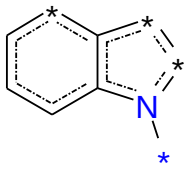
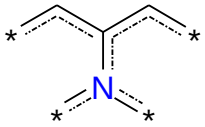
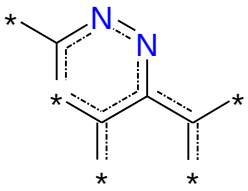
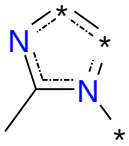
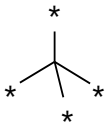
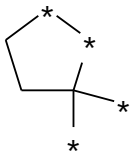
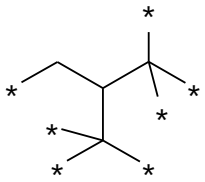
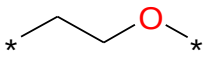
Electronic Supplementary Material (ESI) for Molecular BioSystems.

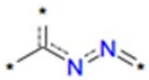
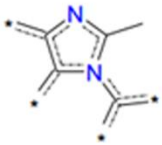
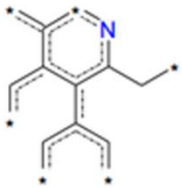
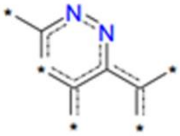
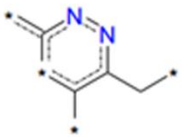
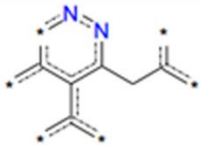
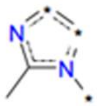
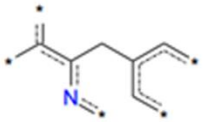
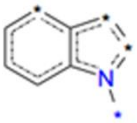
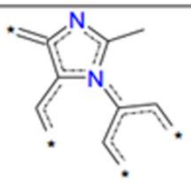
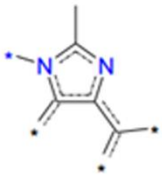
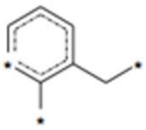
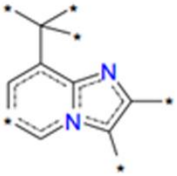
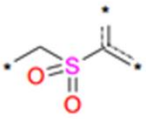
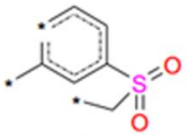
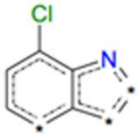
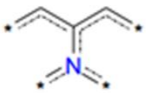
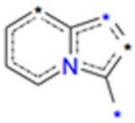
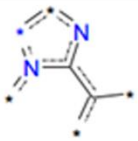
Table S1 Cross-validation results of 16 models derived from structural fingerprints

Models	Training set								Test set							
	TP	**TN**	**FP**	**FN**	**SE**	**SP**	**Q**	**MCC**	**TP**	**TN**	**FP**	**FN**	**SE**	**SP**	**Q**	**MCC**
kNN_ES	61	93	14	8	0.884	0.869	0.875	0.744	19	30	6	3	0.864	0.833	0.845	0.683
kNN_MA	60	95	12	9	0.870	0.888	0.881	0.752	19	28	8	3	0.864	0.778	0.810	0.624
kNN_S	60	95	12	9	0.870	0.888	0.881	0.752	19	30	6	3	0.864	0.833	0.845	0.683
kNN_SC	57	95	12	12	0.826	0.888	0.864	0.714	19	29	7	3	0.864	0.806	0.828	0.653
NB_ ES	64	89	18	5	0.928	0.832	0.869	0.743	20	32	4	2	0.909	0.889	0.897	0.786
NB_ MA	51	97	10	18	0.739	0.907	0.841	0.662	18	30	6	4	0.818	0.833	0.828	0.642
NB_ S	61	97	10	8	0.884	0.907	0.898	0.787	16	35	1	6	0.727	0.972	0.879	0.746
NB_ SC	61	96	11	8	0.884	0.897	0.892	0.776	16	34	2	6	0.727	0.944	0.862	0.705
RP_ ES	60	96	11	9	0.870	0.897	0.886	0.763	14	35	1	8	0.636	0.972	0.845	0.674
RP_ MA	61	94	13	8	0.884	0.879	0.881	0.754	16	34	2	6	0.727	0.944	0.862	0.705
RP_ S	**66**	**93**	**14**	**3**	**0.957**	**0.869**	**0.903**	**0.810**	**21**	**33**	**3**	**1**	**0.955**	**0.917**	**0.931**	**0.858**
RP_ SC	65	94	13	4	0.942	0.879	0.903	0.806	19	33	3	3	0.864	0.917	0.897	0.780
SVM_ ES	63	96	11	6	0.913	0.897	0.903	0.801	17	34	2	5	0.773	0.944	0.879	0.741
SVM_MA	**67**	**104**	**3**	**2**	**0.971**	**0.972**	**0.972**	**0.941**	**20**	**34**	**2**	**2**	**0.909**	**0.944**	**0.931**	**0.854**
SVM_ S	66	96	11	3	0.957	0.897	0.920	0.840	19	34	2	3	0.864	0.944	0.914	0.816
SVM_SC	67	96	11	2	0.971	0.897	0.926	0.853	20	33	3	2	0.909	0.917	0.914	0.819

Table S2 Statistics of the typical privileged fragments and unprivileged fragments.

No.	Fragment	TA	SA	NA*
PS9		23	22	1
PS18		15	14	1
PS4		14	14	0
PS7		12	12	0
NS1		212	71	141
NS3		5	0	5
NS9		29	0	29
NS6		34	1	33

* TA: total fragment appearances. SA: appearances of fragments in selective LXRβ molecules. NA: appearances of fragments in non-selective LXRβ molecules.

 PS1	 PS2	 PS3	 PS4	 PS5
 PS6	 PS7	 PS8	 PS9	 PS10
 PS11	 PS12	 PS13	 PS14	 PS15
 PS16	 PS17	 PS18	 PS19	 PS20

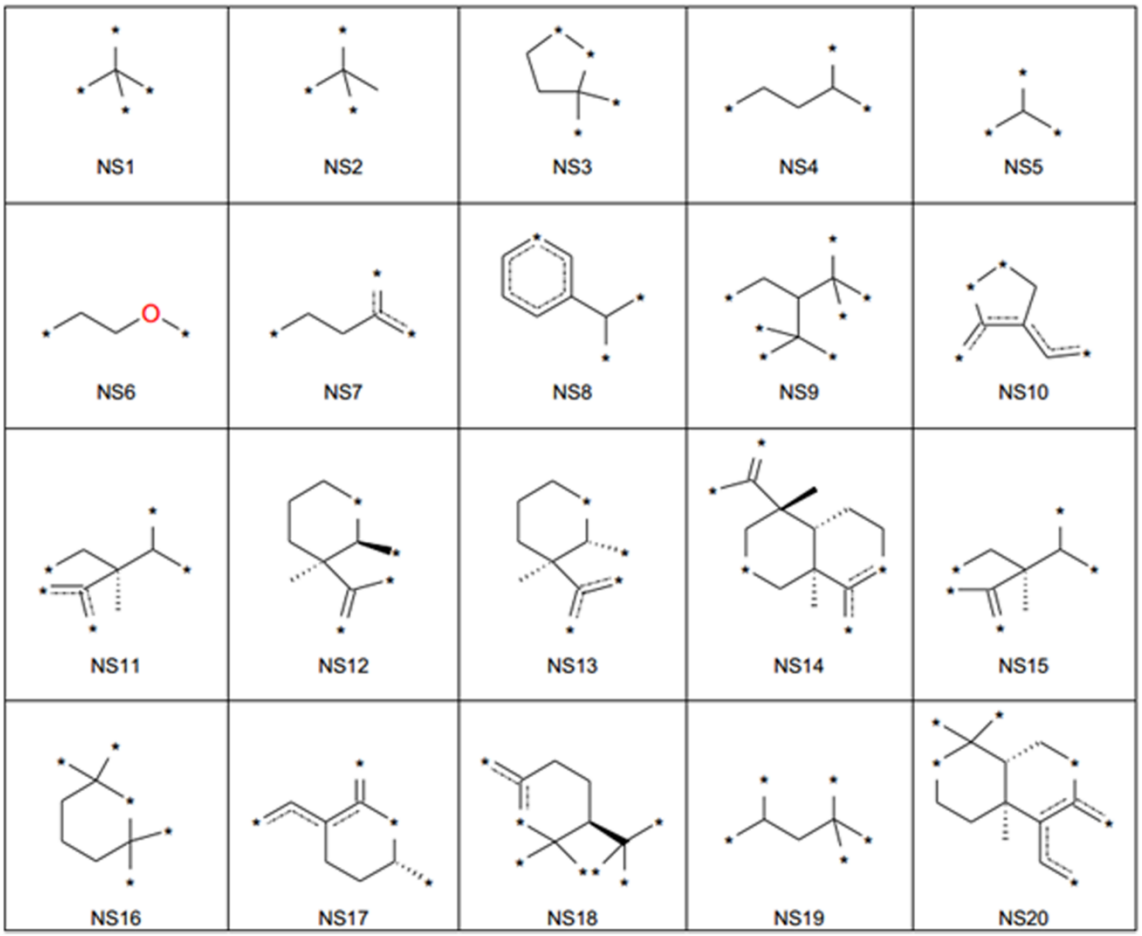


Fig. S1 A: privileged fragments for selective LXRβ agonists (PS1~20). B: Unprivileged fragments for selective LXRβ agonists (NS1~20).