Tomographic docking suggests the mechanism of auxin receptor TIR1 selectivity
Supplementary material

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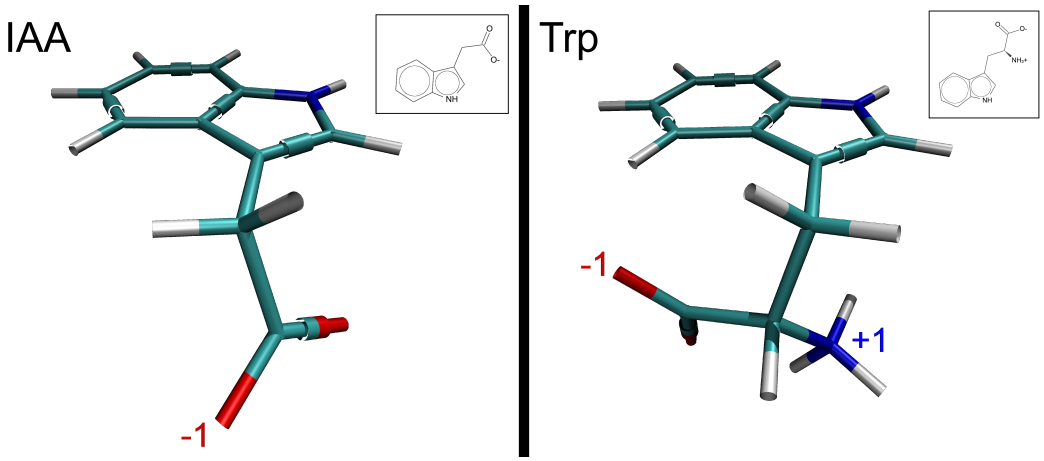

Figure S1: Structures of IAA (on the left) and Trp (on the right), displaying bond orders and charges at pH=7.3. The insets show the respective skeletal structural formulae.

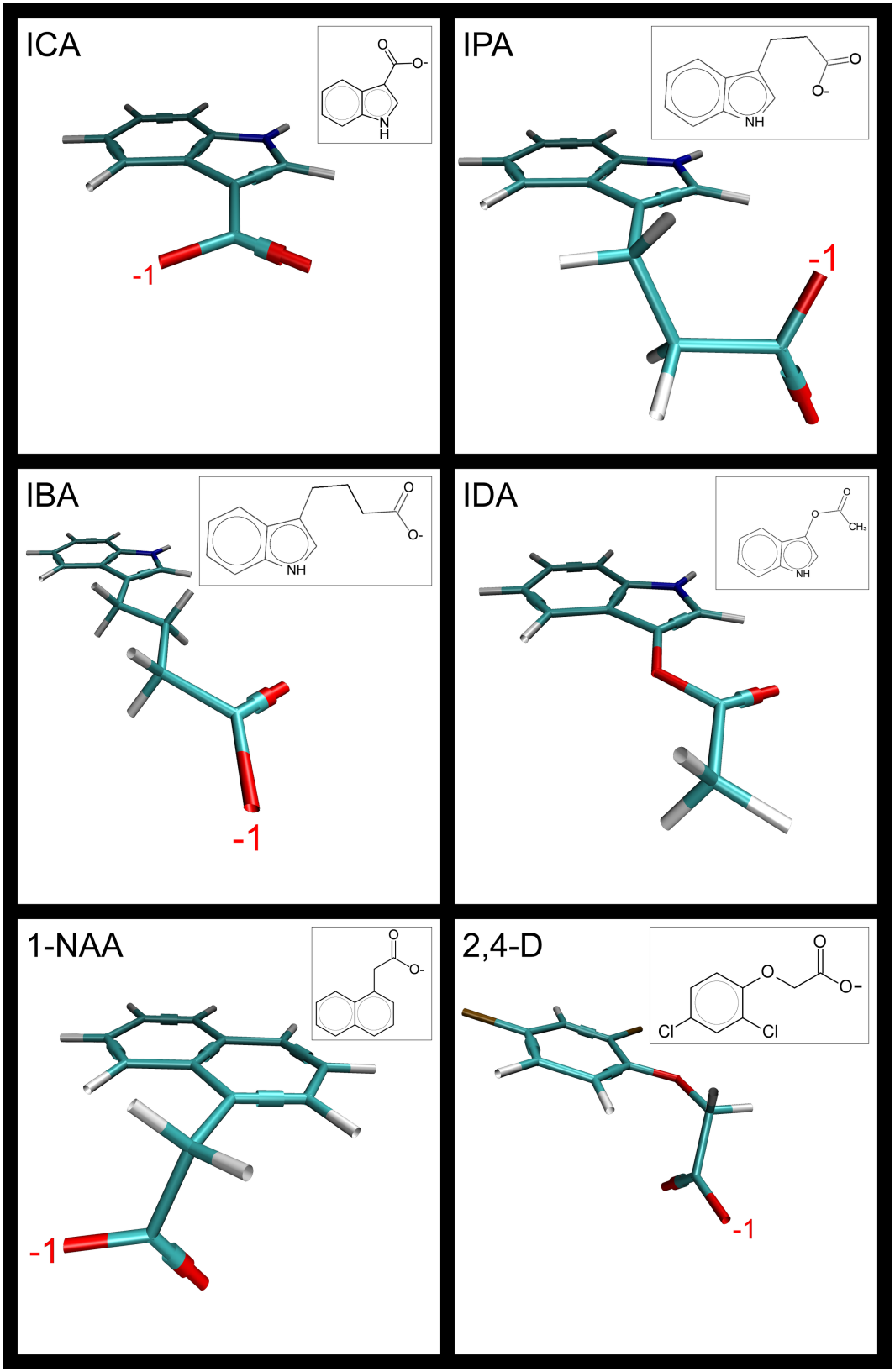

Figure S2: Structure of compounds used for validation. All representations show bond order and charges at pH=7.3, with skeletal structural formulae in the insets. Top-left: indole-3-carboxylic acid (ICA). Top-right: indole-3-propionic acid (IPA). Middle-left: indole-3-butyric acid (IBA). Middle-right: 3-indolyl acetate (IDA). Bottom-left: 1-naphthaleneacetic acid (1-NAA). Bottom-right: 2,4-dichlorophenoxyacetic acid (2,4-D).

	Atoms in search space at step number														
Residue	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
HIS-78	0	0	0	0	0	1	1	3	6	6	6	6	6	6	6
PHE-79	0	1	1	3	4	4	4	4	4	4	4	4	4	4	4
PHE-82	1	3	4	6	7	9	9	9	9	9	9	9	9	9	9
LEU-84	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
VAL-321	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
ARG-344	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
VAL-345	0	0	0	0	0	0	0	0	0	0	0	0	1	2	6
PHE-346	0	0	0	0	0	0	0	0	0	0	1	5	8	11	12
PRO-347	0	0	0	0	0	0	1	3	5	6	6	6	6	6	6
PRO-350	1	2	3	6	6	6	6	6	6	6	6	6	6	6	6
PHE-351	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
MET-353	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
GLU-361	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
LEU-378	0	0	0	0	0	0	0	0	0	0	0	1	3	3	7
TYR-379	0	0	0	0	0	0	0	0	0	0	0	2	3	7	10
PHE-380	0	0	0	0	0	0	0	2	4	9	10	12	12	12	12
CYS-381	0	0	0	0	0	0	1	2	4	5	7	7	7	7	7
GLN-383	0	0	0	0	0	0	0	0	1	2	2	2	2	2	2
MET-384	0	0	0	0	0	0	0	0	1	2	2	2	4	4	4
PHE-402	0	0	0	0	0	0	0	0	0	0	0	0	0	1	4
ARG-403	0	0	0	0	0	0	0	0	0	0	1	4	10	14	17
LEU-404	0	0	0	0	0	0	0	0	1	2	6	9	9	9	9
CYS-405	0	0	0	0	0	1	***1***	***5***	5	7	7	7	7	7	7
ILE-406	0	0	0	1	2	5	7	9	9	9	9	9	9	9	9
ILE-407	0	2	3	5	8	9	9	9	9	9	9	9	9	9	9
GLU-408	7	9	10	10	10	10	10	10	10	10	10	10	10	10	10
PRO-409	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7
LYS-410	10	10	10	10	10	10	10	10	10	10	10	8	7	6	5
ALA-411	1	3	4	4	4	4	4	4	4	4	4	4	4	4	4
PHE-424	0	0	0	0	0	0	0	0	0	2	3	4	4	4	4
ARG-436	0	0	0	0	0	0	0	0	0	0	1	4	6	9	12
LEU-437	0	0	0	0	0	0	0	0	0	0	1	3	7	8	8
SER-438	0	0	0	0	0	0	0	0	***0***	***5***	6	8	8	8	8
LEU-439	0	0	0	0	0	***1***	***4***	***7***	***9***	9	9	9	9	9	9
SER-440	0	0	0	0	0	3	7	8	8	8	8	8	8	8	8
GLY-441	0	0	1	3	4	4	4	4	4	4	4	4	4	4	4
SER-462	0	0	0	0	0	***0***	***2***	***3***	***5***	5	5	5	5	5	5
VAL-463	0	0	2	3	5	5	5	5	5	5	5	5	5	5	5
ALA-464	1	4	5	6	6	6	6	6	6	6	6	6	6	6	6
PHE-465	12	12	12	12	12	12	12	12	12	12	12	12	12	11	9
ALA-466	4	5	5	5	5	5	5	5	5	5	5	5	5	5	5
ARG-489	***9***	***13***	***14***	***16***	16	16	16	16	16	16	16	16	16	16	16
ASP-490	9	9	9	9	9	9	9	9	9	9	9	9	8	5	0
CYS-491	3	3	3	3	3	3	3	3	3	3	3	3	3	3	1
PRO-492	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
SER-515	3	3	3	3	3	3	3	3	3	3	1	0	0	0	0
IHP-601	0	0	0	0	0	0	0	0	0	0	0	0	1	1	2

Table S1: Number of atoms belonging to each residue included in the search space at each step. The residues in violet are those belonging to the engagement niche; those in orange constitute the molecular filter. The steps across which the contribution of the molecular filter residues changes significantly are highlighted in bold italic typefont.