Supplementary Information

Crystal structures of 3,3′,5,5′-tetrabromo-4,4′-bipyridine and Co(II) coordination polymer based thereon

Table S1. Details of XRD experiments

	1	**2**
Chemical formula	$C_{10}H_4Br_4N_2$	$C_{12}H_{12}Br_4CoN_4O_8$
M_r	471.79	718.83
Crystal system, space group	Triclinic, $P^{-}1$	Monoclinic, $C2/c$
a, *b*, *c* (Å)	7.8725 (4), 10.9122 (6), 15.6053 (8)	18.3716 (10), 11.4111 (6), 13.2287 (12)
a, b, g (°)	103.034 (2), 96.915 (2), 92.460 (2)	90, 132.282 (2), 90
V (Å^3)	1293.15 (12)	2051.8 (2)
Z	4	4
m (mm^{-1})	12.42	8.67
No. of measured, independent and observed [$I > 2s(I)$] reflections	57634, 7528, 6176	23514, 4908, 4079
R_{int}	0.097	0.093
$(\sin q/l)_{max}$ (Å^{-1})	0.703	0.854
Range of *h*, *k*, *l*	*h* = -11®11, *k* = -15®15, *l* = -21®21	*h* = −30→25, *k* = −17→19, *l* = −20→22
$R[F^2 > 2s(F^2)]$, $wR(F^2)$, *S*	0.042, 0.107, 1.04	0.032, 0.079, 1.02
No. of reflections	7528	4908
No. of parameters	289	139
$D\rho_{max}$, $D\rho_{min}$ (e Å^{-3})	1.66, -1.57	1.20, −1.85

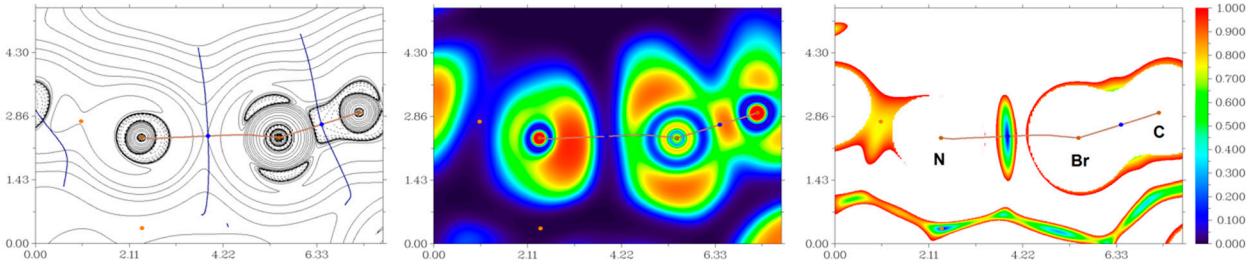

Figure S1. Contour line diagram of the Laplacian of electron density distribution $\nabla^2\rho(\mathbf{r})$, bond paths, and selected zero-flux surfaces (left panel), visualization of electron localization function

(ELF, center panel), and reduced density gradient (RDG, right panel) analyses for halogen bond Br···N (3.088 Å) in **1**. Bond critical points (3, –1) are shown in blue, nuclear critical points (3, –3) in pale brown, ring critical points (3, +1) in orange, and bond paths are shown as pale brown lines, with length units – Å, and the color scale for the ELF and RDG maps is presented in a.u.

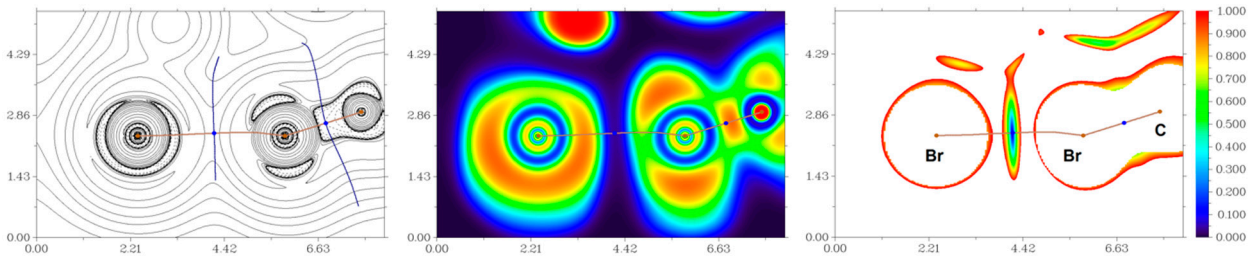

Figure S2. Contour line diagram of the Laplacian of electron density distribution $\nabla^2\rho(\mathbf{r})$, bond paths, and selected zero-flux surfaces (left panel), visualization of electron localization function (ELF, center panel), and reduced density gradient (RDG, right panel) analyses for halogen bond Br···Br (3.459 Å) in **1**. Bond critical points (3, –1) are shown in blue, nuclear critical points (3, –3) in pale brown, bond paths are shown as pale brown lines, length units – Å, and the color scale for the ELF and RDG maps is presented in a.u.

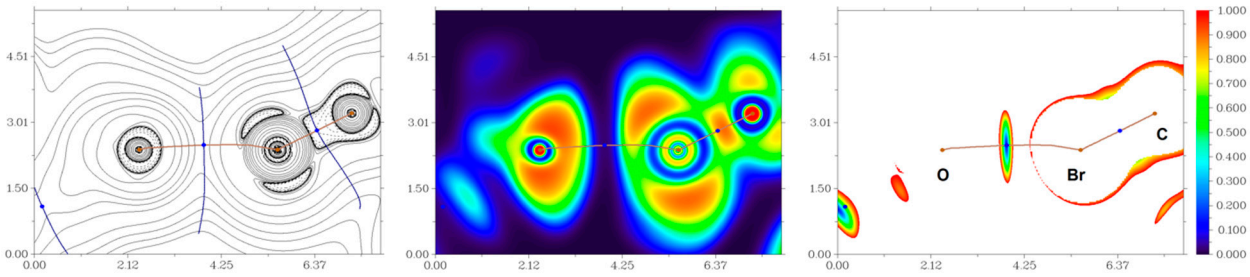

Figure S3. Contour line diagram of the Laplacian of electron density distribution $\nabla^2\rho(\mathbf{r})$, bond paths, and selected zero-flux surfaces (left panel), visualization of electron localization function (ELF, center panel), and reduced density gradient (RDG, right panel) analyses for halogen bond Br···O (3.146 Å) in **2**. Bond critical points (3, –1) are shown in blue, nuclear critical points (3, –3) in pale brown, bond paths are shown as pale brown lines, length units – Å, and the color scale for the ELF and RDG maps is presented in a.u.

Table S2. Cartesian atomic coordinates for model structures.

Atom	X	Y	Z
1 (part with halogen bonds Br···N 3.088 Å)			
C	-0.891618	6.000634	12.558242
C	-1.102966	7.176644	13.288986
C	-1.991819	8.139124	12.843006
H	-2.118368	8.918256	13.372200
N	-2.676543	8.024894	11.711484
C	-2.508025	6.898738	11.013887
H	-3.007321	6.783766	10.214138

C	-1.638115	5.888530	11.399600
C	0.099273	4.983238	12.983128
C	1.410801	4.986625	12.504002
C	2.324755	4.049932	12.942448
H	3.212349	4.087893	12.604844
N	2.014606	3.094867	13.817833
C	0.767294	3.047447	14.266826
H	0.528114	2.358736	14.876161
C	-0.199733	3.958454	13.885634
Br	-0.196992	7.477031	14.913949
Br	-1.518578	4.335470	10.338138
Br	1.948551	6.265311	11.222262
Br	-1.939125	3.773570	14.608543
C	0.324512	11.043110	10.528734
C	1.042581	10.674375	11.660257
C	0.463910	10.777229	12.916834
H	0.970091	10.506899	13.674367
N	-0.778537	11.242776	13.108183
C	-1.482338	11.599621	12.026382
H	-2.363411	11.936047	12.142909
C	-0.971515	11.493089	10.748710
C	0.900928	10.958199	9.160662
C	1.672004	11.967707	8.609214
C	2.164920	11.866608	7.322502
H	2.683849	12.582114	6.973056
N	1.940332	10.804267	6.554092
C	1.195690	9.812102	7.055819
H	1.012199	9.057014	6.509509
C	0.679735	9.844166	8.348557
Br	2.784878	9.945627	11.529175
Br	-2.077215	11.945809	9.278334
Br	2.013471	13.552654	9.588862
Br	-0.318376	8.390544	8.990556
C	-7.547988	11.043110	10.528734
C	-6.829919	10.674375	11.660257
C	-7.408590	10.777229	12.916834
H	-6.902409	10.506899	13.674367
N	-8.651037	11.242776	13.108183
C	-9.354838	11.599621	12.026382
H	-10.235911	11.936047	12.142909
C	-8.844015	11.493089	10.748710
C	-6.971572	10.958199	9.160662
C	-6.200496	11.967707	8.609214
C	-5.707580	11.866608	7.322502
H	-5.188651	12.582114	6.973056
N	-5.932168	10.804267	6.554092
C	-6.676810	9.812102	7.055819
H	-6.860301	9.057014	6.509509
C	-7.192765	9.844166	8.348557
Br	-5.087622	9.945627	11.529175
Br	-9.949715	11.945809	9.278334
Br	-5.859029	13.552654	9.588862

Br	-8.190876	8.390544	8.990556
1 (part with halogen bonds Br···N 3.150 and 3.160 Å)			
C	0.792884	0.140967	10.528734
C	1.510953	-0.227769	11.660257
C	0.932283	-0.124915	12.916834
H	1.438464	-0.395245	13.674367
N	-0.310165	0.340633	13.108183
C	-1.013965	0.697477	12.026382
H	-1.895038	1.033903	12.142909
C	-0.503142	0.590946	10.748710
C	1.369301	0.056056	9.160662
C	2.140377	1.065563	8.609214
C	2.633293	0.964464	7.322502
H	3.152221	1.679970	6.973056
N	2.408704	-0.097876	6.554092
C	1.664062	-1.090042	7.055819
H	1.480571	-1.845130	6.509509
C	1.148107	-1.057978	8.348557
Br	3.253250	-0.956517	11.529175
Br	-1.608843	1.043666	9.278334
Br	2.481844	2.650510	9.588862
Br	0.149997	-2.511600	8.990556
C	6.416919	1.298095	2.508635
C	6.628266	0.122085	1.777892
C	7.517119	-0.840395	2.223871
H	7.643669	-1.619528	1.694677
N	8.201843	-0.726165	3.355394
C	8.033325	0.399991	4.052990
H	8.532622	0.514963	4.852740
C	7.163415	1.410199	3.667278
C	5.426027	2.315491	2.083749
C	4.114499	2.312104	2.562876
C	3.200545	3.248797	2.124430
H	2.312952	3.210836	2.462033
N	3.510694	4.203862	1.249044
C	4.758007	4.251282	0.800051
H	4.997186	4.939993	0.190717
C	5.725033	3.340275	1.181243
Br	5.722292	-0.178303	0.152929
Br	7.043879	2.963259	4.728740
Br	3.576749	1.033418	3.844615
Br	7.464425	3.525159	0.458334
C	-3.334409	-2.305320	17.575513
C	-3.123061	-3.481330	16.844769
C	-2.234208	-4.443809	17.290749
H	-2.107659	-5.222942	16.761555
N	-1.549484	-4.329580	18.422271
C	-1.718002	-3.203424	19.119868
H	-1.218705	-3.088452	19.919617
C	-2.587912	-2.193216	18.734156
C	-4.325300	-1.287924	17.150627
C	-5.636828	-1.291310	17.629753

C	-6.550782	-0.354618	17.191307
H	-7.438375	-0.392579	17.528911
N	-6.240633	0.600447	16.315922
C	-4.993320	0.647867	15.866929
H	-4.754141	1.336578	15.257594
C	-4.026294	-0.263140	16.248121
Br	-4.029035	-3.781717	15.219806
Br	-2.707448	-0.640155	19.795617
Br	-6.174578	-2.569997	18.911493
Br	-2.286902	-0.078256	15.525212
1 (part with halogen bonds Br···Br)			
C	-0.891618	6.000634	12.558242
C	-1.102966	7.176644	13.288986
C	-1.991819	8.139124	12.843006
H	-2.118368	8.918256	13.372200
N	-2.676543	8.024894	11.711484
C	-2.508025	6.898738	11.013887
H	-3.007321	6.783766	10.214138
C	-1.638115	5.888530	11.399600
C	0.099273	4.983238	12.983128
C	1.410801	4.986625	12.504002
C	2.324755	4.049932	12.942448
H	3.212349	4.087893	12.604844
N	2.014606	3.094867	13.817833
C	0.767294	3.047447	14.266826
H	0.528114	2.358736	14.876161
C	-0.199733	3.958454	13.885634
Br	-0.196992	7.477031	14.913949
Br	-1.518578	4.335470	10.338138
Br	1.948551	6.265311	11.222262
Br	-1.939125	3.773570	14.608543
C	0.792884	0.140967	10.528734
C	1.510953	-0.227769	11.660257
C	0.932283	-0.124915	12.916834
H	1.438464	-0.395245	13.674367
N	-0.310165	0.340633	13.108183
C	-1.013965	0.697477	12.026382
H	-1.895038	1.033903	12.142909
C	-0.503142	0.590946	10.748710
C	1.369301	0.056056	9.160662
C	2.140377	1.065563	8.609214
C	2.633293	0.964464	7.322502
H	3.152221	1.679970	6.973056
N	2.408704	-0.097876	6.554092
C	1.664062	-1.090042	7.055819
H	1.480571	-1.845130	6.509509
C	1.148107	-1.057978	8.348557
Br	3.253250	-0.956517	11.529175
Br	-1.608843	1.043666	9.278334
Br	2.481844	2.650510	9.588862
Br	0.149997	-2.511600	8.990556
2 (part with halogen bonds Br···O 3.146 Å)			

Br	4.263331	4.632678	3.379113
Br	6.448013	3.423558	-0.360363
Co	6.960798	9.691790	2.446789
O	6.578897	9.820050	4.505614
O	4.906823	9.781138	2.172063
N	6.960798	0.480293	2.446789
N	7.329434	9.301188	5.378922
N	6.960798	7.572292	2.446789
O	7.893777	8.211998	5.160766
C	6.960798	3.292673	2.446789
O	7.491335	9.850062	6.459522
C	6.960798	4.777485	2.446789
C	5.869112	6.895956	2.825845
H	5.096743	7.377276	3.098613
C	6.713820	1.167812	1.321559
H	6.526156	0.689230	0.522634
C	5.837728	5.508594	2.830054
C	6.722384	2.556771	1.287696
C	4.043127	10.749599	2.777594
H	4.392981	10.992313	3.660396
H	3.144618	10.370408	2.873509
H	4.001623	11.549174	2.211897
H	4.530112	9.459802	1.624668
Br	9.658266	4.632678	1.514464
Br	7.473584	3.423558	5.253940
C	8.052485	6.895956	2.067732
H	8.824854	7.377276	1.794964
C	7.207777	1.167812	3.572018
H	7.395440	0.689230	4.370943
C	8.083869	5.508594	2.063524
C	7.199213	2.556771	3.605881
O	7.342700	9.820050	0.387963
O	9.014774	9.781138	2.721514
N	6.592163	9.301188	-0.485345
O	6.027820	8.211998	-0.267189
O	6.430262	9.850062	-1.565945
C	9.878469	10.749599	2.115983
H	9.528616	10.992313	1.233181
H	10.776979	10.370408	2.020069
H	9.919974	11.549174	2.681680
H	9.391485	9.459802	3.268910
N	6.960798	11.891393	2.446789
Br	4.263331	16.043778	3.379113
Br	6.448013	14.834658	-0.360363
N	6.960798	18.983392	2.446789
C	6.960798	14.703773	2.446789
C	6.960798	16.188585	2.446789
C	5.869112	18.307056	2.825845
H	5.096743	18.788376	3.098613
C	6.713820	12.578912	1.321559
H	6.526156	12.100330	0.522634
C	5.837728	16.919694	2.830054

C	6.722384	13.967871	1.287696
Br	9.658266	16.043778	1.514464
Br	7.473584	14.834658	5.253940
C	8.052485	18.307056	2.067732
H	8.824854	18.788376	1.794964
C	7.207777	12.578912	3.572018
H	7.395440	12.100330	4.370943
C	8.083869	16.919694	2.063524
C	7.199213	13.967871	3.605881
Br	3.977537	10.338228	-6.408041
Br	6.162219	9.129108	-10.147517
Co	6.675005	15.397340	-7.340366
O	6.293104	15.525600	-5.281540
O	4.621029	15.486688	-7.615091
N	6.675005	6.185843	-7.340366
N	7.043640	15.006738	-4.408232
N	6.675005	13.277842	-7.340366
O	7.607984	13.917548	-4.626388
C	6.675005	8.998223	-7.340366
O	7.205541	15.555612	-3.327632
C	6.675005	10.483035	-7.340366
C	5.583318	12.601506	-6.961309
H	4.810950	13.082826	-6.688541
C	6.428026	6.873362	-8.465595
H	6.240363	6.394780	-9.264520
C	5.551934	11.214144	-6.957101
C	6.436590	8.262321	-8.499458
C	3.757334	16.455149	-7.009560
H	4.107187	16.697863	-6.126759
H	2.858824	16.075958	-6.913646
H	3.715830	17.254724	-7.575257
H	4.244318	15.165352	-8.162487
Br	9.372472	10.338228	-8.272690
Br	7.187790	9.129108	-4.533214
C	7.766691	12.601506	-7.719422
H	8.539060	13.082826	-7.992190
C	6.921983	6.873362	-6.215137
H	7.109647	6.394780	-5.416211
C	7.798076	11.214144	-7.723631
C	6.913419	8.262321	-6.181273
O	7.056906	15.525600	-9.399192
O	8.728980	15.486688	-7.065640
N	6.306369	15.006738	-10.272499
O	5.742026	13.917548	-10.054344
O	6.144468	15.555612	-11.353099
C	9.592676	16.455149	-7.671172
H	9.242822	16.697863	-8.553973
H	10.491186	16.075958	-7.767086
H	9.634180	17.254724	-7.105474
H	9.105691	15.165352	-6.518245
N	6.675005	17.596943	-7.340366
Br	3.977537	21.749328	-6.408041

Br	6.162219	20.540208	-10.147517
N	6.675005	24.688942	-7.340366
C	6.675005	20.409323	-7.340366
C	6.675005	21.894135	-7.340366
C	5.583318	24.012606	-6.961309
H	4.810950	24.493926	-6.688541
C	6.428026	18.284462	-8.465595
H	6.240363	17.805880	-9.264520
C	5.551934	22.625244	-6.957101
C	6.436590	19.673421	-8.499458
Br	9.372472	21.749328	-8.272690
Br	7.187790	20.540208	-4.533214
C	7.766691	24.012606	-7.719422
H	8.539060	24.493926	-7.992190
C	6.921983	18.284462	-6.215137
H	7.109647	17.805880	-5.416211
C	7.798076	22.625244	-7.723631
C	6.913419	19.673421	-6.181273
2 (part with halogen bonds Br···O 3.290 Å)			
Br	4.263331	4.632678	3.379113
Br	6.448013	3.423558	-0.360363
Co	6.960798	9.691790	2.446789
O	6.578897	9.820050	4.505614
O	4.906823	9.781138	2.172063
N	6.960798	0.480293	2.446789
N	7.329434	9.301188	5.378922
N	6.960798	7.572292	2.446789
O	7.893777	8.211998	5.160766
C	6.960798	3.292673	2.446789
O	7.491335	9.850062	6.459522
C	6.960798	4.777485	2.446789
C	5.869112	6.895956	2.825845
H	5.096743	7.377276	3.098613
C	6.713820	1.167812	1.321559
H	6.526156	0.689230	0.522634
C	5.837728	5.508594	2.830054
C	6.722384	2.556771	1.287696
C	4.043127	10.749599	2.777594
H	4.392981	10.992313	3.660396
H	3.144618	10.370408	2.873509
H	4.001623	11.549174	2.211897
H	4.530112	9.459802	1.624668
Br	9.658266	4.632678	1.514464
Br	7.473584	3.423558	5.253940
C	8.052485	6.895956	2.067732
H	8.824854	7.377276	1.794964
C	7.207777	1.167812	3.572018
H	7.395440	0.689230	4.370943
C	8.083869	5.508594	2.063524
C	7.199213	2.556771	3.605881
O	7.342700	9.820050	0.387963
O	9.014774	9.781138	2.721514

N	6.592163	9.301188	-0.485345
O	6.027820	8.211998	-0.267189
O	6.430262	9.850062	-1.565945
C	9.878469	10.749599	2.115983
H	9.528616	10.992313	1.233181
H	10.776979	10.370408	2.020069
H	9.919974	11.549174	2.681680
H	9.391485	9.459802	3.268910
N	6.960798	11.891393	2.446789
Br	4.263331	16.043778	3.379113
Br	6.448013	14.834658	-0.360363
N	6.960798	18.983392	2.446789
C	6.960798	14.703773	2.446789
C	6.960798	16.188585	2.446789
C	5.869112	18.307056	2.825845
H	5.096743	18.788376	3.098613
C	6.713820	12.578912	1.321559
H	6.526156	12.100330	0.522634
C	5.837728	16.919694	2.830054
C	6.722384	13.967871	1.287696
Br	9.658266	16.043778	1.514464
Br	7.473584	14.834658	5.253940
C	8.052485	18.307056	2.067732
H	8.824854	18.788376	1.794964
C	7.207777	12.578912	3.572018
H	7.395440	12.100330	4.370943
C	8.083869	16.919694	2.063524
C	7.199213	13.967871	3.605881
Br	14.108269	18.189522	-3.379113
Br	11.923587	19.398642	0.360363
Co	11.410802	13.130410	-2.446789
O	11.792703	13.002150	-4.505614
O	13.464777	13.041062	-2.172063
N	11.410802	22.341907	-2.446789
N	11.042166	13.521012	-5.378922
N	11.410802	15.249908	-2.446789
O	10.477823	14.610202	-5.160766
C	11.410802	19.529527	-2.446789
O	10.880265	12.972138	-6.459522
C	11.410802	18.044715	-2.446789
C	12.502488	15.926244	-2.825845
H	13.274857	15.444924	-3.098613
C	11.657780	21.654388	-1.321559
H	11.845444	22.132970	-0.522634
C	12.533872	17.313606	-2.830054
C	11.649216	20.265429	-1.287696
C	14.328473	12.072601	-2.777594
H	13.978619	11.829887	-3.660396
H	15.226982	12.451792	-2.873509
H	14.369977	11.273026	-2.211897
H	13.841488	13.362398	-1.624668
Br	8.713334	18.189522	-1.514464

Br	10.898016	19.398642	-5.253940
C	10.319115	15.926244	-2.067732
H	9.546746	15.444924	-1.794964
C	11.163823	21.654388	-3.572018
H	10.976160	22.132970	-4.370943
C	10.287731	17.313606	-2.063524
C	11.172387	20.265429	-3.605881
O	11.028900	13.002150	-0.387963
O	9.356826	13.041062	-2.721514
N	11.779437	13.521012	0.485345
O	12.343780	14.610202	0.267189
O	11.941338	12.972138	1.565945
C	8.493131	12.072601	-2.115983
H	8.842984	11.829887	-1.233181
H	7.594621	12.451792	-2.020069
H	8.451626	11.273026	-2.681680
H	8.980115	13.362398	-3.268910
N	11.410802	10.930807	-2.446789
Br	14.108269	6.778422	-3.379113
Br	11.923587	7.987542	0.360363
N	11.410802	3.838808	-2.446789
C	11.410802	8.118427	-2.446789
C	11.410802	6.633615	-2.446789
C	12.502488	4.515144	-2.825845
H	13.274857	4.033824	-3.098613
C	11.657780	10.243288	-1.321559
H	11.845444	10.721870	-0.522634
C	12.533872	5.902506	-2.830054
C	11.649216	8.854329	-1.287696
Br	8.713334	6.778422	-1.514464
Br	10.898016	7.987542	-5.253940
C	10.319115	4.515144	-2.067732
H	9.546746	4.033824	-1.794964
C	11.163823	10.243288	-3.572018
H	10.976160	10.721870	-4.370943
C	10.287731	5.902506	-2.063524
C	11.172387	8.854329	-3.605881

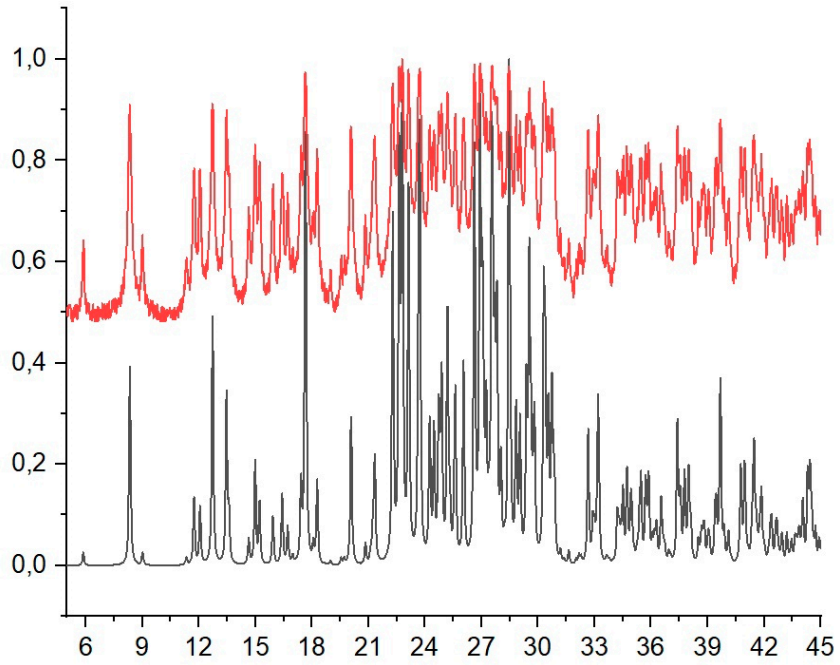

Figure S4. PXRD data for **1**

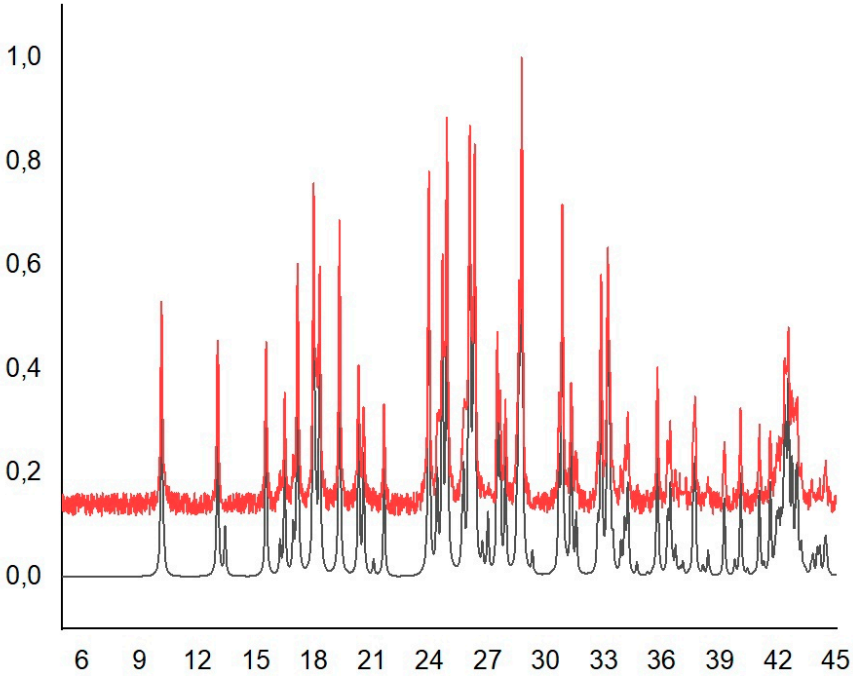

Figure S5. PXRD data for **2**