

## 咪唑类离子液体与酪氨酸相互作用及机理的密度泛函理论研究

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## Interaction and Mechanism between Imidazolium Ionic Liquids and Zwitterionic Amino Acid Tyr: a DFT study

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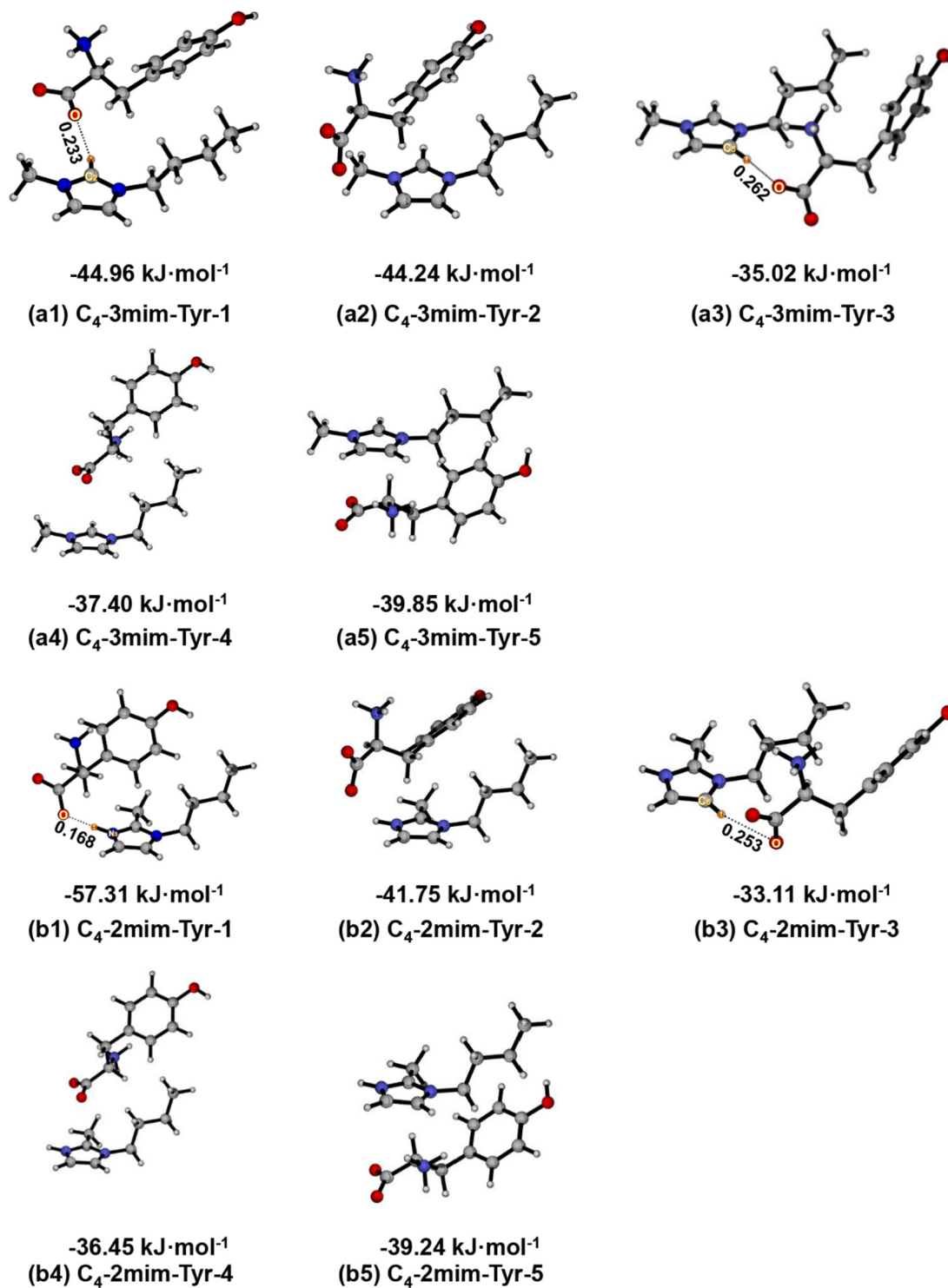
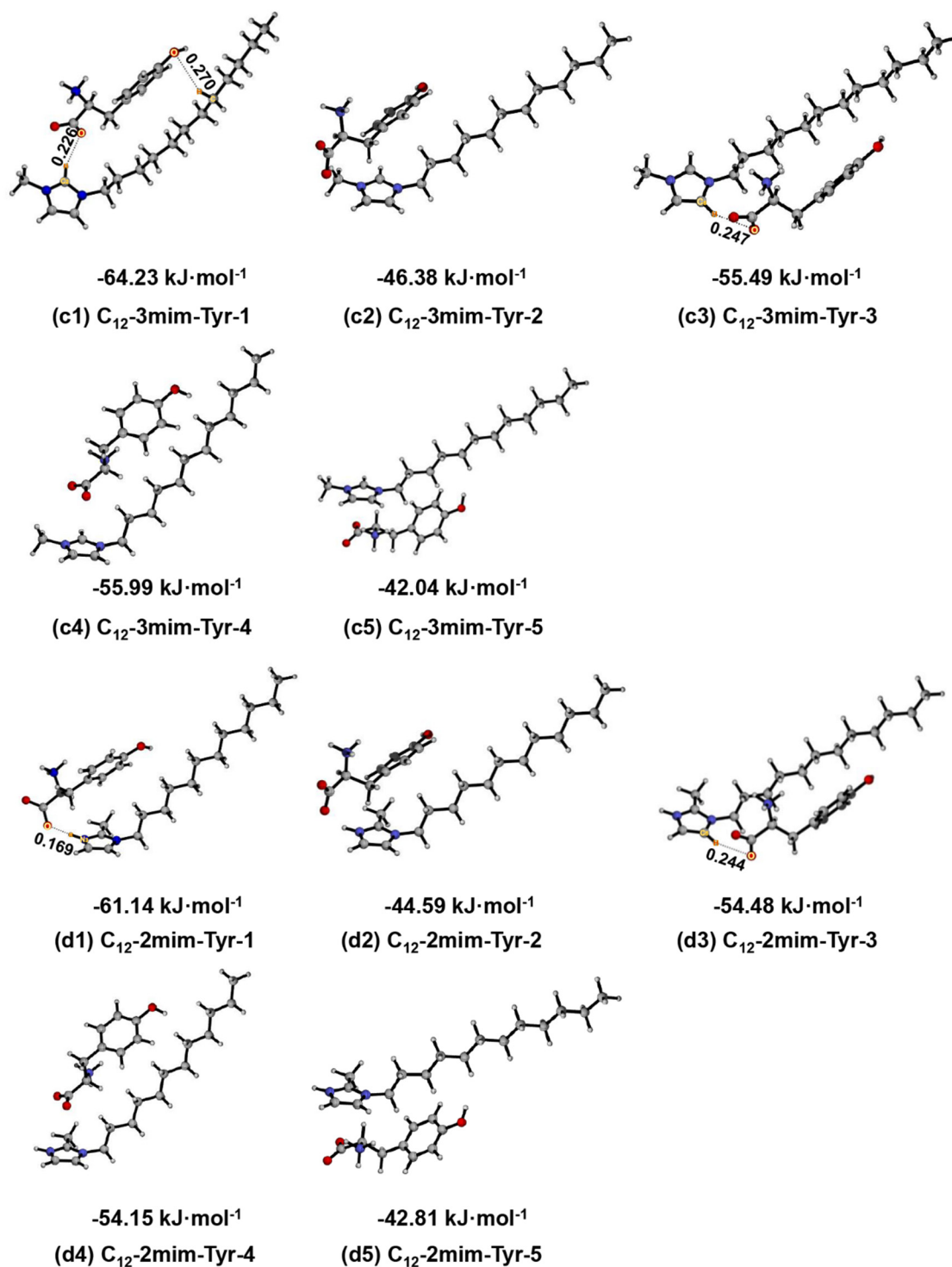


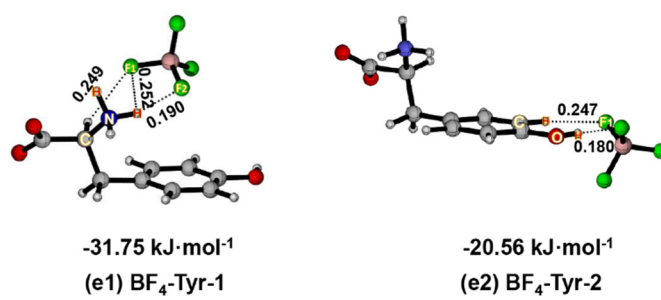
Fig. S1 The optimized conformers of  $\text{C}_4\text{-3mim-Tyr}/\text{C}_4\text{-2mim-Tyr}$  complexes.

The unit of the distances of H-bond labeled in picture is nm.



**Fig. S2** The optimized conformers of C<sub>12</sub>-3mim-Tyr/C<sub>12</sub>-2mim-Tyr complexes.

The unit of the distances of H-bond labeled in picture is nm.



**Fig. S3** The optimized conformers of BF<sub>4</sub>-Tyr complexes.

The unit of the distances of H-bond labeled in picture is nm.

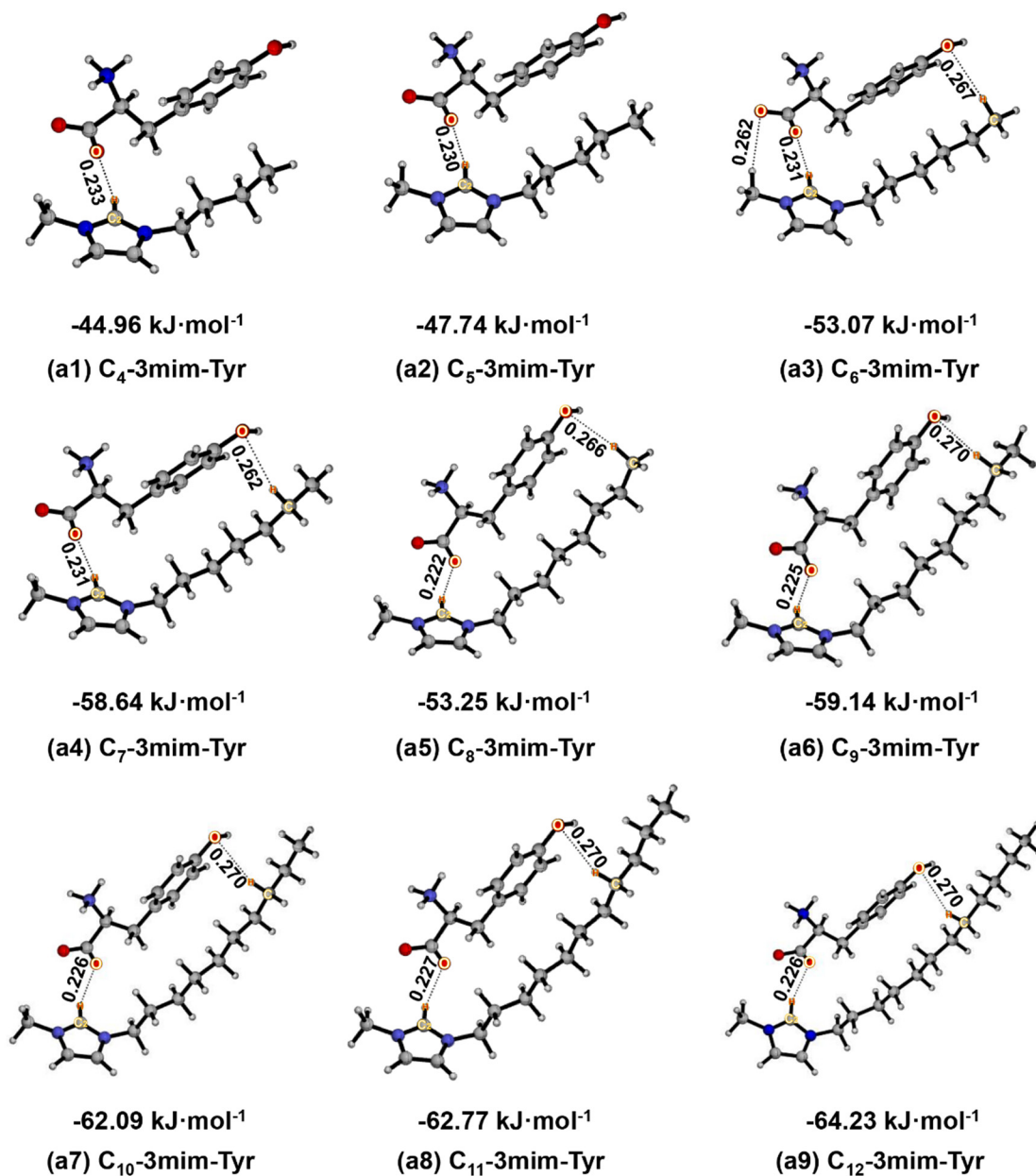


Fig. S4 The optimized conformers of  $C_n$ -3mim complexes.

Chain length  $n$  increase from 4 to 12, the unit of the distances of H-bond labeled in picture is nm.

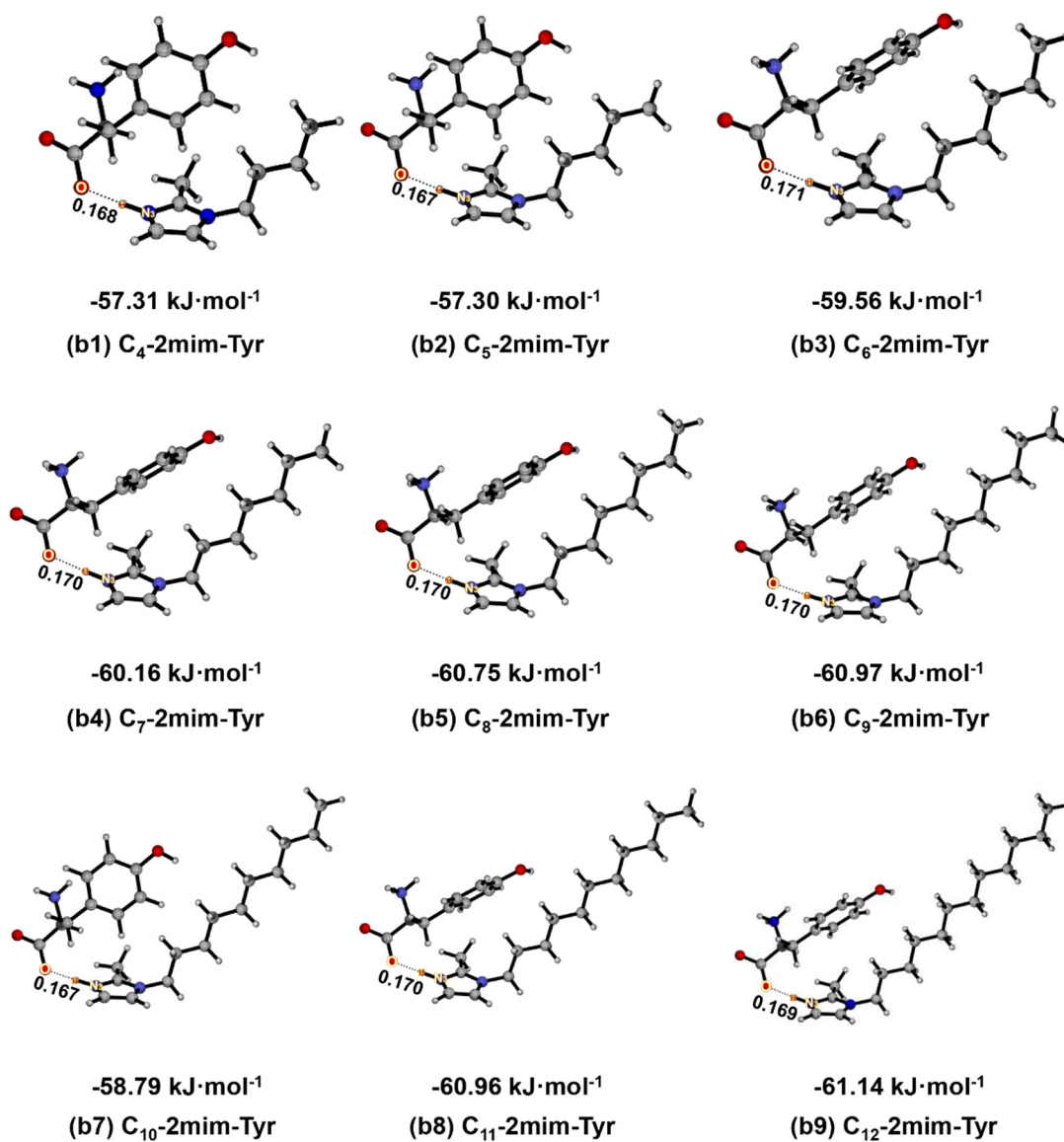
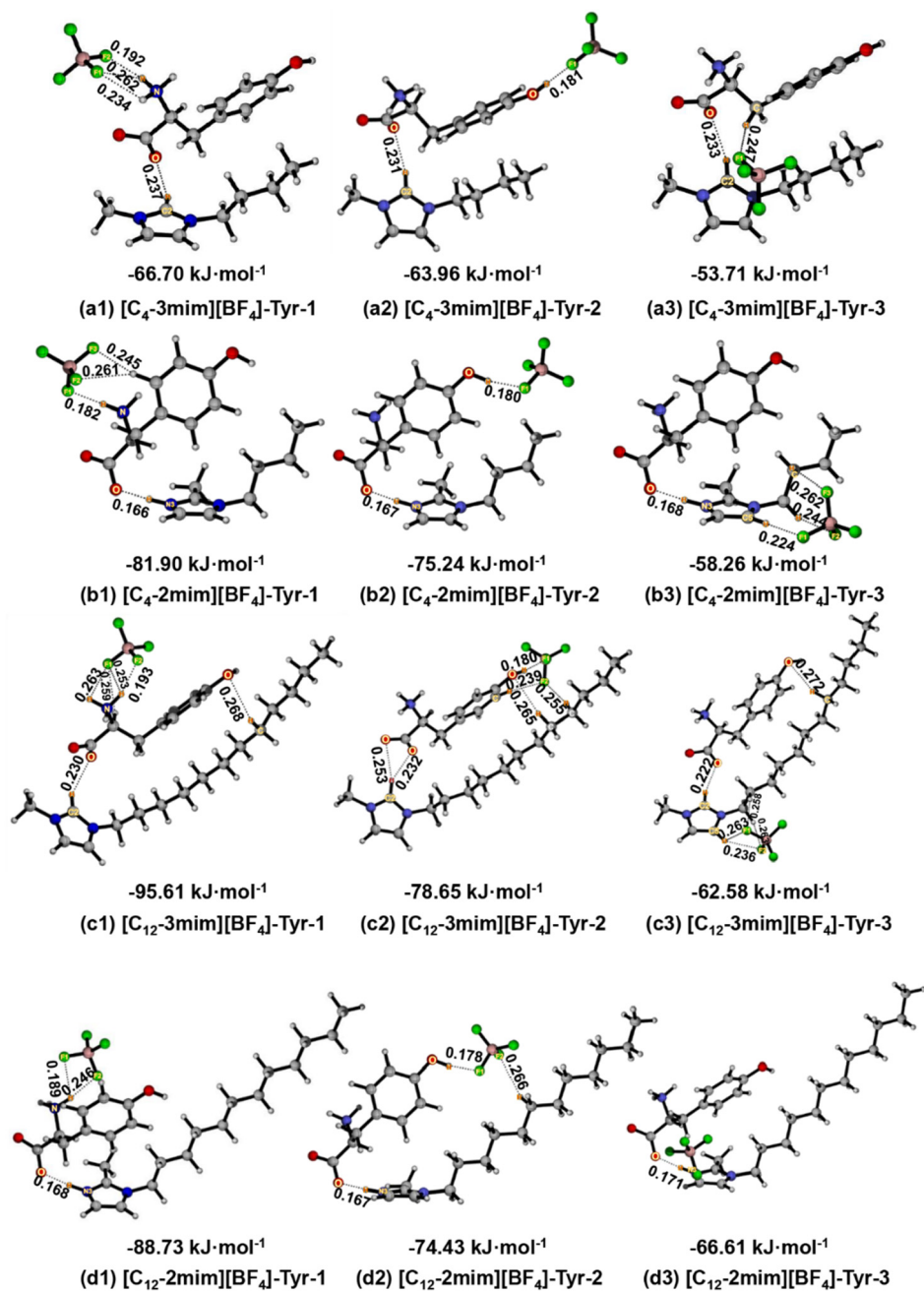


Fig. S5 The optimized conformers of  $C_n$ -2mim complexes.

Chain length  $n$  increase from 4 to 12, the unit of the distances of H-bond labeled in picture is nm.



**Fig. S6** The optimized conformers of ILs-Tyr complexes.

The unit of the distances of H-bond labeled in picture is nm.

**Table S1 H-bonds and interaction energy of cation/anion-Tyr complexes.**

Structures	H-bond	Distance/nm	Angle/(°)	$\Delta E/(\text{kJ}\cdot\text{mol}^{-1})$	$\Delta\Delta E/(\text{kJ}\cdot\text{mol}^{-1})$
C <sub>4</sub> -3mim-Tyr -1	C2-H $\cdots$ O <sub>COO</sub>	0.233	155.0	-44.96	0.00
C <sub>4</sub> -3mim-Tyr -2	N/A	N/A	N/A	-44.24	0.72
C <sub>4</sub> -3mim-Tyr -3	C5-H $\cdots$ O <sub>COO</sub>	0.262	167.0	-35.02	9.94
C <sub>4</sub> -3mim-Tyr -4	N/A	N/A	N/A	-37.40	7.56
C <sub>4</sub> -3mim-Tyr -5	N/A	N/A	N/A	-39.85	5.11
C <sub>4</sub> -2mim-Tyr -1	N3-H $\cdots$ O <sub>COO</sub>	0.168	174.7	-57.31	0.00
C <sub>4</sub> -2mim-Tyr -2	N/A	N/A	N/A	-41.75	15.56
C <sub>4</sub> -2mim-Tyr -3	C5-H $\cdots$ O <sub>COO</sub>	0.253	155.0	-33.11	24.20
C <sub>4</sub> -2mim-Tyr -4	N/A	N/A	N/A	-36.45	20.86
C <sub>4</sub> -2mim-Tyr -5	N/A	N/A	N/A	-39.24	18.07
C <sub>12</sub> -3mim-Tyr -1	C2-H $\cdots$ O <sub>COO</sub>	0.226	151.3	-64.23	0.00
	C <sub>Alkyl</sub> -H $\cdots$ O <sub>OH</sub>	0.270	132.7	N/A	N/A
C <sub>12</sub> -3mim-Tyr -2	N/A	N/A	N/A	-46.38	17.85
C <sub>12</sub> -3mim-Tyr -3	C5-H $\cdots$ O <sub>COO</sub>	0.247	156.2	-55.49	8.74
C <sub>12</sub> -3mim-Tyr -4	N/A	N/A	N/A	-55.99	8.24
C <sub>12</sub> -3mim-Tyr -5	N/A	N/A	N/A	-42.04	22.19
C <sub>12</sub> -2mim-Tyr -1	N3-H $\cdots$ O <sub>COO</sub>	0.169	168.9	-61.14	0.00
C <sub>12</sub> -2mim-Tyr -2	N/A	N/A	N/A	-44.59	16.55
C <sub>12</sub> -2mim-Tyr -3	C5-H $\cdots$ O <sub>COO</sub>	0.244	157.8	-54.48	6.66
C <sub>12</sub> -2mim-Tyr -4	N/A	N/A	N/A	-54.15	6.99
C <sub>12</sub> -2mim-Tyr -5	N/A	N/A	N/A	-42.81	18.33
BF <sub>4</sub> -Tyr-1	N <sub>Tyr</sub> -H $\cdots$ F2	0.190	161.8	-31.75	N/A
	C <sub>Amino</sub> -H $\cdots$ F1	0.249	124.6	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F1	0.252	106.9	N/A	N/A
BF <sub>4</sub> -Tyr-2	O <sub>OH</sub> -H $\cdots$ F1	0.180	170.2	-20.56	11.19
	C <sub>Ben</sub> -H $\cdots$ F1	0.247	173.0	N/A	N/A

**Table S2 H-bonds and interaction energy of ILs-Tyr complexes.**

Structure	H-bond	Distance/nm	Angle/(°)	$\Delta E/(\text{kJ}\cdot\text{mol}^{-1})$	$\Delta\Delta E/(\text{kJ}\cdot\text{mol}^{-1})$
[C <sub>4</sub> -3mim][BF <sub>4</sub> ]-Tyr-1	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.237	153.2	-66.70	0.00
	N <sub>Tyr</sub> -H $\cdots$ F1	0.234	115.3	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F1	0.262	96.6	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F2	0.192	155.2	N/A	N/A
[C <sub>4</sub> -3mim][BF <sub>4</sub> ]-Tyr-2	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.231	156.3	-63.96	2.74
	O <sub>OH</sub> -H $\cdots$ F1	0.181	175.4	N/A	N/A
[C <sub>4</sub> -3mim][BF <sub>4</sub> ]-Tyr-3	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.233	158.5	-53.71	12.99
	C <sub>Amino</sub> -H $\cdots$ F1	0.247	157.7	N/A	N/A
[C <sub>4</sub> -2mim][BF <sub>4</sub> ]-Tyr-1	N <sub>3</sub> -H $\cdots$ O <sub>COO</sub>	0.166	177.5	-81.90	0.00
	N <sub>Tyr</sub> -H $\cdots$ F1	0.182	179.4	N/A	N/A
	C <sub>Ben</sub> -H $\cdots$ F2	0.261	151.0	N/A	N/A
	C <sub>Ben</sub> -H $\cdots$ F3	0.245	151.1	N/A	N/A
[C <sub>4</sub> -2mim][BF <sub>4</sub> ]-Tyr-2	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.167	176.0	-75.24	6.66
	O <sub>OH</sub> -H $\cdots$ F1	0.180	166.4	N/A	N/A
[C <sub>4</sub> -2mim][BF <sub>4</sub> ]-Tyr-3	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.168	175.8	-58.26	23.64
	C <sub>5</sub> -H $\cdots$ F1	0.224	180.0	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ F2	0.244	150.5	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ F3	0.262	129.8	N/A	N/A
[C <sub>12</sub> -3mim][BF <sub>4</sub> ]-Tyr-1	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.230	143.5	-95.61	0.00
	C <sub>Alkyl</sub> -H $\cdots$ O <sub>OH</sub>	0.268	137.2	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F2	0.193	158.7	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F1	0.253	100.4	N/A	N/A
	C <sub>Amino</sub> -H $\cdots$ F1	0.259	75.9	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F1	0.263	95.0	N/A	N/A
[C <sub>12</sub> -3mim][BF <sub>4</sub> ]-Tyr-2	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.232	153.3	-78.65	16.96
	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.253	139.4	N/A	N/A
	O <sub>OH</sub> -H $\cdots$ F1	0.180	168.1	N/A	N/A
[C <sub>12</sub> -3mim][BF <sub>4</sub> ]-Tyr-2	C <sub>Ben</sub> -H $\cdots$ F2	0.239	168.6	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ F2	0.255	122.5	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ O <sub>OH</sub>	0.265	156.1	N/A	N/A
[C <sub>12</sub> -3mim][BF <sub>4</sub> ]-Tyr-3	C <sub>2</sub> -H $\cdots$ O <sub>COO</sub>	0.222	156.5	-62.58	33.03
	C <sub>Alkyl</sub> -H $\cdots$ O <sub>OH</sub>	0.272	131.2	N/A	N/A
	C <sub>5</sub> -H $\cdots$ F2	0.236	146.4	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ F1	0.258	157.4	N/A	N/A
	C <sub>5</sub> -H $\cdots$ F1	0.263	130.0	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ F2	0.263	130.8	N/A	N/A
[C <sub>12</sub> -2mim][BF <sub>4</sub> ]-Tyr-1	N <sub>3</sub> -H $\cdots$ O <sub>COO</sub>	0.168	173.9	-88.73	0.00
	N <sub>Tyr</sub> -H $\cdots$ F1	0.189	116.7	N/A	N/A
	N <sub>Tyr</sub> -H $\cdots$ F2	0.246	146.8	N/A	N/A
[C <sub>12</sub> -2mim][BF <sub>4</sub> ]-Tyr-2	N <sub>3</sub> -H $\cdots$ O <sub>COO</sub>	0.167	175.9	-74.43	14.30
	O <sub>OH</sub> -H $\cdots$ F1	0.178	168.1	N/A	N/A
	C <sub>Alkyl</sub> -H $\cdots$ F2	0.266	138.2	N/A	N/A
[C <sub>12</sub> -2mim][BF <sub>4</sub> ]-Tyr-2	N <sub>3</sub> -H $\cdots$ O <sub>COO</sub>	0.171	168.2	-66.61	22.12