Electronic Supplementary Information

1,2,4-Triazole based molecular switches: crystal structures, Hirshfeld surface analysis and optical properties

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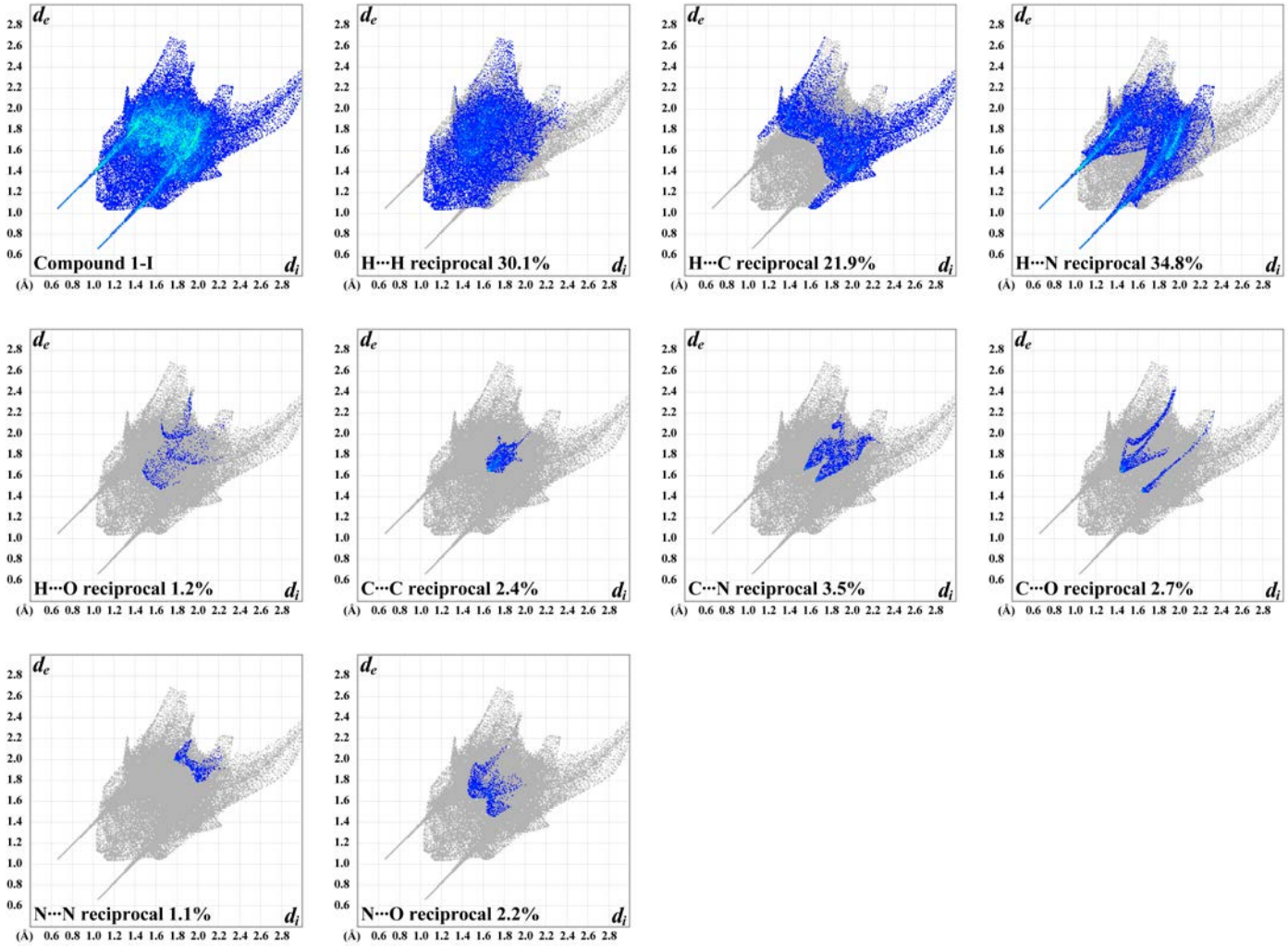


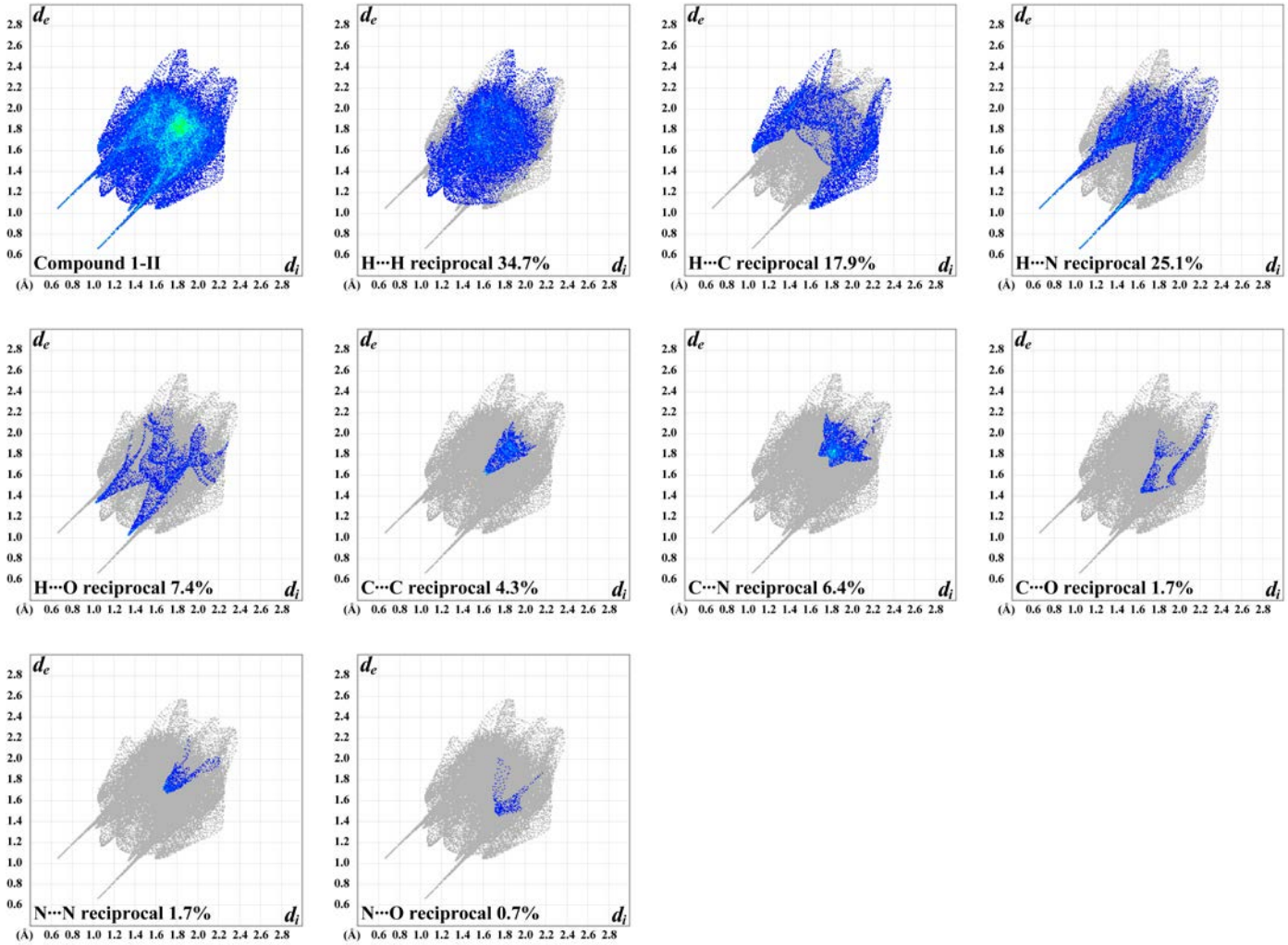


Fig. S1 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for two independent molecules of **1**.

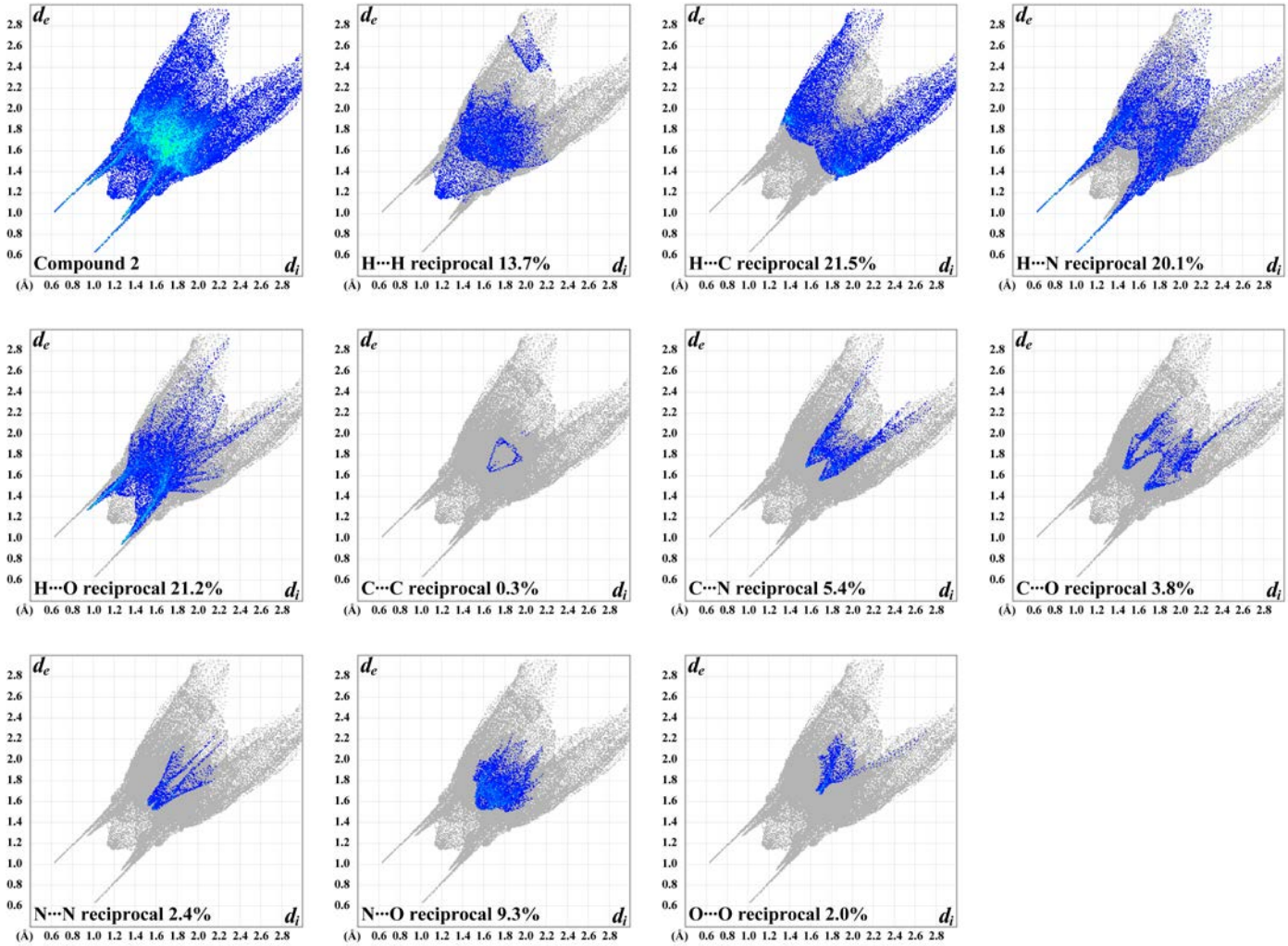


Fig. S2 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for **2**.

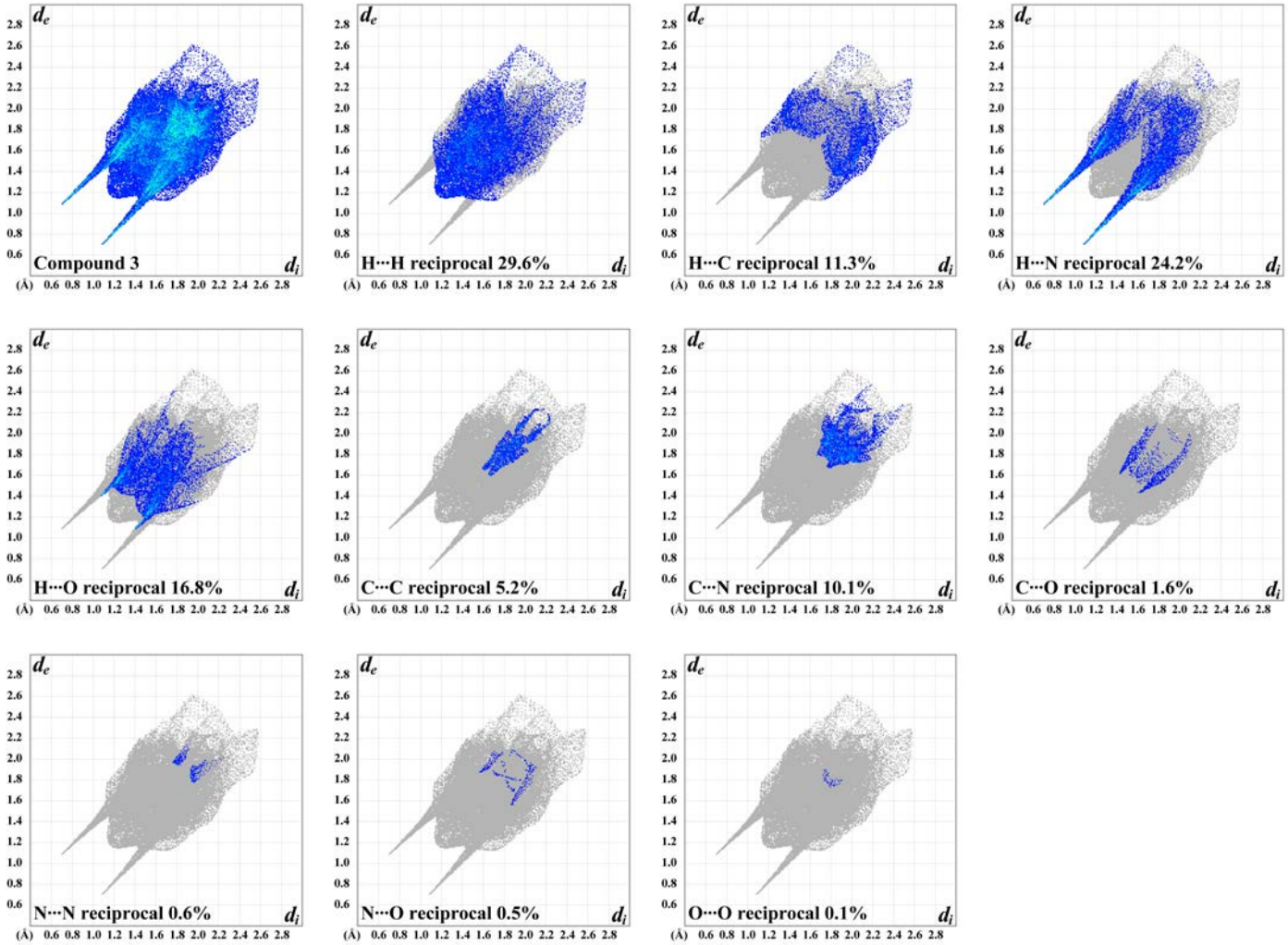


Fig. S3 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for **3**.

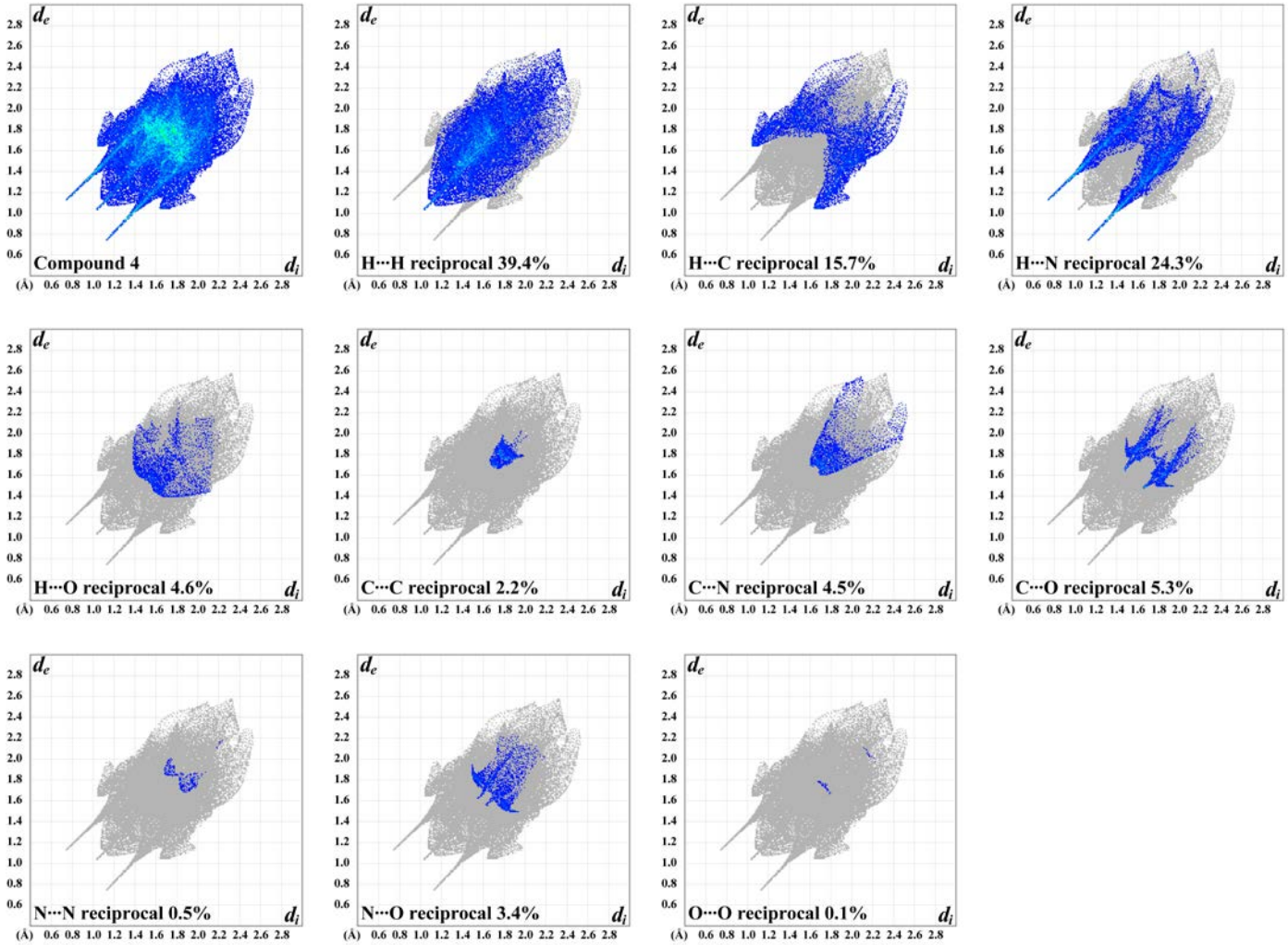


Fig. S4 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for **4**.

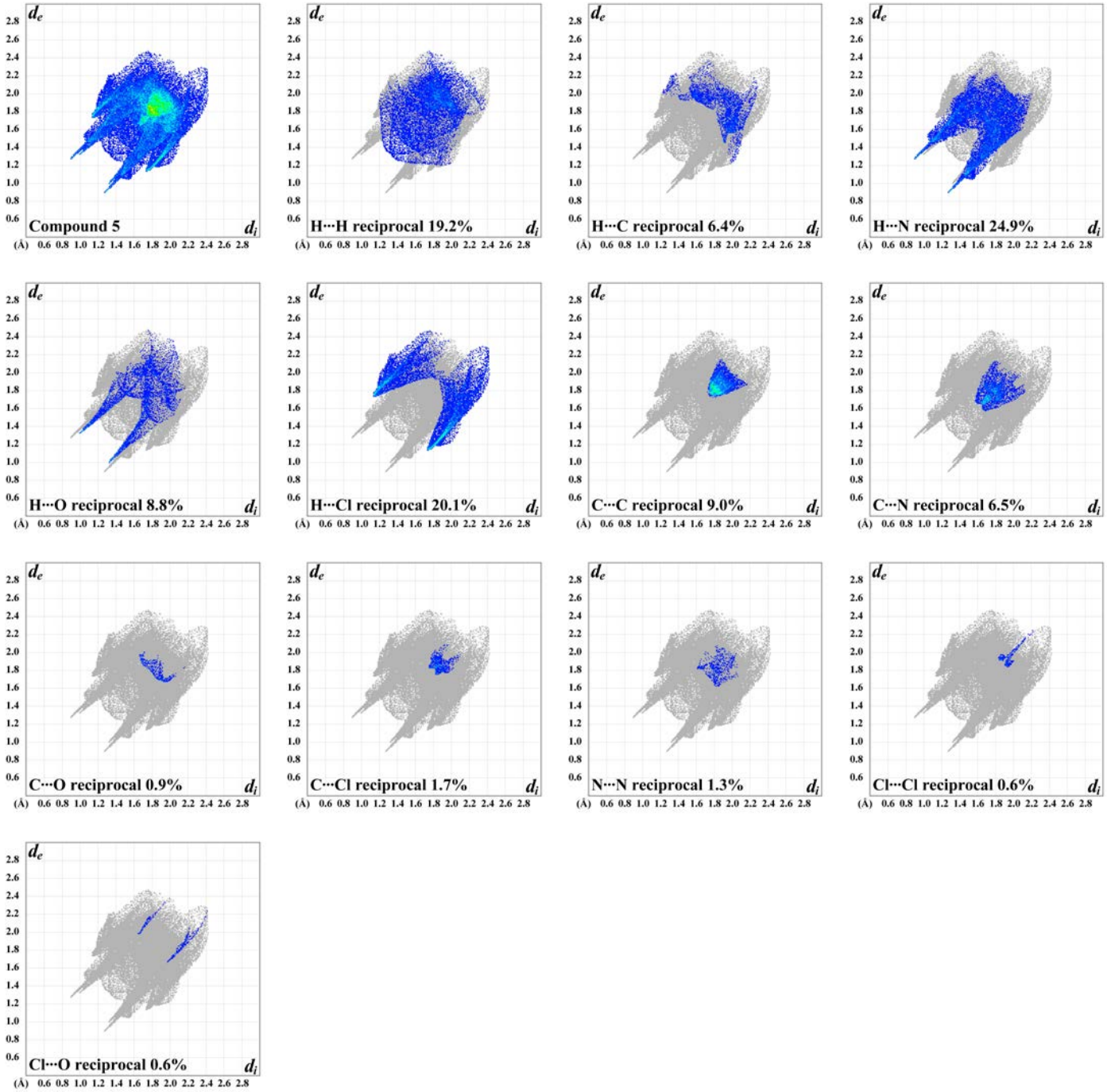


Fig. S5 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for **5**.

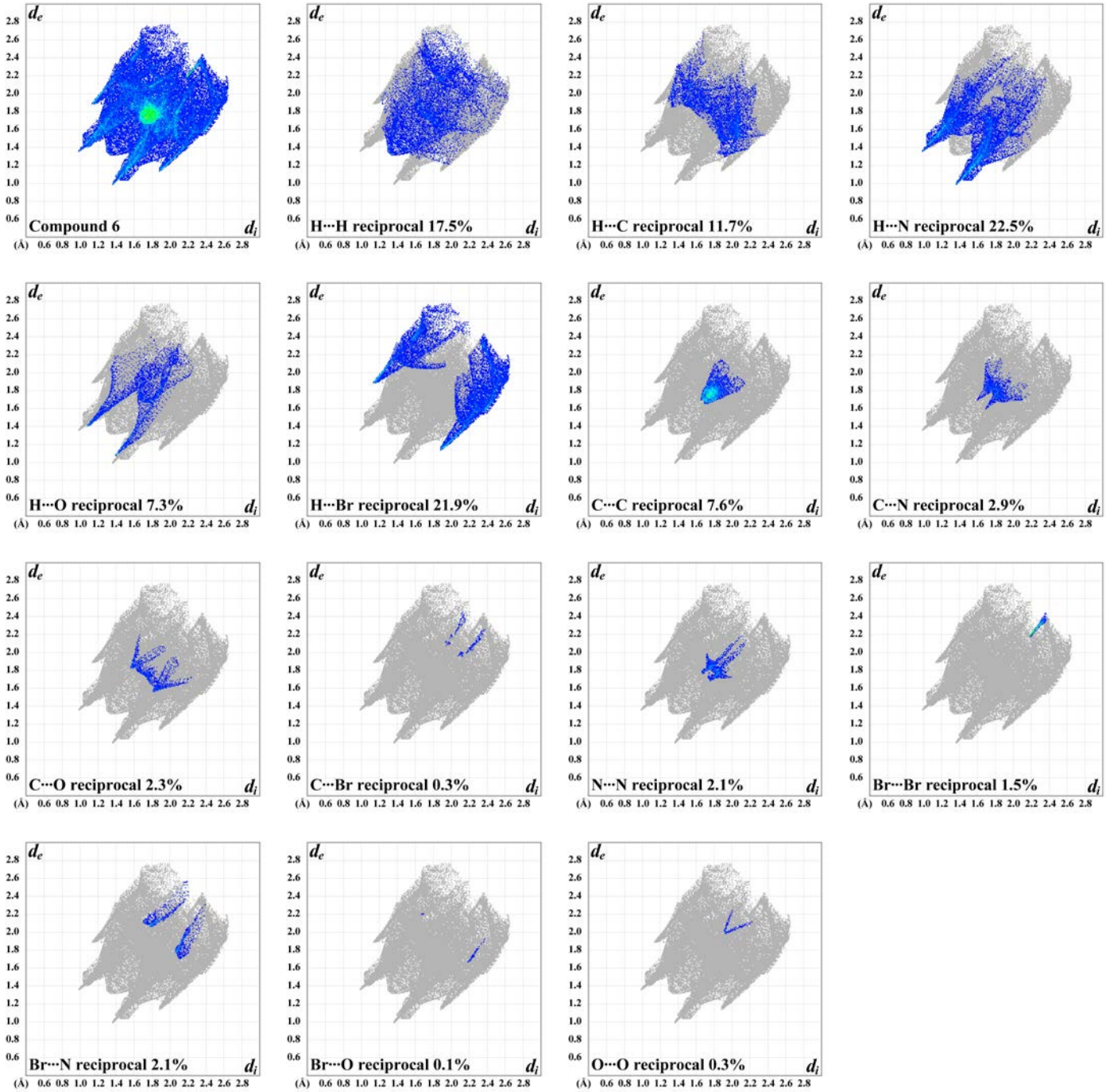
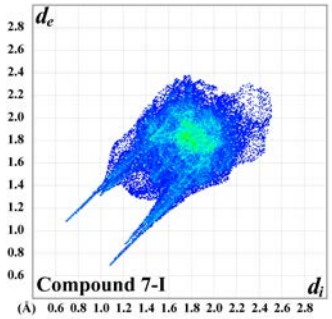
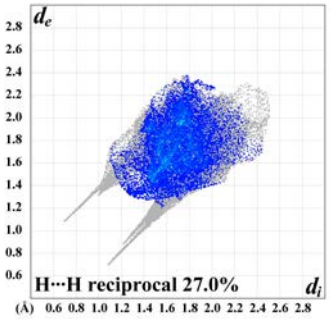


Fig. S6 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for **6**.


d_e
Compound 7-I
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8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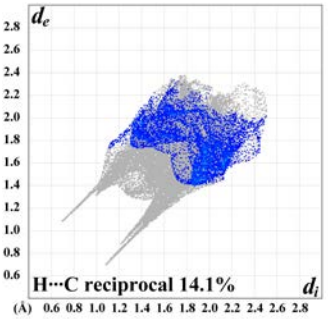
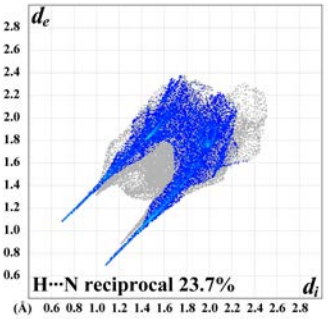
H···H reciprocal 27.0%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
H···C reciprocal 14.1%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8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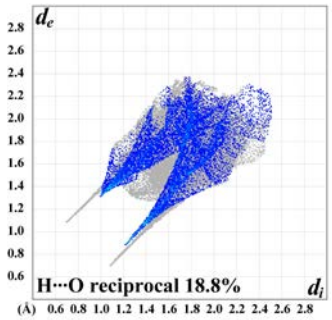
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d_i
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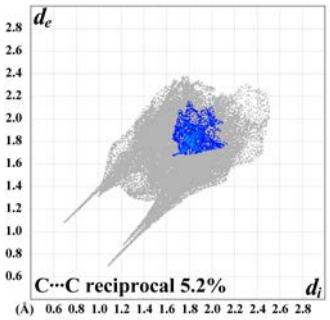
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d_i
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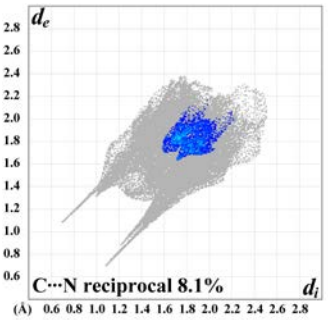
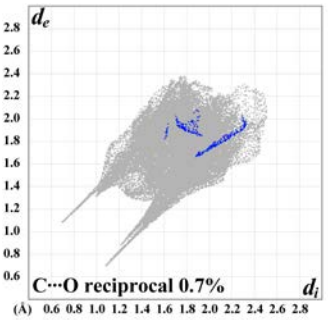

d_e
C···N reciprocal 8.1%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8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C···O reciprocal 0.7%
d_i
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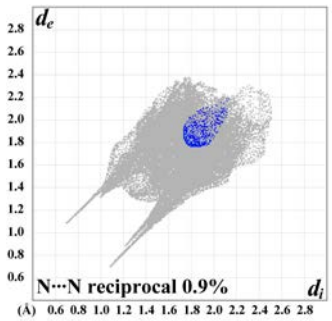
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d_i
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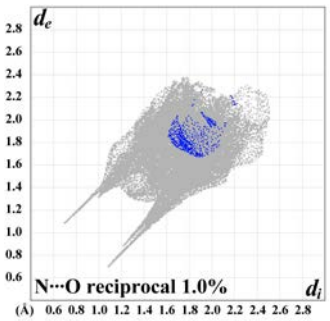
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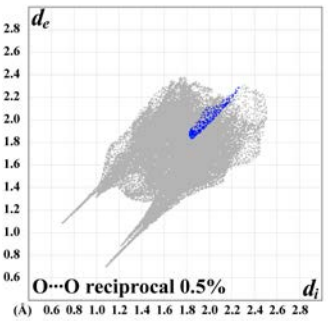
N···O reciprocal 1.0%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8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O···O reciprocal 0.5%
d_i
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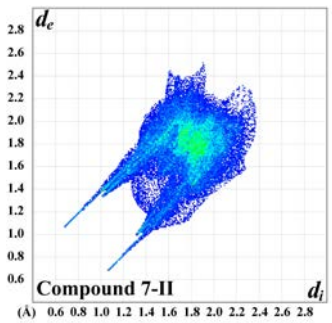
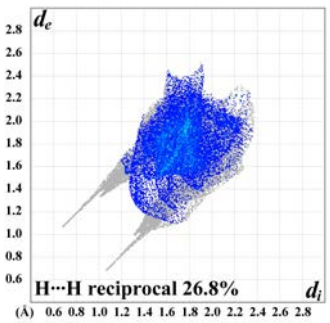
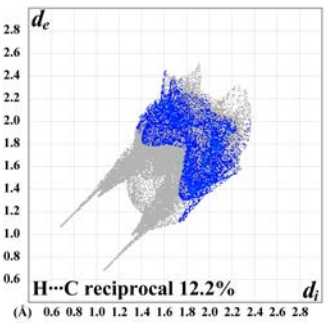

d_e
Compound 7-II
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
H···H reciprocal 26.8%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8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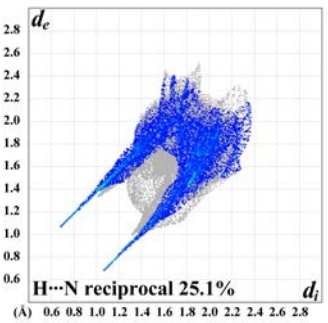
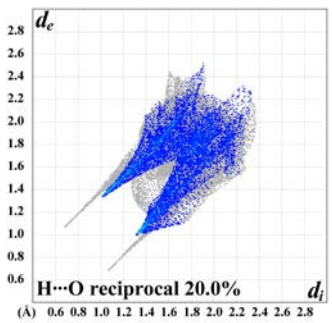
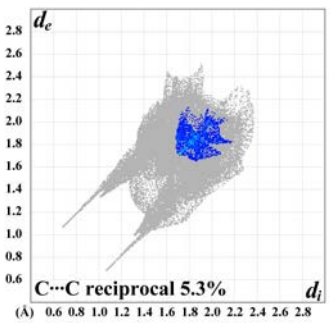
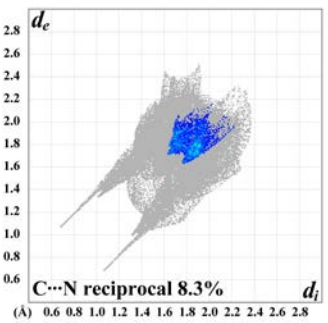
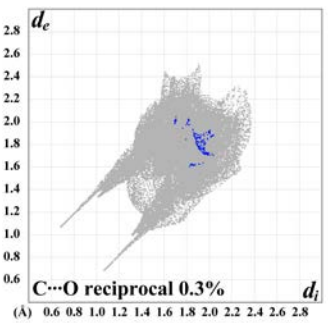
H···C reciprocal 12.2%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
H···N reciprocal 25.1%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
H···O reciprocal 20.0%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
C···C reciprocal 5.3%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
C···N reciprocal 8.3%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8


d_e
C···O reciprocal 0.3%
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

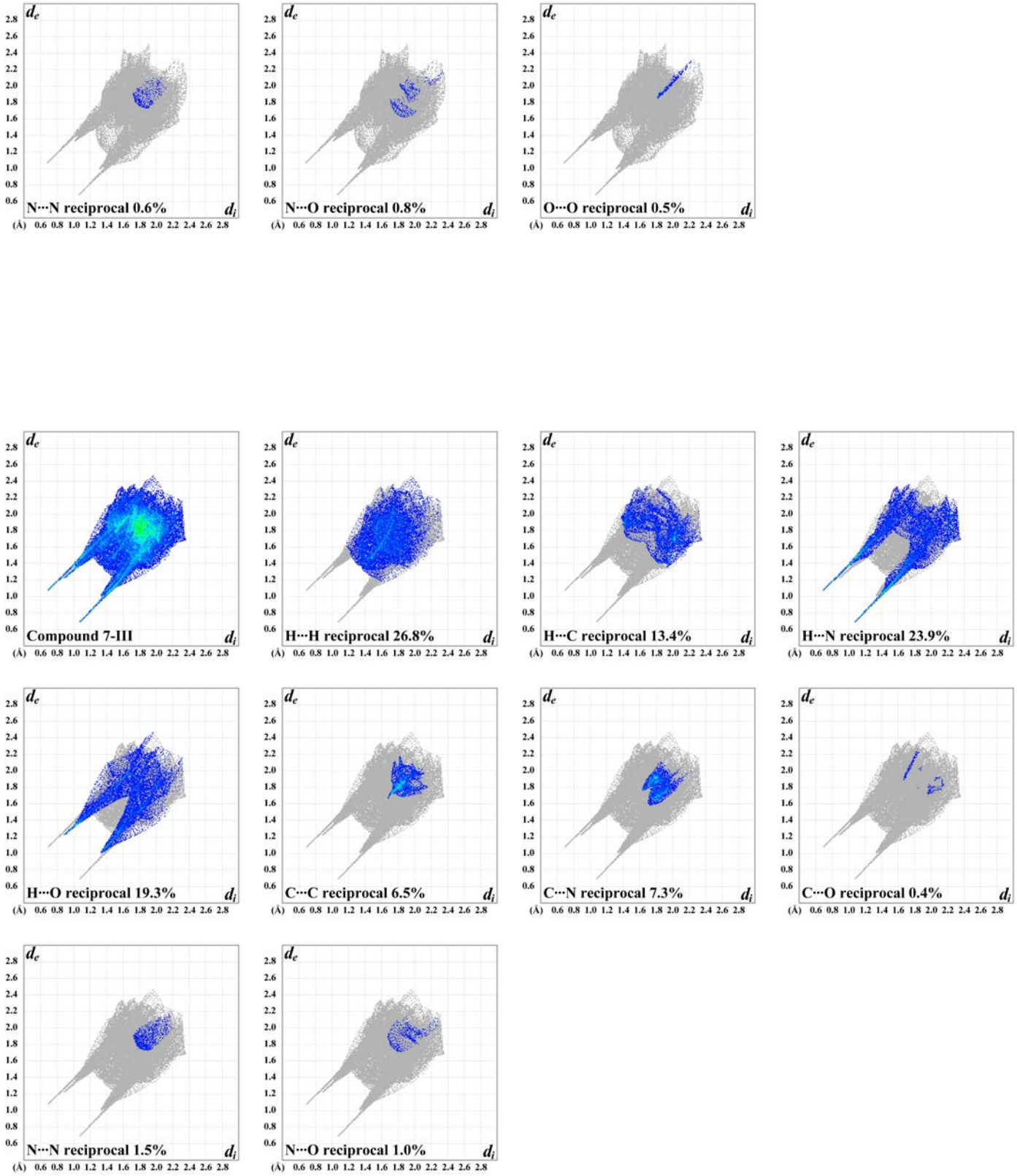


Fig. S7 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for three independent molecules of **7**.

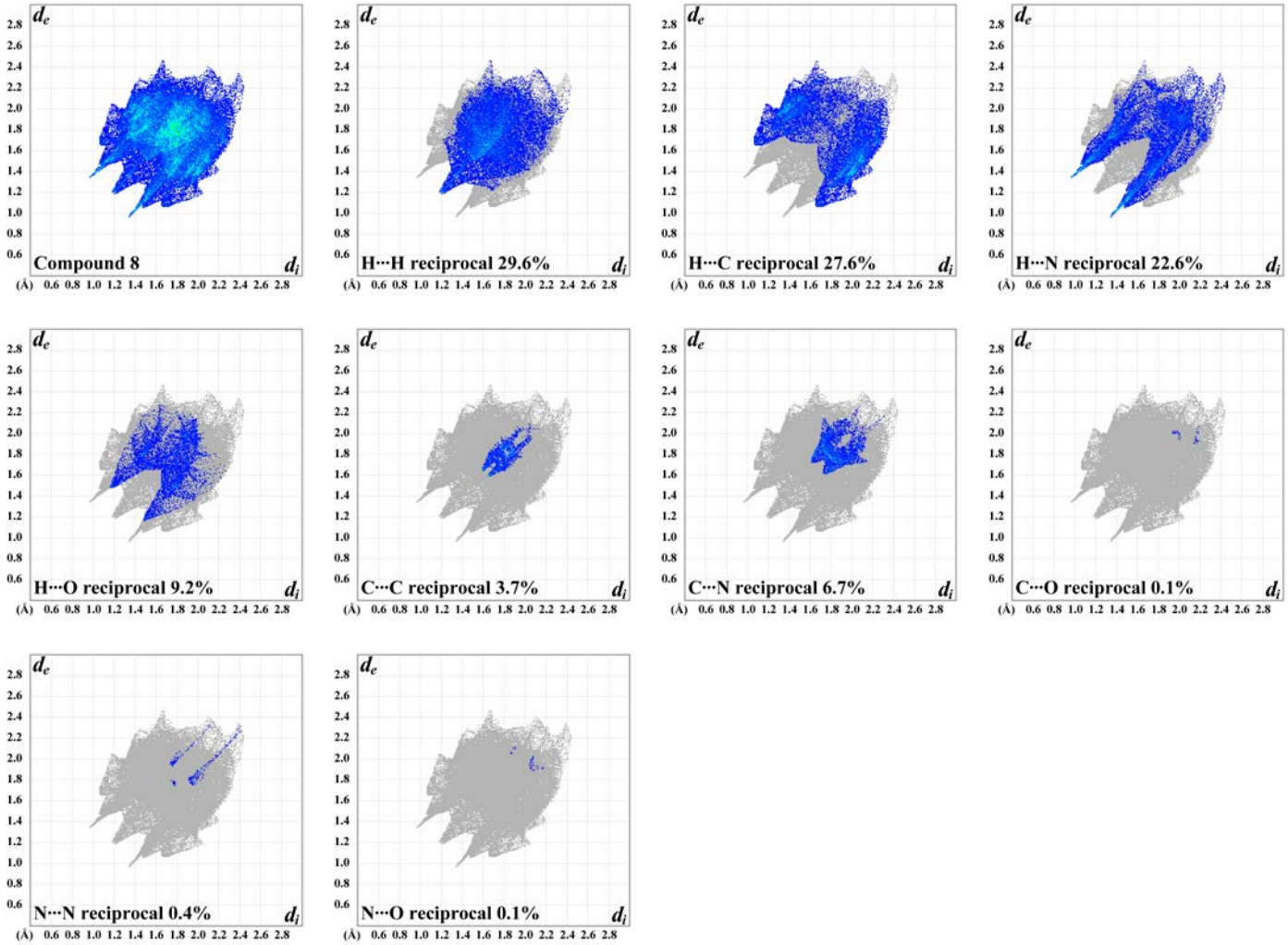


Fig. S8 2D fingerprint plots and decomposed 2D fingerprint plots of observed contacts for **8**.

Table S1 Selected bond lengths (Å) and angles (°) for **1-II**, **7-II** and **7-III**[a]

	1-II	**7-II**	**7-III**
Bond lengths			
C–N	1.279(2)	1.266(17)	1.258(14)
C–C	1.457(2)	1.424(19)	1.469(14)
C–O	1.350(2)	1.360(17)	1.366(13)
N–N	1.401(2)	1.399(15)	1.391(12)
Bond angles			
C–C–N	120.62(14)	121.4(10)	122.1(9)
N–N–C	115.76(13)	117.9(9)	117.2(8)
Torsion angles			
C–C–N–N	–179.67(14)	179.5(9)	178.5(10)
Dihedral angles (Φ)			
Phenol–Triazole	6.1	6.6	2.0

[a]Values with respect to the moieties marked by bold in Scheme 2 of the main text.

Table S2 Classical hydrogen bond lengths (Å) and angles (°) for **1–8**

	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
1[a]	O(14)–H(14)···N(102)$^{\#1}$	0.95(2)	1.74(2)	2.667(2)	163.3(19)
	O(114)–H(114)···N(1)$^{\#2}$	0.93(2)	1.76(2)	2.685(2)	174(2)
2[b]	O(14)–H(14)···N(1)$^{\#1}$	0.84	1.79	2.621(4)	168
3[c]	O(14)–H(14)···N(2)$^{\#1}$	0.82	2.02	2.766(12)	150
	O(15)–H(15)···N(1)$^{\#2}$	0.82	1.94	2.725(12)	160
4[d]	O(14)–H(14)···N(1)$^{\#1}$	0.82	2.04	2.788(3)	151
5	O(14)–H(14)···N(6)	0.84	1.95	2.67(2)	143
6	O(14)–H(14)···N(6)	0.84	1.95	2.684(8)	145
7[e]	O(14)–H(14)···N(6)	0.82	1.96	2.658(13)	142
	O(15)–H(15)···N(1)$^{\#1}$	0.82	1.92	2.710(16)	160
	O(34)–H(34)···N(26)	0.82	1.94	2.648(14)	145
	O(35)–H(35)···N(21)$^{\#1}$	0.82	1.91	2.698(17)	162
	O(54)–H(54)···N(46)	0.82	1.97	2.687(11)	146
	O(55)–H(55)···N(41)$^{\#2}$	0.82	1.92	2.697(12)	158
8	O(14)–H(14)···N(6)	0.82	1.90	2.618(4)	146

[a]Symmetry transformations used to generate equivalent atoms: #1 –1 + *x*, *y*, *z*; #2 –3/2 + *x*, 1/2 – *y*, 1/2 + *z*.

[b]Symmetry transformations used to generate equivalent atoms: #1 3/2 + *x*, 3/2 – *y*, 1/2 + *z*.

[c]Symmetry transformations used to generate equivalent atoms: #1 3/2 + *x*, 1/2 – *y*, 1/2 + *z*; #2 2 + *x*, *y*, 1 + *z*.

[d]Symmetry transformations used to generate equivalent atoms: #1 1/2 + *x*, 1 – *y*, 3/2 + *z*.

[e]Symmetry transformations used to generate equivalent atoms: #1 1 + *x*, *y*, *z*; #2 *x*, –1 + *y*, *z*.

Table S3 Hirshfeld contact surfaces and derived "random contacts" and "enrichment ratios" for **1-II**, **7-II** and **7-III**

	1-II				**7-II**				**7-III**			
	H	C	N	O	H	C	N	O	H	C	N	O
Contacts (*C*, %)[b]												
H	34.7	–	–	–	26.8	–	–	–	26.8	–	–	–
C	17.9	4.3	–	–	12.2	5.3	–	–	13.4	6.5	–	–
N	25.1	6.4	1.7	–	25.1	8.3	0.6	–	23.9	7.3	1.5	–
O	7.4	1.7	0.7	0.0	20.0	0.3	0.8	0.5	19.3	0.4	1.0	0.0
Surface (*S*, %)												
	59.9	17.3	17.8	4.9	55.5	15.7	17.7	11.1	55.1	17.1	17.6	10.4
Random contacts (*R*, %)												
H	35.9	–	–	–	30.8	–	–	–	30.4	–	–	–
C	20.7	3.0	–	–	17.4	2.5	–	–	18.8	2.9	–	–
N	21.3	1.1	3.2	–	19.6	0.9	3.1	–	19.4	1.0	3.1	–
O	5.9	1.7	1.7	0.2	12.3	3.5	3.9	1.2	11.5	3.6	3.7	1.1
Enrichment (*E*)[c]												
H	0.97	–	–	–	0.87	–	–	–	0.88	–	–	–
C	0.86	1.43	–	–	0.70	2.12	–	–	0.71	2.24	–	–
N	1.18	5.82	0.53	–	1.28	9.22	0.19	–	1.23	7.30	0.48	–
O	1.25	1.00	0.41	–	1.63	0.09	0.21	0.42	1.68	0.11	0.27	0.00

[a]Values are obtained from CrystalExplorer 3.1.[1]

[b]The enrichment ratios were not computed when the "random contacts" were lower than 0.9%, as they are not meaningful.[2]

References

1 S. K. Wolff, D. J. Grimwood, J. J. McKinnon, M. J. Turner, D. Jayatilaka and M. A. Spackman, *CrystalExplorer 3.1*, University of Western Australia, 2012.

2 C. Jelsch, K. Ejsmont and L. Huder, *IUCrJ*, 2014, **1**, 119.