Supporting information

The significance of halogen bonding in ligand-receptor interactions – the lesson learned from Molecular Dynamic simulations of the D_4 receptor

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Figure S1. The XSAR matrix for D_4R target.

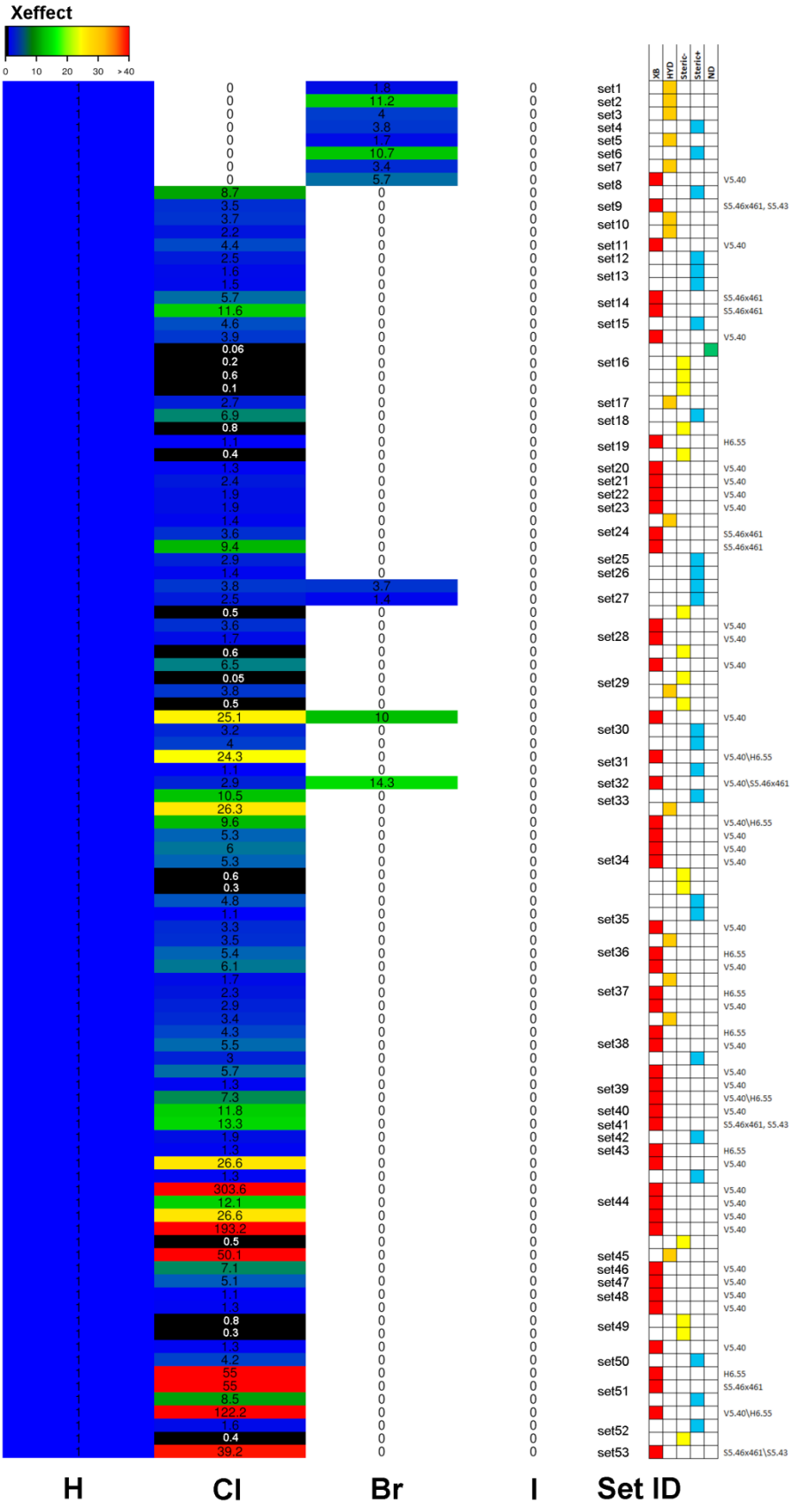
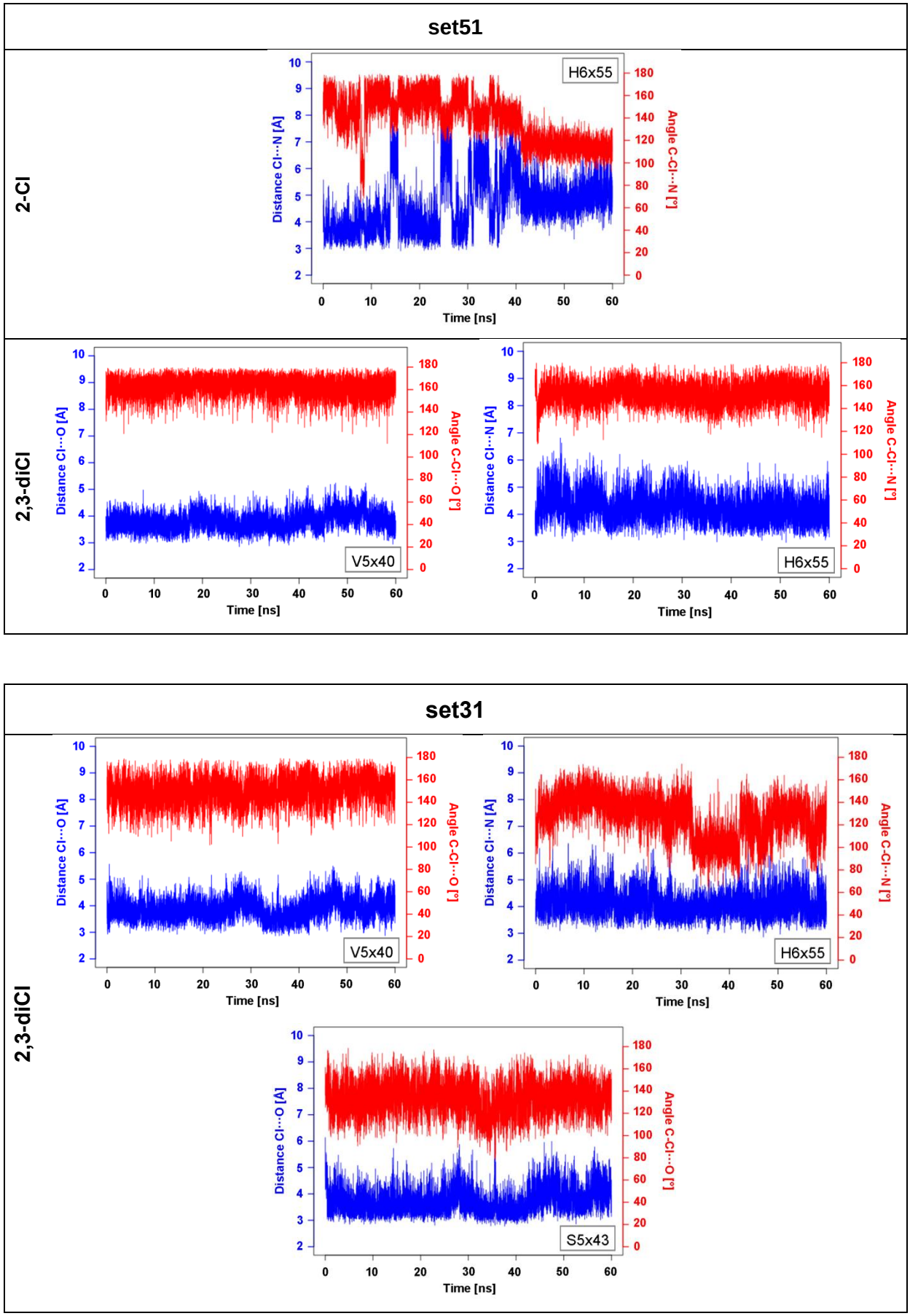
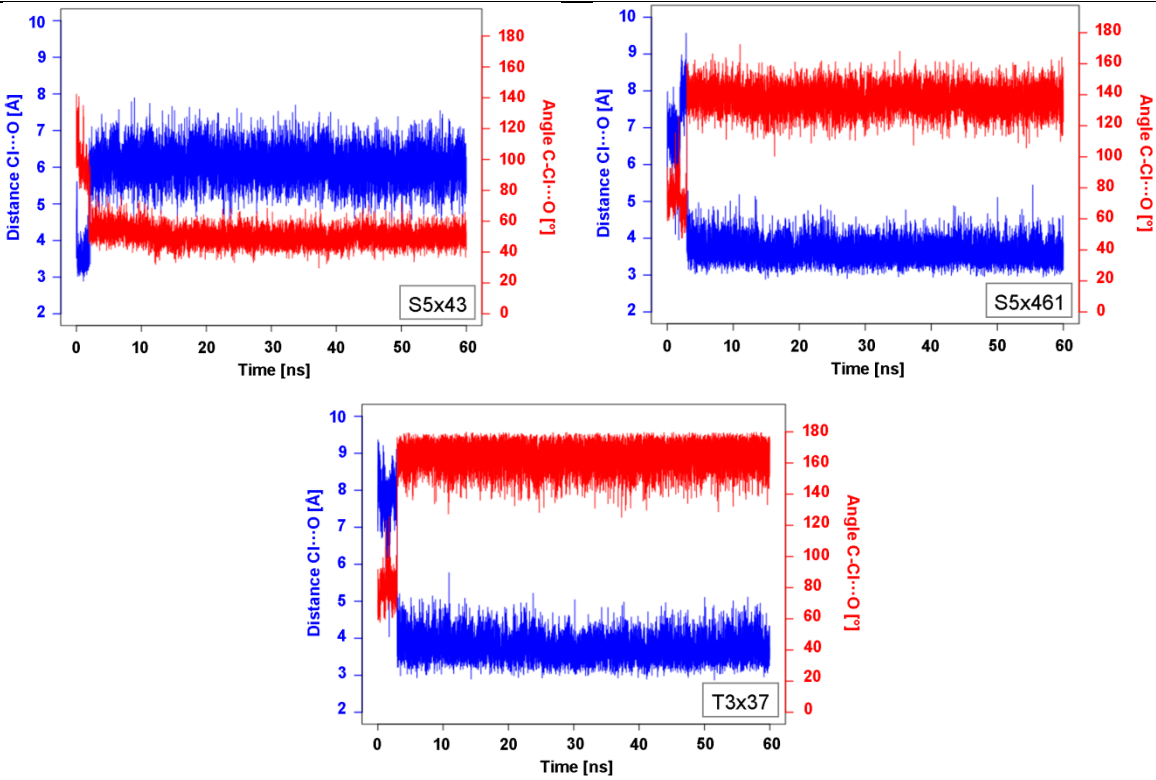


Figure S2. The dependency of the change in length (blue line) and angle (red line) of the halogen bond formed between the analog of the XSAR library and the selected amino acid of the D_4 receptor binding site.



set27

3-Cl



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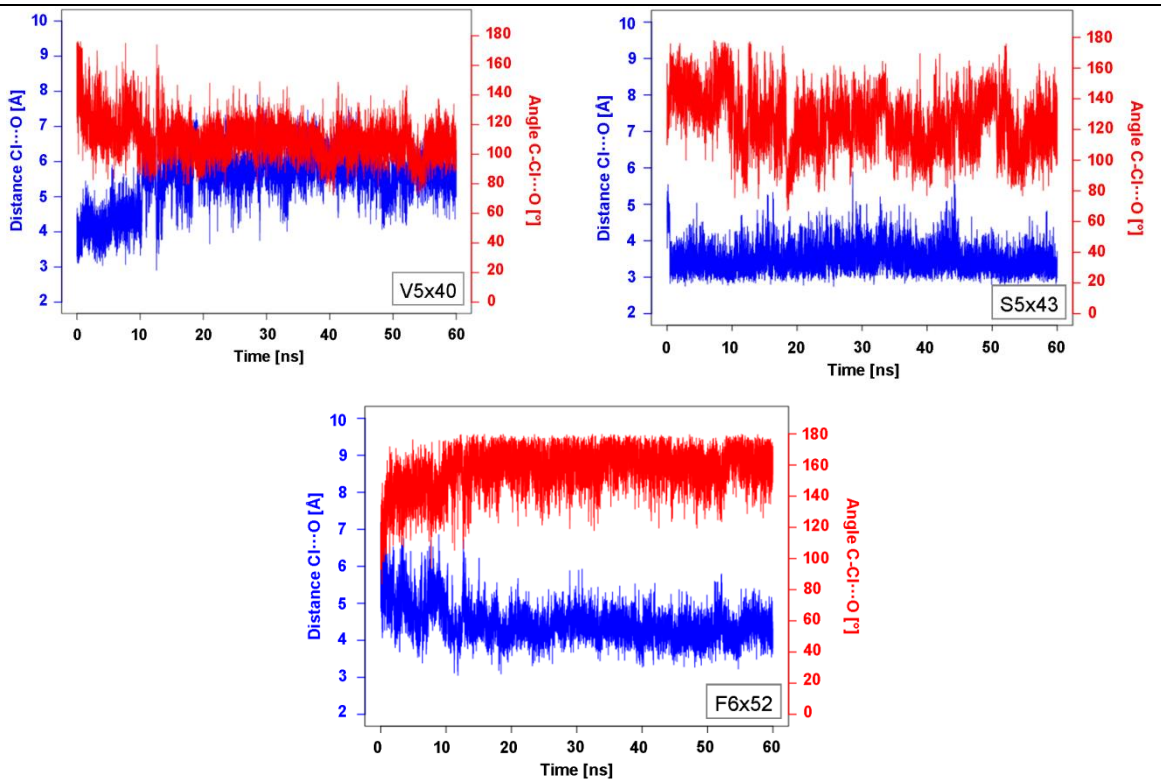
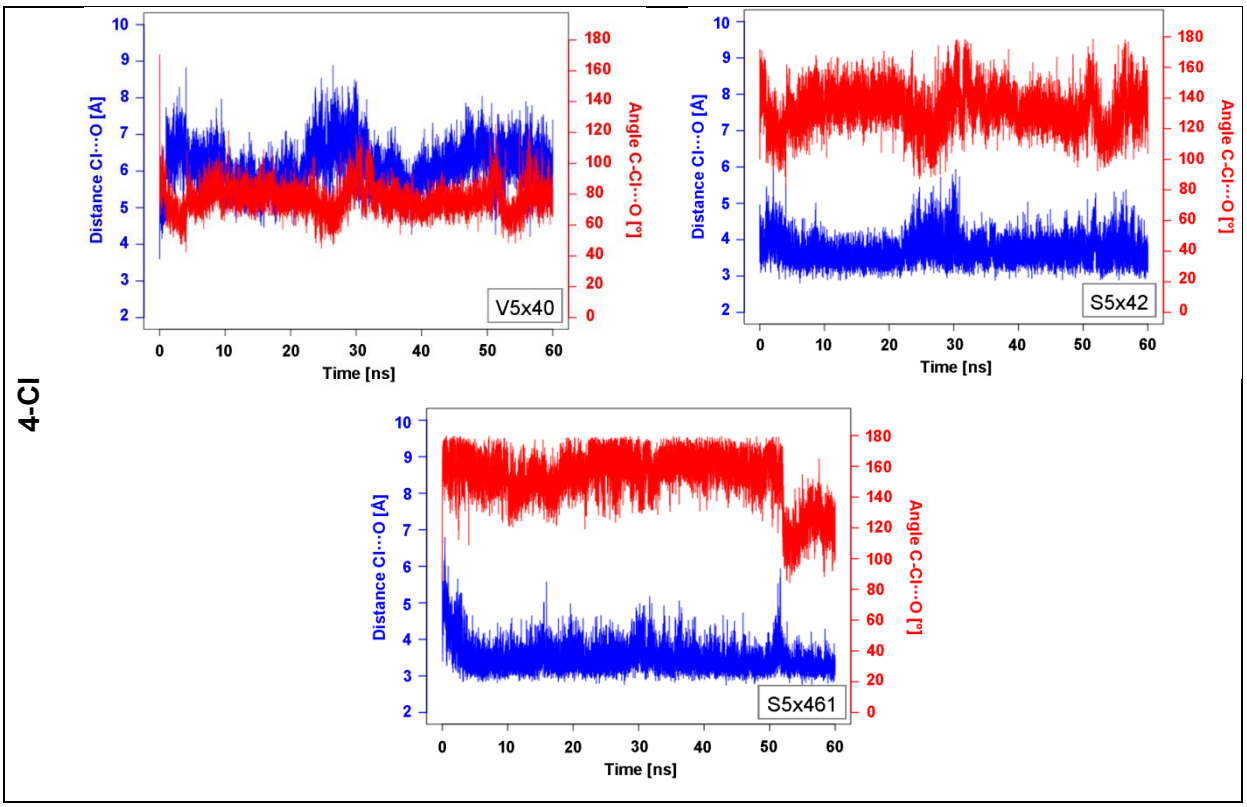



4-Cl
Distance Cl···O [Å]
Angle C-Cl···O [°]
Time [ns]
V5x40
S5x42
S5x461

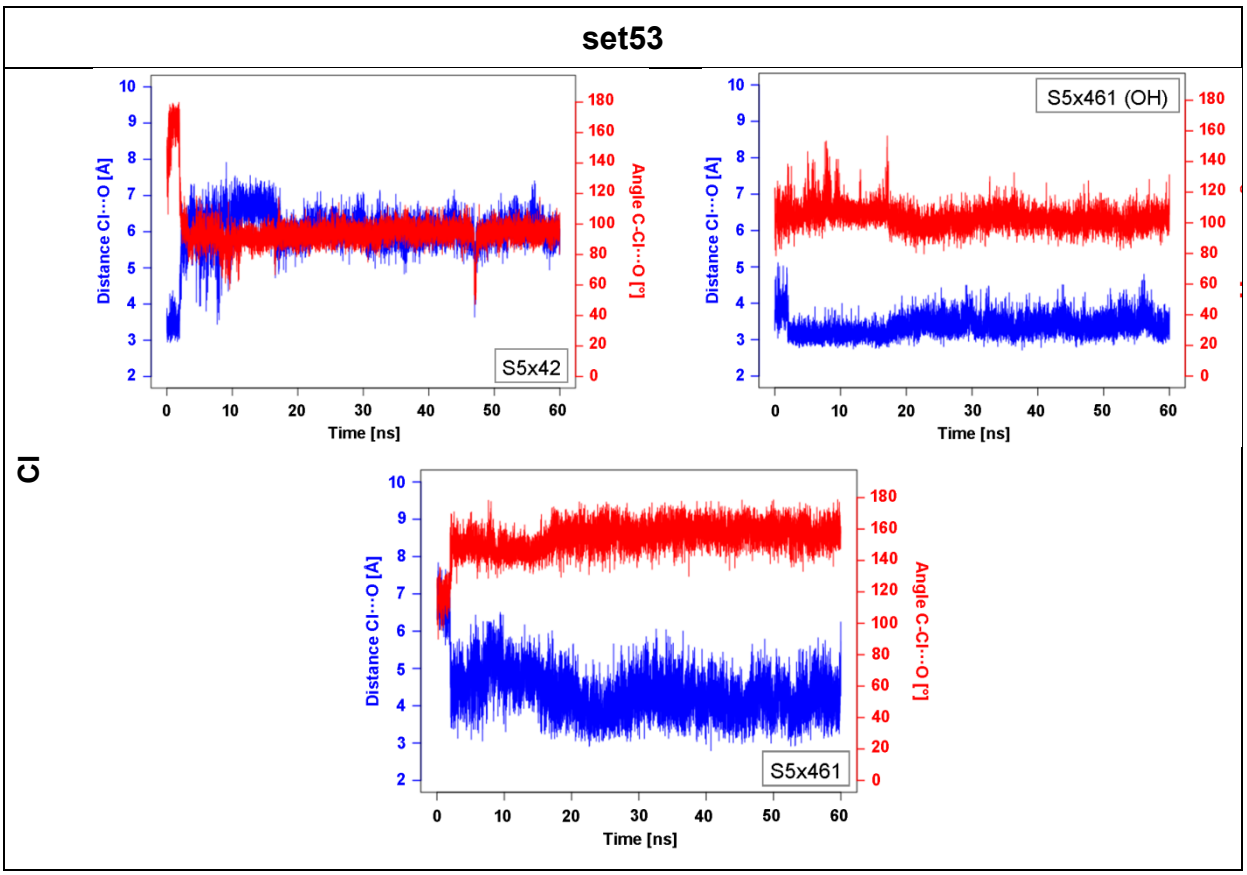
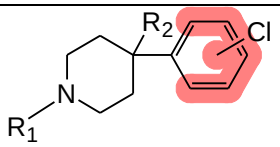

set53
Cl
Distance Cl···O [Å]
Angle C-Cl···O [°]
Time [ns]
S5x42
S5x461 (OH)
S5x461

Table S1. Analysis of the XSAR scaffolds.



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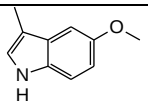
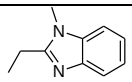
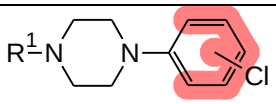
32		OH	-	-	2.9
52		H	-	0.4	1.6



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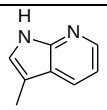
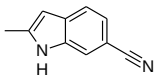
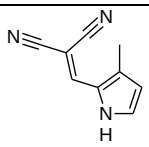
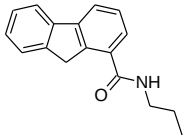
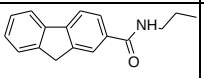
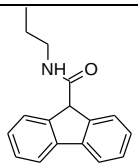
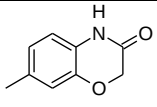
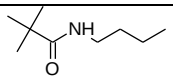
11		–	–	4.4
19		1.1	–	–
			0.4	
20		–	–	1.3
21		2.4		–
22		1.9		–
23		1.9		–
26		–	–	1.4
30		4.0	3.2	25.1
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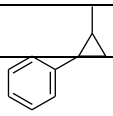
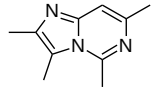
34		6	0.6	9.6

		5.3		
		–	4.8	
35		–	–	1.1
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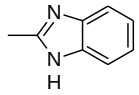
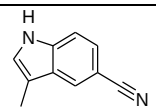
36		6.1	5.4	3.5
37		2.9	–	1.7
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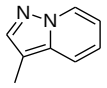
38		5.7	4.3	5.5
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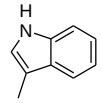
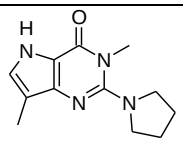
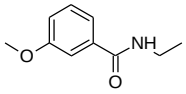
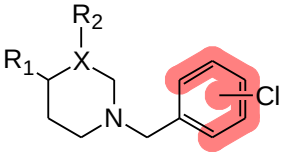
39		1.3		7.3
46		–	–	7.1
48		–	3.4	
49		1.3	–	0.3
		1.3		
		–	0.8	
51		55	8.5	55
		122		



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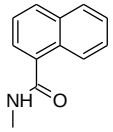
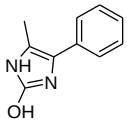
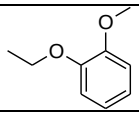
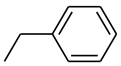
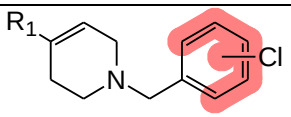
27		–	C	0.5	1.4	3.8
43		–	C	0.3	1.3	0.5
44	–		O	–	1.3	26.6

					26.6	
47	–		O	–	–	5.1



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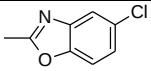
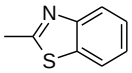
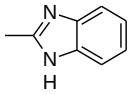
14		–	–	2.1
16		0.1	0.6	3.9
24		–	–	1.4