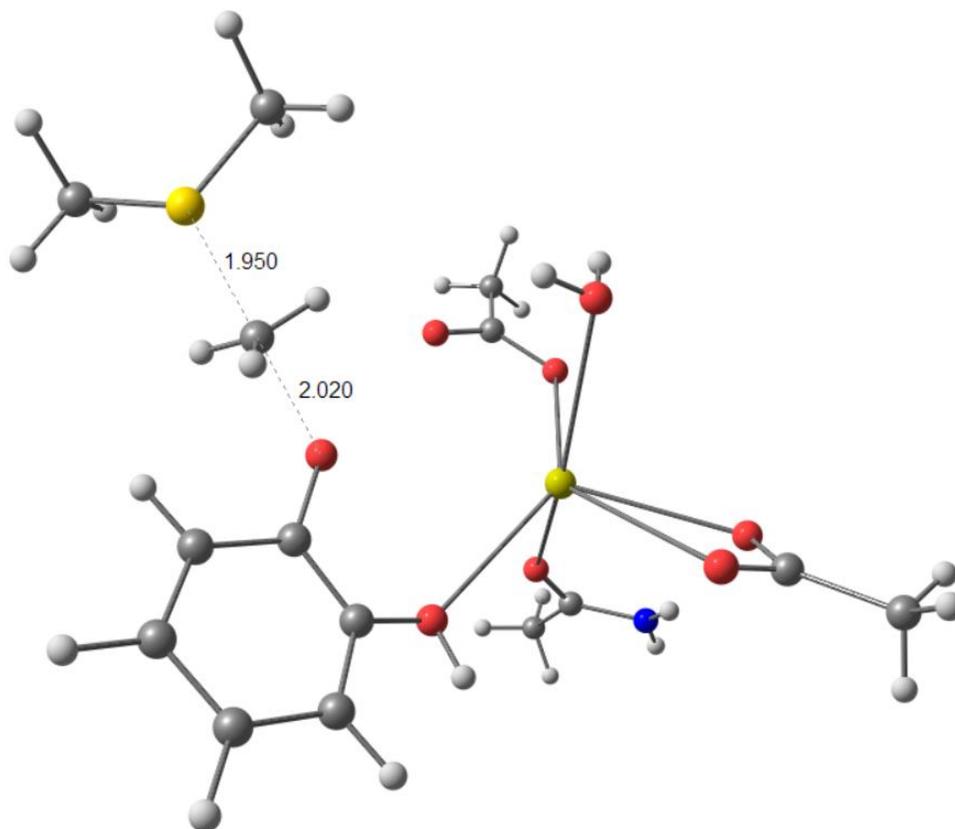


Figure S1. Initial geometry used to generate all other conformations.

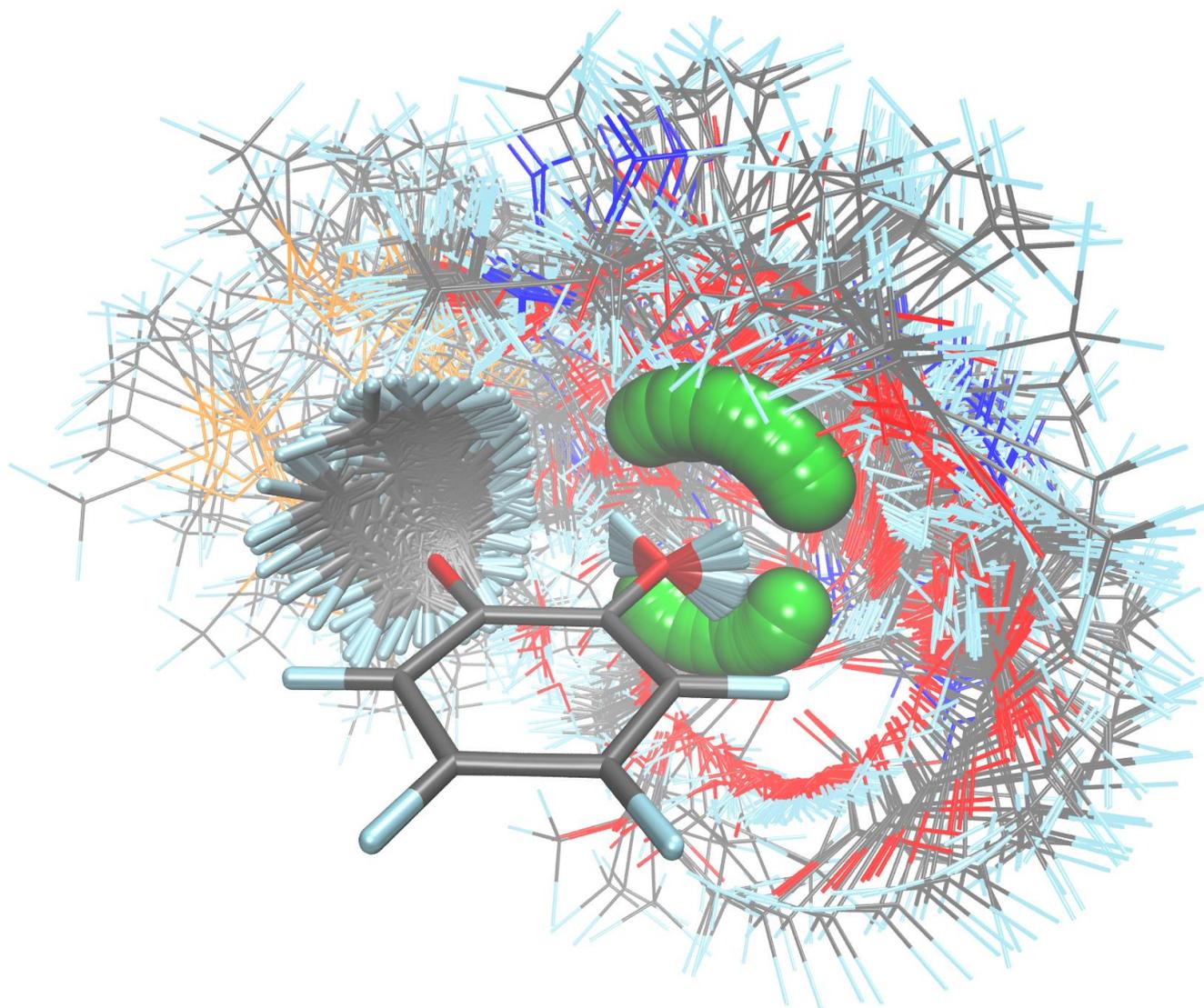


Figure S2. Overview of all generated TS conformations guesses aligned by catechol C and O.

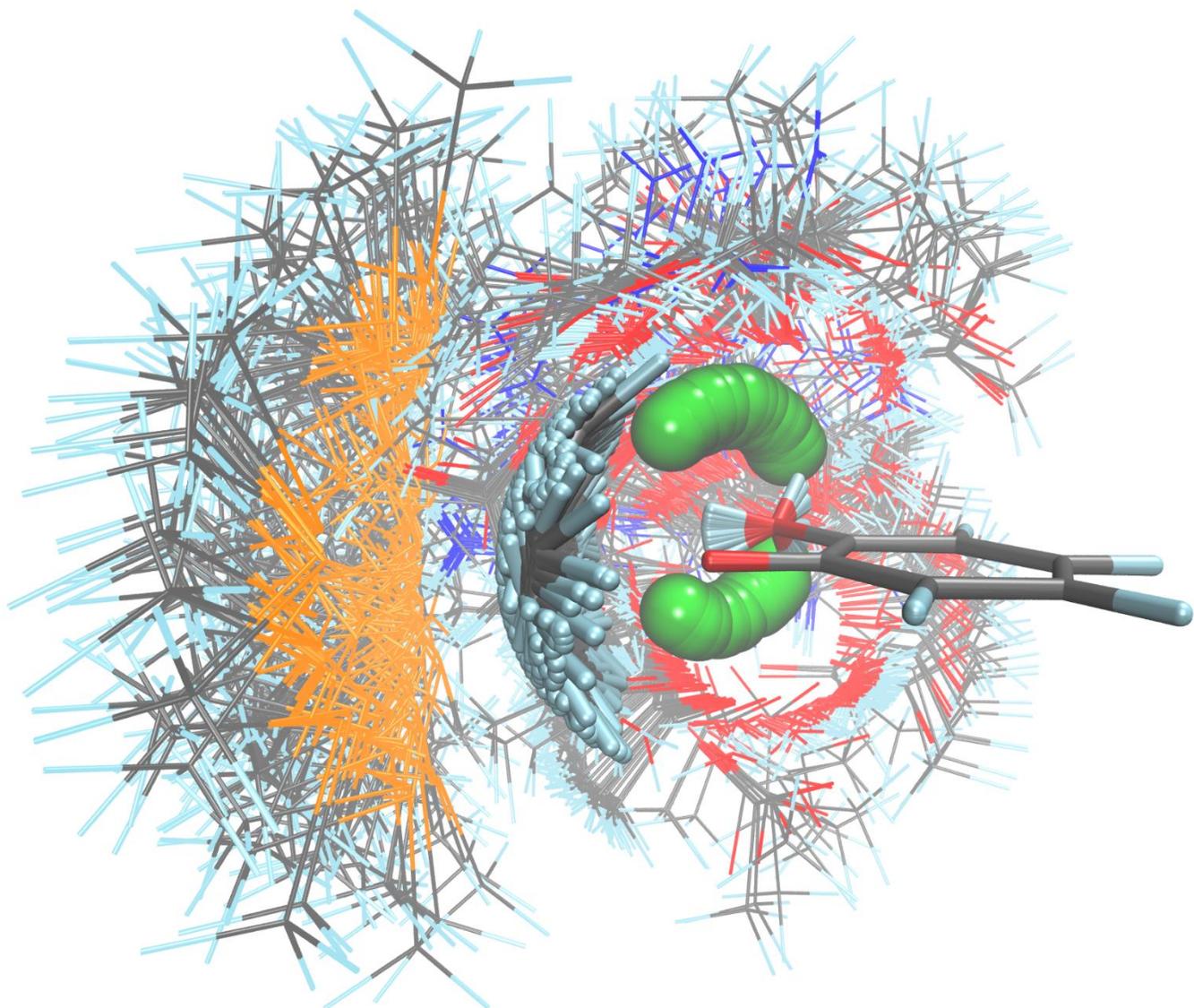


Figure S3. Another overview of all generated TS conformations guesses aligned by catechol C and O.

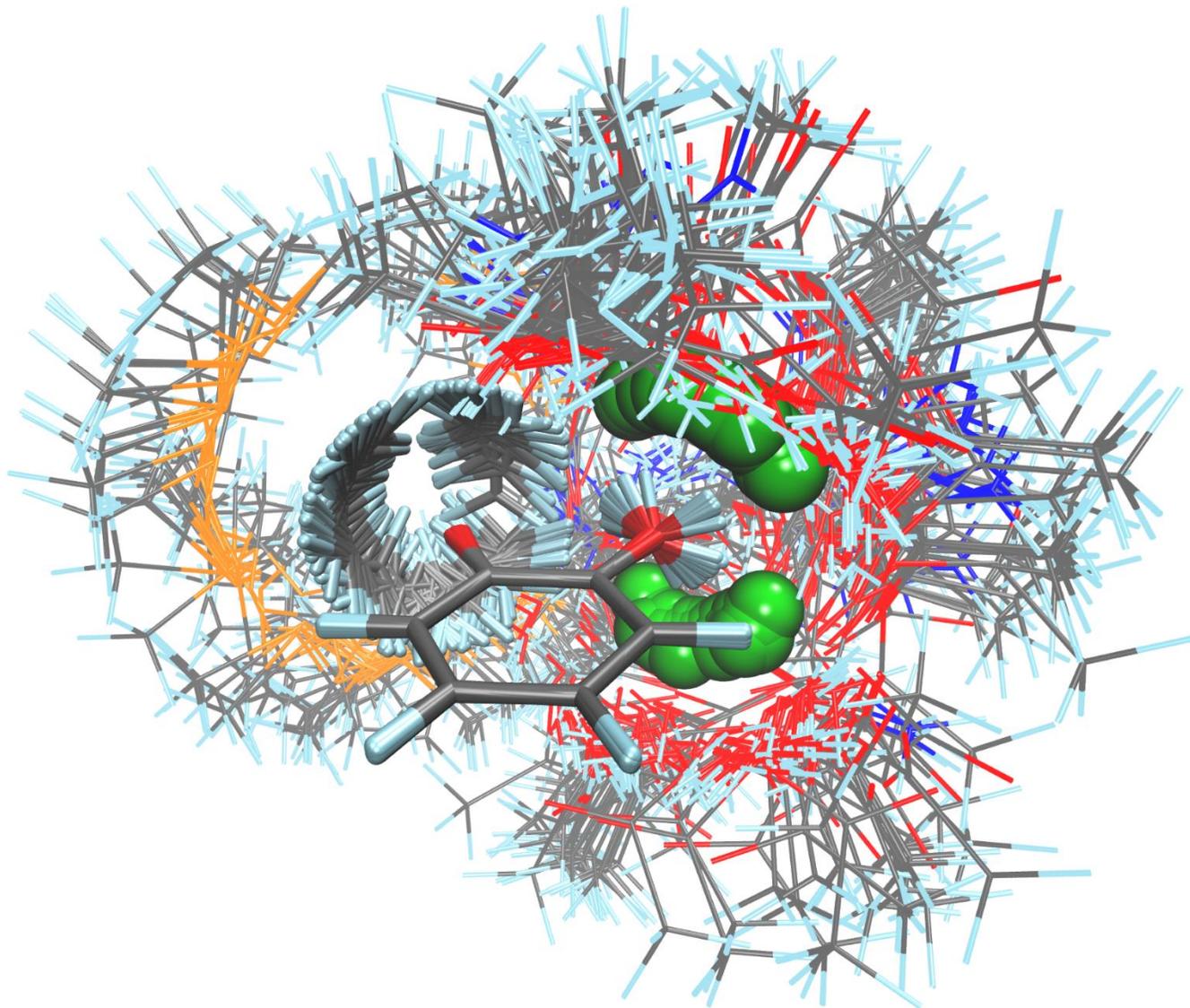


Figure S4. Overview of all located TS conformations aligned by catechol C and O.

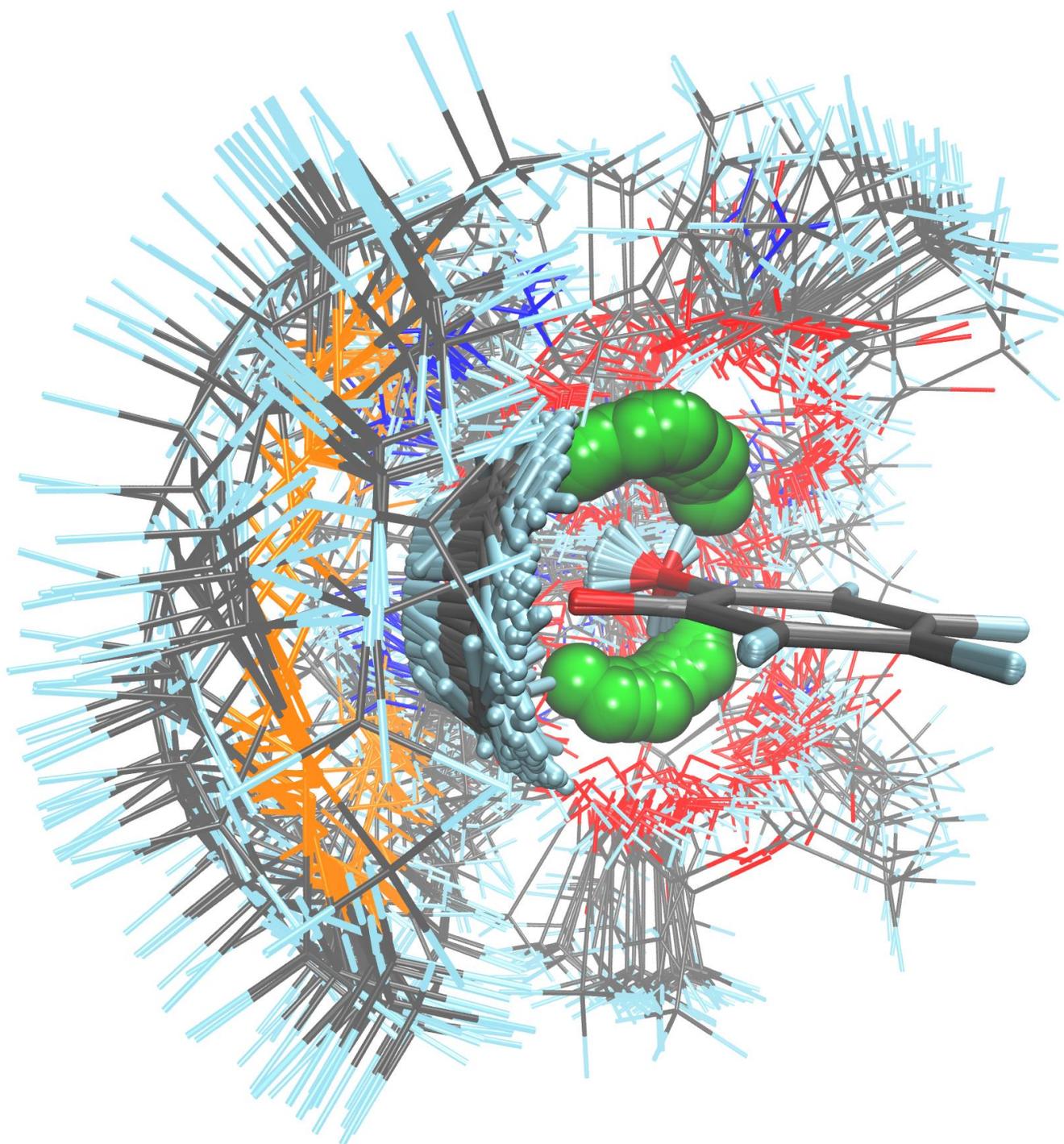


Figure S5. Another overview of all located TS conformations aligned by catechol C and O.

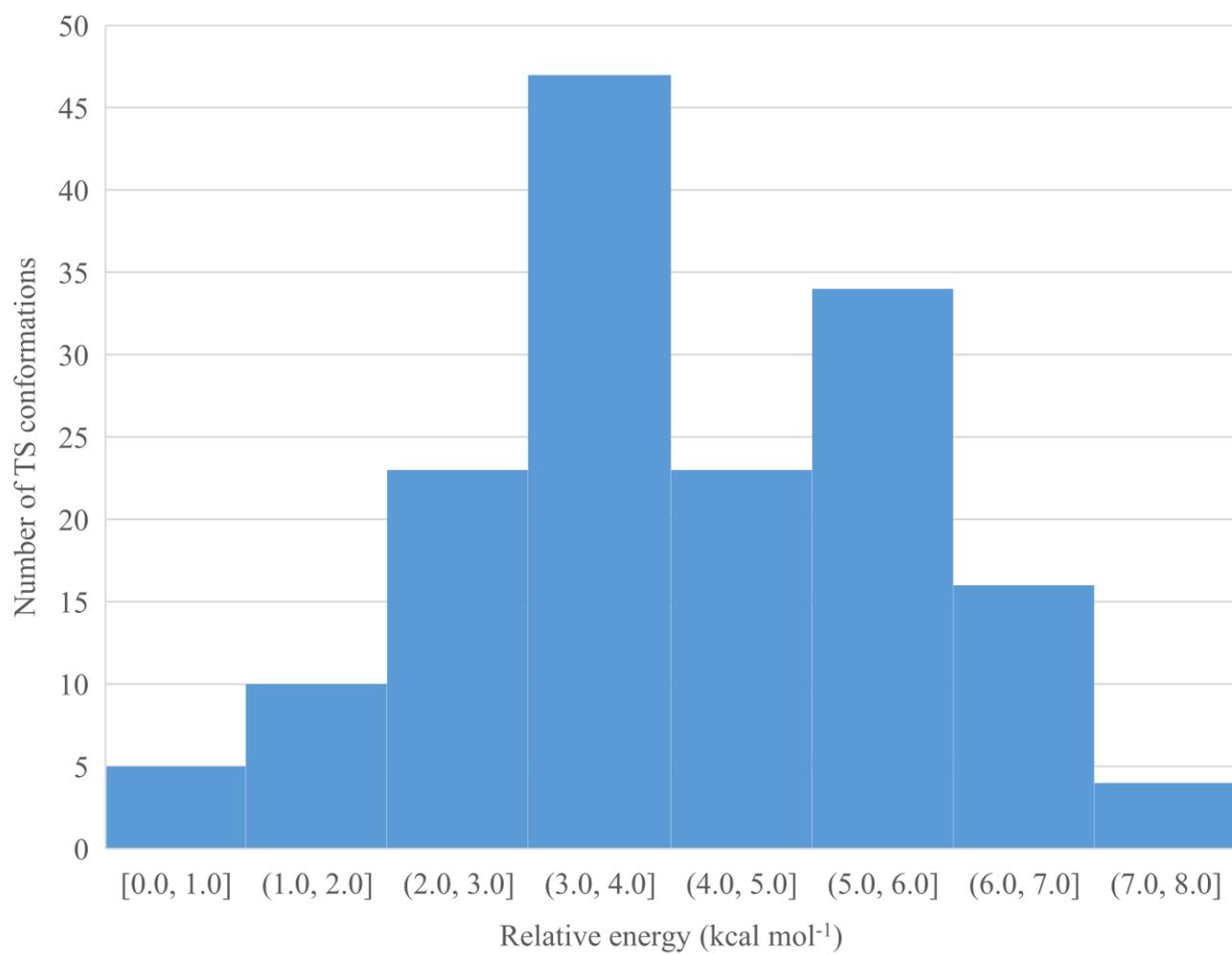


Figure S6. Relative energies of located conformations.

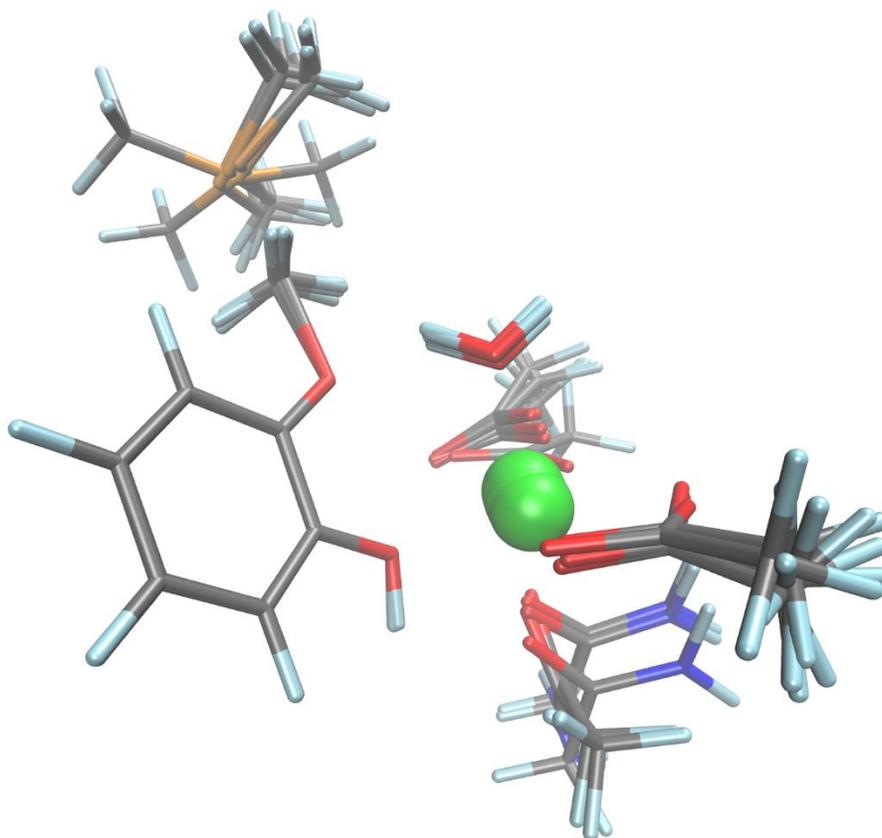


Figure S7. Overview of located TS conformations which are similar to the reaction taking part in COMT enzyme. Aligned by catechol C and O.

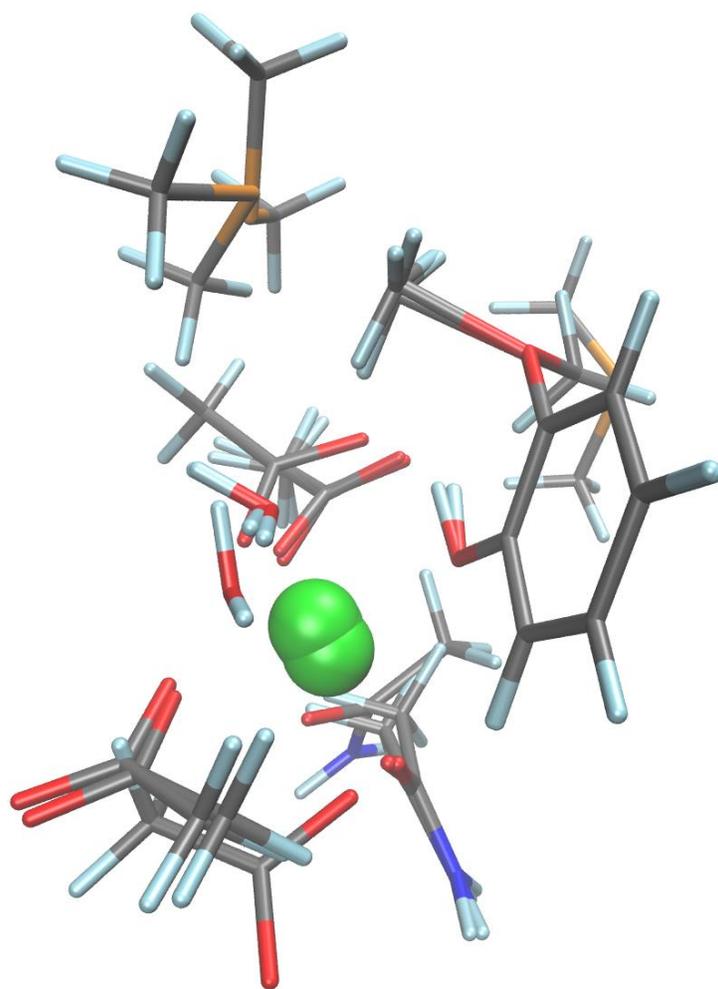


Figure S8. Overview of the lowest-lying located TS conformations. Aligned by catechol C and O.

Table S1. Relative energies of all conformations.

TS №	E_{rel} kcal·mol ⁻¹						
0	5.87	38	1.76	78	3.12	118	6.91
1	5.38	39	4.72	79	5.92	119	2.44
2	3.52	40	2.03	80	1.81	120	2.10
3	3.81	41	2.54	81	3.07	121	4.74
4	5.63	42	1.26	82	6.01	122	4.87
5	0.73	43	7.30	83	4.31	123	7.09
6	5.91	44	4.29	84	0.76	124	5.28
7	4.35	45	3.85	85	3.45	125	6.28
8	2.19	46	3.41	86	5.10	126	5.56
9	3.52	47	4.21	87	4.85	127	6.08
10	2.82	48	6.14	88	3.79	128	6.43
11	5.84	49	3.74	89	5.57	129	2.66
12	5.76	50	5.94	90	4.88	130	1.41
13	5.01	51	5.94	91	0.60	131	7.01
14	1.88	52	2.83	92	2.16	132	1.75
15	3.32	53	2.04	93	6.15	133	3.09
16	4.19	54	2.40	94	3.66	134	4.32
17	4.02	55	5.44	95	5.62	135	3.08
18	3.88	56	0.33	96	3.97	136	4.32
19	4.31	57	5.91	97	1.96	137	5.25
20	3.96	58	6.52	98	4.00	138	4.38
21	5.66	59	3.36	99	0.00	139	4.52
22	6.02	60	6.83	100	2.94	140	4.57
23	5.18	61	3.56	101	2.70		
24	6.29	62	5.64	102	3.45		
25	2.38	63	5.98	103	3.43		
26	5.84	64	5.28	104	3.27		
27	5.62	65	1.68	105	4.68		
28	5.75	66	1.78	106	3.16		
29	3.53	67	2.39	107	3.54		
30	3.14	68	4.97	108	3.61		
31	2.29	69	6.52	109	4.49		
32	4.74	70	5.43	110	2.63		
33	6.25	71	5.85	111	2.41		
34	5.94	72	5.03	112	2.40		
35	3.60	73	3.18	113	3.29		
36	5.28	74	3.12	114	5.53		
37	6.89	75	2.55	115	3.63		
		76	4.21	116	5.53		
		77	2.61	117	2.14		