New powder diffraction data of some *N*-derivatives of 4-chloro-3, 5-dimethylphenoxyacetamide-potential pesticides

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N-derivatives of 4-chloro-3,5-dimethylphenoxyacetamide—2-(4-chloro-3,5-dimethylphenoxy)-*N*-(4-fluorophenyl)acetamide, 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-fluorophenyl) acetamide, 2-(4-chloro-3,5-dimethylphenoxy)-*N*-[4-chloro-3-(trifluoromethyl)phenyl] acetamide, 2-(4-chloro-3,5-dimethylphenoxy)-*N*-[3-chloro-4-methylphenyl]acetamide, 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(2,4,6-tribromophenyl) acetamide, 2-(4-chloro-3,5-dimethylphenoxy)-*N*-pyridin-2-ylacetamide, 1-[(4-chloro-3,5-dimethylphenoxy)acetyl]-4-methylpiperazine, and 1-benzyl-4-[(4-chloro-3,5-dimethylphenoxy)acetyl]piperazine—have been characterized by X-ray powder diffraction. These organic compounds are potential pesticides. Experimental 2θ peak positions, relative peak intensities, values of d and Miller indices, and unit-cell parameters are presented. © *2011 International Centre for Diffraction Data.* [DOI: 10.1154/1.3652921]

Key words: X-ray powder diffraction, pesticide, 4-chloro-3,5-dimethylphenoxyacetamide

I. INTRODUCTION

Derivatives of fluorophenoxyalkane acids show high biological activity. The salts, esters, amides, and other derivatives of these acids were applied widely in many areas of agriculture, with many as herbicides, fungicides, and regulators of the plant growth (Newman *et al*., 1947; Berhenke *et al*., 1951; Melnikov, 1987). The chemical properties of these herbicides result from the aromatic radical (phenyl) and the presence of derivatives of the carboxyl group (Gruzdyev *et al*., 1988).

The physiological activity of phenoxyacetic acid increases when a halogen such as fluorine or chlorine is introduced into the aromatic radical, and the position of the halogen is very important. For example, in the chlorophenoxyacetic acid series, 4-chlorophenoxyacetic acid has the highest physiological activity.

In the Department of Organic Chemistry at Maria Curie Sklodowska University (Lublin, Poland), investigations have been carried out for many years in order to search for new organic compounds of potential biological activity (Tarasiuk *et al*., 2000; Tarasiuk, 2007). Lately, it has concentrated on research related to the synthesis of *N*-fluorophenyl-pyridine-2-yl-amides and derivatives of 4-chloro-3,5-dimethylphenoxyacetic acid. Other groups of potential herbicides have been described (Olszewska *et al*., 2008; Olszewska *et al*., 2009).

The derivatives of 4-chloro-3,5-dimethylphenoxyacetamides have interesting pesticide activity. Highest pesticide activity will establish the derivatives of 2-(4-chloro-3,5-dimethylphenoxy)-*N*-[4-chloro-3-(trifluoromethyl)phenyl]acetamide and 1-benzyl-4-[(4-chloro-3,5-dimethylphenoxy) acetyl]piperazin.

II. SYNTHESIS

A. Materials

4-fluoroaniline (bp = 187 °C/767 mm Hg), 3-chloro-4-fluoroaniline (mp = 41–44 °C), 4-chloro-3-(trifluoromethyl) aniline (mp = 35–37 °C), 3-chloro-4-methylaniline (bp = 237–238 °C), 2,4,6-tribromoaniline (mp = 120–122 °C), 2-aminopyridine (mp = 58–60 °C), 4-methylpiperazine (bp = 138 °C), 1-benzylpiperazine (refractive index n20/D = 1.547), 4-chloro-3,5-dimethylphenol (mp = 114–116 °C), methyl bromoacetate (bp = 51–52 °C/15 mm Hg), thionyl chloride (bp = 79 °C), dimethyl sulfoxide (DMSO; bp = 189 °C), and phosphorus oxychloride (bp = 105 °C) were used. All reagents were supplied by Aldrich Chemical Company.

B. Synthesis of 4-chloro-3,5-dimethylphenoxyacetic acid

A mixture of the 4-chloro-3,5-dimethylphenol, methyl bromoacetate, potassium carbonate, and potassium iodide in dimethyl sulfoxide at solvent was stirred at 80 °C for 6 h.

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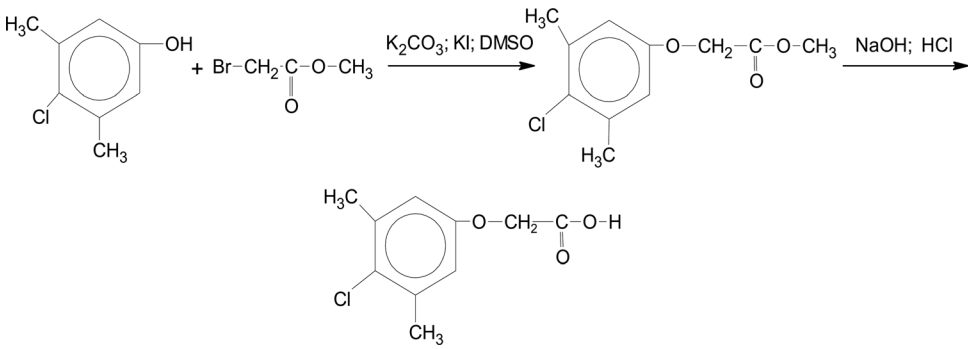

Figure 1. Scheme of producing the 4-chloro-3,5-dimethylphenoxyacetic acid.

The DMSO was removed by evaporation in vacuum, and the solid was water added to the residue. The resulting solid was filtered and washed with 1N NaOH and water. The appropriate methyl 4-chloro-3,5-dimethylphenoxyacetate were hydrolysed for 2 h in a water ethanol solution of sodium hydroxide at 80 °C. Free acid were separated from the reaction mixture by adding a 10% water solution of hydrochloric acid. The product was purified by crystallisation from ethanol–water. Yield of acid was 89%; mp 150–151.5 °C; mp150–151 °C acc (Baker, 1972).

The course of reaction that produced the 4-chloro-3,5-dimethylphenoxyacetic acid is presented in a general scheme in Figure 1. The chloride of 4-chloro-3,5-dimethylphenoxyacetic acid was received in the reaction of the acids with an excess of thionyl chloride. *N*-Derivatives-2-(4-chloro-3,5-dimethylphenoxy)acetamides were synthesised in reaction of acid chloride with an excess of 2-aminopyridine or derivatives of piperazine in benzene, or 4-chloro-3,5-dimethylphenoxyacetic acid with fluoroanilines and phosphorus oxychloride in toluene.

C. Synthesis of the *N*-fluorophenyl-4-chloro-3,5-dimethylphenoxyacetamides—procedure I

In a round bottom three-necked flask of 250 cm^3, equipped with a 0.025 mol of fluoroaniline, 100 cm^3 of dry toluene, 0.02 mol of a 4-chloro-3,5-dimethylphenoxyacetic acid, and 2.3 g (0.015 mol) phosphorus oxychloride were placed. The mixture was heated at 110 °C for 5 h. The solution was then concentrated under diminished pressure while heating on the boiling water bath. After cooling to 5 °C, it was mixed with water. The crystals were carefully filtered. The raw compound was purified by crystallization from ethanol or benzene. The course of reaction, procedure I that produced the derivatives in question, is presented in a general scheme in Figure 2. This procedure was used to obtain samples 1–5.

D. Synthesis of the *N*-derivatives of 4-chloro-3,5-dimethylphenoxyacetamides—procedure II

In a round bottom three-necked flask of 250 cm^3, equipped with a mechanical stirrer, a thermometer, (0.025 mol) of 2-aminopyridine or derivatives of piperazine, 50 cm^3 of dry benzene, and 6.0 g (0.06 mol) pyridine were placed. While stirring the contents of the flask, a solution of 0.02 mol of 4-chloro-3,5-dimethylphenoxyacetic chloride was being added to 100 cm^3 of dry benzene for 30 min, keeping in that period of time the temperature between 8 and 15 °C. While carrying out the reaction, colorless fine-crystal sediments of pyridine hydrochloride started to set out. After the whole amount of acid chloride was introduced into the reaction mixture, the whole of it was still stirred for 3 h at 30–35 °C. The sediments of pyridine hydrochloride were filtered and washed with dry warm benzene. Then, the solution was concentrated under diminished pressure while heating on the boiling water bath. After it was cooled down to 5 °C, the crystals were carefully filtered. The raw compound was purified by crystallization from toluene. Procedure II is presented in general scheme in Figure 3. This process was used to obtain samples 6–8.

The structure of investigated compounds is presented in a general scheme in Figure 4. The chemical structures of the synthesized samples were confirmed by elemental analysis, FTIR, and ^{1}H-NMR. Characteristics of investigated samples are presented in Table I.

III. EXPERIMENTAL

Powder diffraction data were collected at room temperature in the 2θ range from 3 to 90° on a modified DRON-3.0 SEIFERT automated diffractometer by step scanning with a step equal 0.02° and a count time 6 s/step. Other experimental conditions were as follows: Cu target X-ray tube operated at 45 kV and 30 mA, 6° take-off angle, 1° divergence slit, 0.15 mm receiving slit, and scintillation counter with pulse

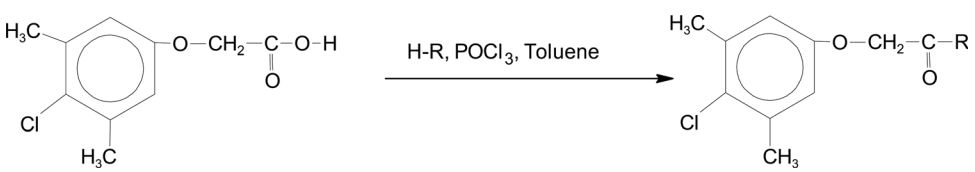

Figure 2. Scheme of synthesis of derivatives of 4-chloro-3,5-dimethylphenoxyacetic acid (procedure I).

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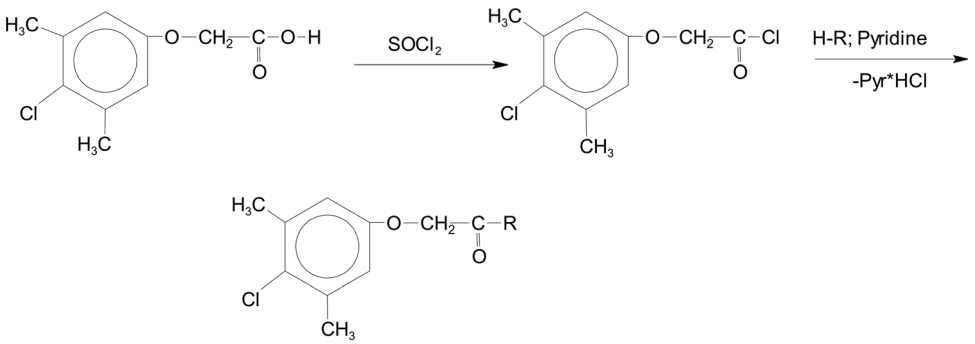
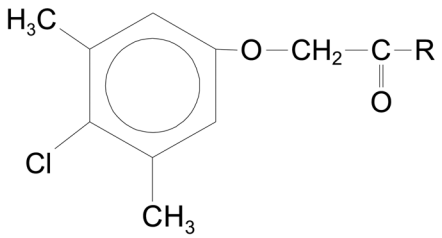


Figure 3. Scheme of synthesis of derivatives of 4-chloro-3,5-imethyl-phenoxyacetic acid (procedure II).



where

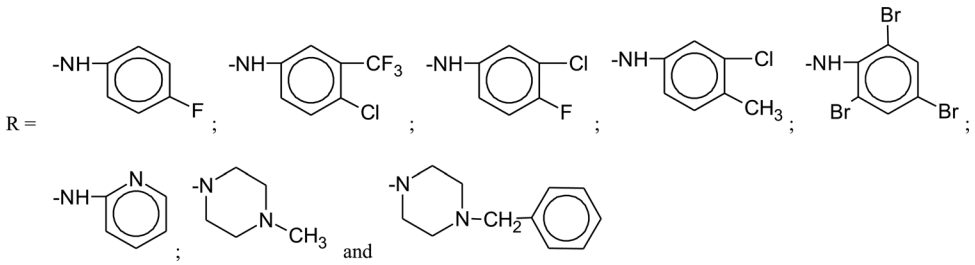
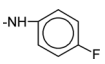
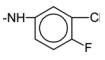
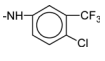
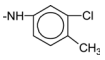
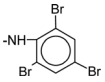
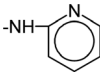
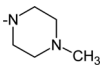
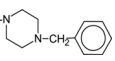


Figure 4. Structural formulas for *N*-derivatives of 4-chloro-3,5-dimethyl-phenoxyacetic acid.

TABLE I. Chemical names, formulas, molecular masses, melting points, and solubility of derivatives for 4-chloro-3,5-dimethylphenoxyacetic acid.

Nr Sample	Name of sample	Substituent R	Procedure	Formula	Molecular mass	Melting point (°C)	Solubility (g/100 cm^3) Acetone	Ethanol	Water
1	2-(4-chloro-3,5-dimethylphenoxy)-*N*-(4-fluorophenyl)acetamide		I	$C_{16}H_{15}ClFNO_2$	307.75	151–152.5	18	7.5	–
2	2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-fluorophenyl)acetamide		I	$C_{16}H_{14}Cl_2FNO_2$	342.19	186–187	11	6.0	–
3	2-(4-chloro-3,5-dimethylphenoxy)-*N*-[4-chloro-3-(trifluoromethyl)phenyl]-acetamide		I	$C_{17}H_{14}Cl_2F_3NO_2$	392.20	169–170.5	25	9.0	–
4	2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-methylophenyl)acetamide		I	$C_{17}H_{17}Cl_2NO_2$	338.23	203.5–204.5	15	6.0	–
5	2-(4-chloro-3,5-dimethylphenoxy)-*N*-(2,4,6-tribromophenyl)acetamide		I	$C_{16}H_{13}Br_3ClNO_2$	526.45	215–216	10	5.5	–
6	2-(4-chloro-3,5-dimethylphenoxy)-*N*-pyridin-2-ylacetamide		II	$C_{15}H_{15}ClN_2O_2$	290.75	98–99	26	10.5	0.05
7	1-[(4-chloro-3,5-dimethylphenoxy)-acetyl]-4-methylpiperazine		II	$C_{15}H_{21}ClN_2O_2$	296.79	87–88	7	2.5	0.2
8	1-benzyl-4-[(4-chloro-3,5-dimethyl-phenoxy)acetyl]piperazine		II	$C_{21}H_{25}ClN_2O_2$	372.89	129–130	6.5	2.0	0.05

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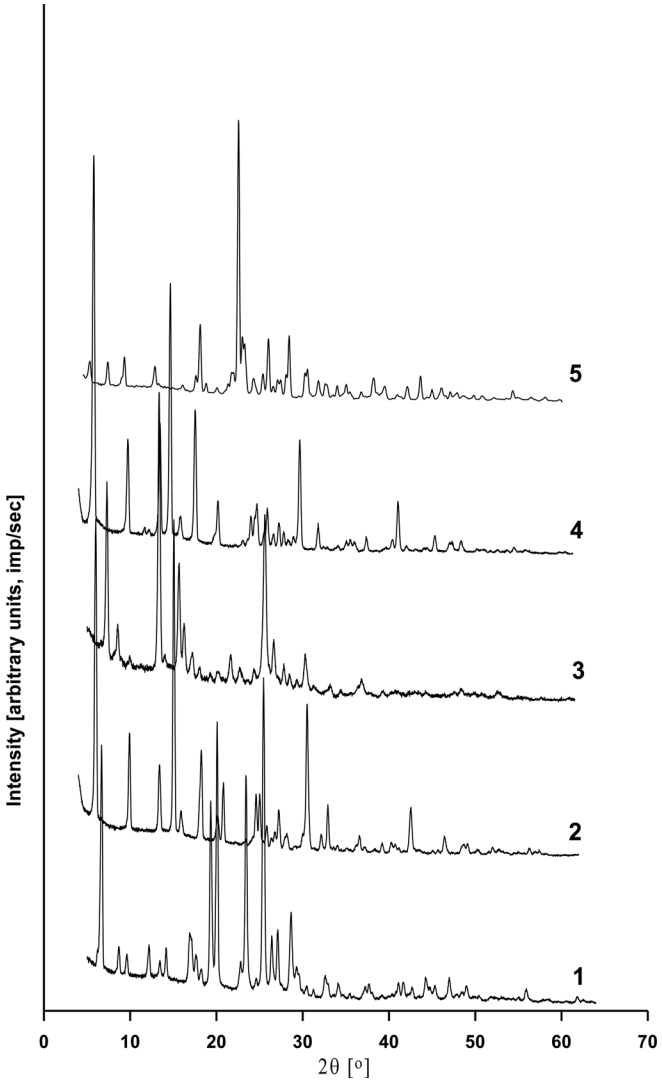

Figure 5. X-ray powder diffraction patterns for samples: (1) 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(4-fluorophenyl)acetamide; (2) 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-fluorophenyl)acetamide; (3) 2-(4-chloro-3,5-dimethylphenoxy)-*N*-[4-chloro-3-(trifluoromethyl)phenyl]-acetamide; (4) 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-methylophenyl)acetamide; (5) 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(2,4,6-tribromophenyl)acetamide.

height analyzer. The diffractometer was calibrated by using a SRM 1976 standard. Throughout the XRD measurements, the ambient temperature was maintained at 20 ± 1 °C. The XRAYAN program (Marciniak and Diduszko, 1994) was used for determining peak intensities and positions. The second derivative method used to determine peak observed positions, $2\theta_{obs}$.

IV. RESULTS AND DISCUSSION

Figure 5 shows the experimental X-ray diffraction patterns for derivatives of chloro-3,5-dimethylphenoxyacetamide (samples 1–5). Figure 6 shows the patterns for the sample 2-(4-chloro-3,5-dimethylphenoxy)-*N*-pyridin-2-ylacetamide (sample 6), 1-[(4-chloro-3,5-dimethylphenoxy)-acetyl]-4-methylpiperazine (sample 7), and 1-benzyl-4-[(4-chloro-3,5-dimethyl-phenoxy)acetyl]piperazine (sample 8). In each diffraction pattern, all observed 2θ peak positions

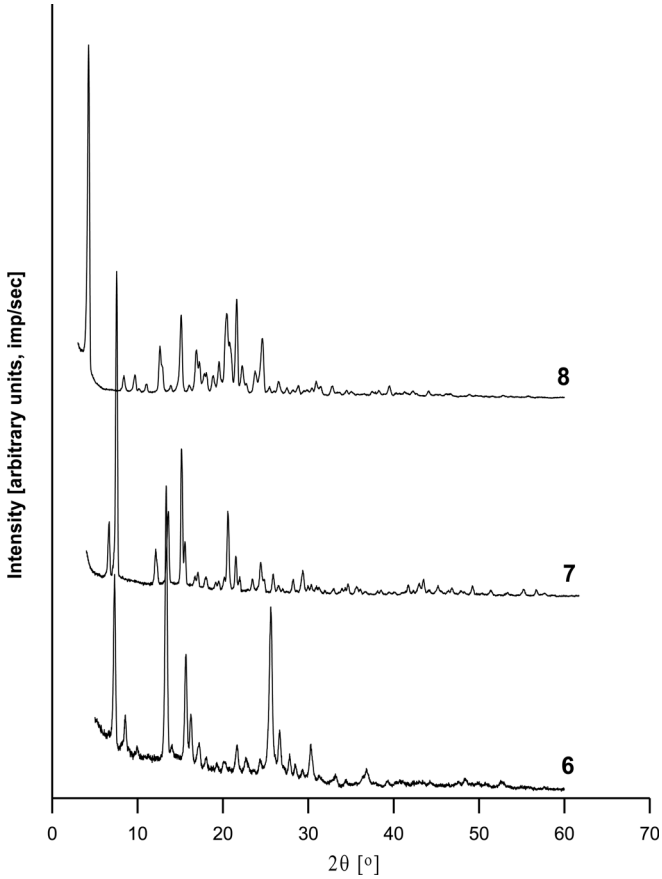

Figure 6. X-ray powder diffraction patterns for samples: (6) 2-(4-chloro-3,5-dimethylphenoxy)-*N*-pyridin-2-ylacetamide; (7) 1-[(4-chloro-3,5-dimethylphenoxy)-acetyl]-4-methylpiperazine; (8) 1-benzyl-4-[(4-chloro-3,5-dimethyl-phenoxy)acetyl]piperazine.

were used in the calculation. Pattern indexing was carried out using the personal computer version of the TREOR program (Werner *et al.*, 1985). The observed and calculated powder diffraction data for the eight compounds are given in Tables II–IX. Unit-cell data, values of M_{30} (de Wolff, 1968), and F_{30} (Smith and Snyder, 1979) are presented in the Table X.

Powder patterns for four of the eight samples can be found in Powder Diffraction File: 1-[(4-chloro-3,5-dimethylphenoxy)-acetyl]-4-methylpiperazine (PDF 00-60-1123), 2-(4-chloro-3,5-dimethylphenoxy)-*N*-pyridin-2-ylacetamide (PDF 00-60-1124), 1-benzyl-4-[(4-chloro-3,5-dimethyl-phenoxy)acetyl]piperazine (PDF 00-60-1125), and 2-(4-chloro-3,5-dimethylphenoxy)-*N*-[4-chloro-3-(trifluoromethyl)phenyl]-acetamide (PDF 00-60-1135) (ICDD, 2010).

As shown in Figures 5 and 6, all the samples of new pesticides are well crystallized. Seven out of the eight compounds crystallize in triclinic system, and only sample 4 ($C_{17}H_{17}Cl_2NO_2$) crystallizes in monoclinic system. For the samples 1–3 where we have different substituents (F, Cl, CF_3, and Br), unit-cell volumes are similar. A little smaller volume for the sample 4 (Cl and CH_3 as substituents) was obtained. The changes in type of substituent cause considerable structural changes revealing differences in intensity and position of diffraction peaks (see diffraction patterns in Figure 5) as well as in different unit cell parameters. This fact

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TABLE II. Powder diffraction data for 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(4-fluorophenyl)acetamide $C_{16}H_{15}ClFNO_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
6.683	13.2164	74	0	0	1	6.703	13.1829	−0.020
8.681	10.1778	10	0	1	0	8.647	10.2230	0.034
9.600	9.2055	7	0	−1	1	9.635	9.1768	−0.035
12.180	7.2606	10	0	1	1	12.122	7.2991	0.058
13.419	6.5928	5	0	0	2	13.430	6.5910	−0.011
14.152	6.2530	10	0	−1	2	14.192	6.2388	−0.040
16.854	5.2562	8	−2	−1	2	16.855	5.2586	−0.001
17.126	5.1735	5	0	−2	1	17.081	5.1895	0.045
17.631	5.0263	8	0	1	2	17.618	5.0325	0.013
18.223	4.8644	5	−1	2	0	18.215	4.8689	0.008
19.314	4.5919	55	0	−2	2	19.339	4.5884	−0.025
20.062	4.4224	91	0	−1	3	20.049	4.4275	0.013
22.774	3.9016	6	−2	1	4	22.787	3.9013	−0.013
23.403	3.7981	71	0	−2	3	23.424	3.7966	−0.021
24.568	3.6206	3	−3	1	4	24.559	3.6237	0.009
25.433	3.4994	100	0	−3	1	25.424	3.5023	0.009
26.383	3.3755	16	0	−1	4	26.409	3.3739	−0.026
27.069	3.2914	20	1	−1	3	27.070	3.2930	−0.001
28.616	3.1170	20	0	−2	4	28.607	3.1194	0.008
29.265	3.0493	4	−1	3	2	29.282	3.0490	−0.017
30.449	2.9333	3	−1	−3	4	30.421	2.9374	0.028
31.229	2.8618	3	−4	−1	3	31.188	2.8669	0.041
32.538	2.7497	5	−3	2	5	32.545	2.7504	−0.008
32.950	2.7162	3	−1	3	3	32.969	2.7160	−0.019
34.077	2.6289	4	−4	−2	4	34.090	2.6292	−0.012
35.414	2.5326	2	−4	−2	3	35.414	2.5339	0.000
37.235	2.4129	2	−4	−1	1	37.223	2.4148	0.011
37.643	2.3877	4	−2	−4	3	37.653	2.3882	−0.011
41.066	2.1962	5	1	−2	5	41.071	2.1970	−0.006
41.614	2.1685	5	−4	−2	1	41.617	2.1694	−0.003
42.664	2.1176	3	−2	−4	6	42.645	2.1195	0.018
44.223	2.0464	5	4	−2	1	44.221	2.0475	0.003
44.728	2.0245	2	−2	2	7	44.774	2.0235	−0.046
45.311	1.9998	3	−6	−1	5	45.330	2.0000	−0.019
46.957	1.9335	7	4	−3	1	46.953	1.9345	0.003
48.329	1.8817	1	−1	−2	8	48.324	1.8828	0.006
48.925	1.8602	4	−6	−2	8	48.918	1.8613	0.007
55.825	1.64551	4	2	−2	6	55.819	1.6464	0.006
61.777	1.50048	2	−4	−6	6	61.747	1.5018	0.029

TABLE III. Powder diffraction data for 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-fluorophenyl)acetamide $C_{16}H_{14}Cl_2FNO_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
5.994	14.7331	91	0	0	1	6.000	14.7258	−0.006
9.909	8.9193	31	0	1	0	9.933	8.9022	−0.024
13.381	6.6116	19	1	−1	1	13.421	6.5954	−0.040
15.045	5.8838	100	0	1	1	15.078	5.8741	−0.033
15.859	5.5836	6	1	0	1	15.851	5.5893	0.008
18.236	4.8611	24	1	1	0	18.257	4.8578	−0.021
20.123	4.4091	6	1	−1	3	20.131	4.4096	−0.008
20.779	4.2715	19	0	1	2	20.743	4.2809	0.035
23.413	3.7964	2	0	−1	5	23.385	3.8029	0.028
24.564	3.6211	14	−1	−3	3	24.576	3.6212	−0.012
24.990	3.5604	15	0	2	1	24.954	3.5672	0.036
25.817	3.4482	6	1	0	3	25.806	3.4513	0.011

TABLE III. (*Continued*.)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
26.312	3.3844	2	0	−4	4	26.377	3.3779	−0.065
26.741	3.3311	3	1	2	0	26.754	3.3311	−0.013
27.201	3.2758	11	−2	0	4	27.199	3.2776	0.002
27.862	3.1995	1	−1	0	5	27.855	3.2019	0.007
28.142	3.1683	2	1	1	2	28.122	3.1721	0.020
30.474	2.9310	40	−2	−3	5	30.455	2.9342	0.019
32.128	2.7838	5	0	−5	6	32.128	2.7851	0.000
32.886	2.7213	14	−2	−2	1	32.970	2.7159	−0.084
33.568	2.6676	1	0	−5	8	33.585	2.6676	−0.017
34.019	2.6332	2	−1	−4	9	34.018	2.6346	0.001
36.565	2.4555	4	−2	−4	5	36.542	2.4582	0.023
39.169	2.2981	3	0	−5	10	39.154	2.3000	0.014
40.209	2.2410	2	−2	−5	8	40.163	2.2445	0.046
40.716	2.2142	2	−3	3	0	40.683	2.2170	0.034
41.172	2.1908	1	−3	−3	5	41.110	2.1950	0.061
42.498	2.1254	12	3	1	0	42.498	2.1265	0.000
42.978	2.1028	1	0	0	7	42.981	2.1037	−0.003
46.386	1.9559	4	0	−5	1	46.401	1.9563	−0.015
48.669	1.8694	1	−1	5	0	48.669	1.8703	−0.001
49.059	1.8554	3	−3	2	5	49.037	1.8571	0.023
51.949	1.75879	2	−1	−5	1	51.960	1.7593	−0.011
56.253	1.63400	2	0	0	9	56.201	1.6362	0.052
57.410	1.60378	1	−1	2	7	57.409	1.6046	0.001

TABLE IV. Powder diffraction data for 2-(4-chloro-3,5-dimethylphenoxy)-*N*-[4-chloro-3-(trifluoromethyl)phenyl]acetamide $C_{17}H_{14}Cl_2F_3NO_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
5.486	16.0950	17	0	0	1	5.484	16.1102	0.002
7.682	11.4990	8	0	1	0	7.705	11.4706	−0.023
12.941	6.8357	12	1	0	0	12.979	6.8190	−0.024
13.995	6.3230	9	1	1	0	14.050	6.3015	−0.055
15.472	5.7223	10	−1	−2	1	15.474	5.7247	−0.002
16.625	5.3281	100	0	1	2	16.584	5.3439	0.041
17.753	4.9921	2	−1	0	3	17.733	5.0002	0.020
18.305	4.8427	5	−1	−3	3	18.305	4.8452	0.000
18.900	4.6915	4	0	−1	4	18.867	4.7021	0.033
19.399	4.5720	1	0	−3	2	19.398	4.5746	0.001
23.120	3.8439	0.9	−2	−1	2	23.119	3.8460	0.001
23.761	3.7416	3	−1	−4	4	23.773	3.7417	−0.012
24.197	3.6752	2	0	−1	5	24.187	3.6786	0.010
25.058	3.5508	21	−2	−3	3	25.048	3.5540	0.010
26.072	3.4150	7	2	1	0	26.090	3.4144	−0.018
27.957	3.1889	0.9	−2	−1	5	27.943	3.1920	0.014
29.235	3.0524	2	−2	1	2	29.246	3.0527	−0.012
29.666	3.0090	1	−1	−4	7	29.666	3.0104	0.000
30.007	2.9755	2	1	−3	4	30.008	2.9769	−0.001
30.901	2.8915	1	0	3	2	30.946	2.8888	−0.046
31.370	2.8493	2	2	0	2	31.363	2.8513	0.007
32.406	2.7605	3	0	−3	7	32.407	2.7618	−0.001
33.310	2.6877	1	0	0	6	33.359	2.6851	−0.050
33.991	2.6354	2	−2	1	4	34.007	2.6354	−0.017
34.756	2.5791	0.6	−2	2	2	34.728	2.5823	0.027
35.243	2.5445	0.8	0	−1	7	35.251	2.5452	−0.008
38.312	2.3475	0.5	−1	4	1	38.310	2.3487	0.001
39.562	2.2761	2	−3	−4	8	39.590	2.2757	−0.028
40.378	2.2320	1	3	2	0	40.366	2.2337	0.012
40.979	2.2006	8	0	−1	8	40.964	2.2025	0.016

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TABLE IV. (*Continued*.)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
41.446	2.1769	2	−1	−6	9	41.455	2.1775	−0.009
45.097	2.0088	0.5	1	−5	7	45.092	2.0100	0.005
45.511	1.9915	0.8	2	3	3	45.517	1.9922	−0.007
46.906	1.9354	2	0	−4	10	46.909	1.9363	−0.002
49.627	1.8355	0.9	−1	−1	10	49.624	1.8365	0.003
50.611	1.80210	0.5	−3	−6	2	50.606	1.8031	0.005
51.554	1.77134	0.8	−1	6	0	51.575	1.7715	−0.020
52.291	1.74809	0.4	−4	−4	2	52.312	1.7483	−0.021
57.411	1.60375	0.5	−2	2	8	57.415	1.6044	−0.005
59.907	1.54277	0.6	3	−4	5	59.877	1.5442	0.029

TABLE V. Powder diffraction data for 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(3-chloro-4-methylphenyl)acetamide $C_{17}H_{17}Cl_2NO_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
5.777	15.2860	100	1	0	0	5.827	15.1626	−0.050
9.728	9.0843	26	−2	0	1	9.735	9.0828	−0.007
11.656	7.5858	2	2	0	0	11.669	7.5814	−0.013
12.203	7.2473	1	1	0	1	12.206	7.2490	−0.003
13.432	6.5866	30	−2	0	2	13.394	6.6086	0.038
14.636	6.0474	71	−3	0	1	14.610	6.0612	0.026
15.807	5.6020	5	0	0	2	15.876	5.5806	−0.069
17.517	5.0588	34	3	0	0	17.542	5.0542	−0.025
20.157	4.4018	11	−3	0	3	20.149	4.4057	0.008
23.034	3.8581	1	3	0	1	23.037	3.8595	−0.003
23.962	3.7107	8	0	0	3	23.910	3.7205	0.052
24.677	3.6048	8	0	2	1	24.644	3.6114	0.033
25.872	3.4409	10	3	1	1	25.860	3.4442	0.012
26.590	3.3496	3	0	1	3	26.646	3.3444	−0.056
27.222	3.2733	7	2	1	2	27.228	3.2742	−0.006
27.773	3.2096	5	1	0	3	27.711	3.2182	0.062
28.248	3.1567	1	−3	2	2	28.210	3.1624	0.038
28.904	3.0866	2	−3	1	4	28.911	3.0873	−0.007
29.629	3.0126	29	−2	1	4	29.588	3.0182	0.041
31.764	2.8149	6	−6	1	2	31.758	2.8167	0.005
34.085	2.6283	1	2	2	2	34.103	2.6282	−0.018
35.042	2.5587	2	−5	2	1	34.990	2.5636	0.053
35.488	2.5275	2	−3	2	4	35.491	2.5286	−0.003
35.954	2.4959	1	−5	1	5	35.943	2.4978	0.010
37.356	2.4053	3	−5	2	4	37.368	2.4057	−0.012
40.370	2.2324	3	0	0	5	40.394	2.2322	−0.024
41.017	2.1987	14	−6	0	6	40.958	2.2028	0.059
42.038	2.1476	1	−4	3	3	42.025	2.1493	0.013
45.288	2.0007	4	−7	2	5	45.295	2.0014	−0.006
46.969	1.9330	1	−4	2	6	46.988	1.9332	−0.019
47.319	1.9195	2	−9	1	5	47.290	1.9215	0.029
48.308	1.8825	3	−9	1	2	48.305	1.8835	0.003
54.442	1.68400	2	9	0	0	54.447	1.6846	−0.005

TABLE VI. Powder diffraction data for 2-(4-chloro-3,5-dimethylphenoxy)-*N*-(2,4,6-tribromophenyl)acetamide $C_{16}H_{13}Br_3ClNO_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
5.320	16.5993	6	0	0	1	5.323	16.5971	−0.003
7.394	11.9460	8	0	1	0	7.411	11.9250	−0.017
9.325	9.4765	10	0	1	1	9.314	9.4368	0.011

TABLE VI. (*Continued*.)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
12.855	6.8808	6	1	0	3	12.919	6.8505	−0.064
13.991	6.3248	0.9	1	1	0	13.971	6.3370	0.020
16.064	5.5128	2	0	0	3	16.051	5.4960	0.013
17.584	5.0396	4	−1	−1	1	17.586	5.0416	−0.002
18.097	4.8980	23	0	1	3	18.108	4.8974	−0.011
18.788	4.7192	3	1	−1	4	18.799	4.7190	−0.011
21.310	4.1662	2	2	1	4	21.307	4.1688	0.003
21.692	4.0937	3	1	2	4	21.707	4.0929	−0.015
21.968	4.0428	3	−1	−1	2	21.972	4.0441	−0.004
22.543	3.9410	100	0	2	3	22.548	3.9421	−0.005
22.957	3.8709	11	1	3	1	22.971	3.8705	−0.014
23.260	3.8211	8	2	1	1	23.274	3.8208	−0.014
24.254	3.6667	4	−1	2	1	24.292	3.6629	−0.038
25.361	3.5092	7	0	3	2	25.360	3.5111	0.001
26.003	3.4239	18	2	0	6	26.005	3.4254	−0.002
26.552	3.3544	3	1	−3	1	26.540	3.3575	0.012
27.041	3.2948	4	0	0	5	27.031	3.2976	0.010
27.432	3.2487	4	1	−1	6	27.464	3.2466	−0.032
28.016	3.1823	5	2	3	2	28.083	3.1764	−0.067
28.399	3.1403	22	2	3	4	28.388	3.1430	0.011
29.493	3.0262	0.7	2	3	1	29.492	3.0278	0.001
30.200	2.9570	6	1	4	2	30.186	2.9599	0.014
30.526	2.9261	7	1	−2	6	30.574	2.9231	−0.048
31.791	2.8125	5	2	3	0	31.806	2.8126	−0.015
32.555	2.7482	3	0	0	6	32.575	2.7479	−0.020
32.828	2.7260	2	−1	−3	3	32.909	2.7208	−0.081
33.487	2.6738	0.8	1	4	4	33.504	2.6738	−0.017
33.970	2.6369	4	2	4	4	34.031	2.6336	−0.061
35.024	2.5599	4	1	−2	7	35.034	2.5604	−0.010
35.452	2.5300	2	2	−3	1	35.457	2.5309	−0.005
36.735	2.4446	2	1	0	8	36.740	2.4455	−0.005
38.185	2.3550	6	3	−2	3	38.180	2.3564	0.005
39.511	2.2789	3	3	4	4	39.534	2.2787	−0.023
40.927	2.2033	1	1	−5	2	40.917	2.2049	0.010
42.096	2.1448	4	4	0	7	42.091	2.1461	0.005
43.628	2.0730	9	0	−4	6	43.629	2.0740	−0.001
44.368	2.0401	0.7	4	3	5	44.367	2.0411	0.001
44.955	2.0148	4	−2	−5	1	44.932	2.0167	0.023
46.047	1.9695	3	2	−3	9	46.034	1.9710	0.013
46.526	1.9504	0.9	2	5	7	46.527	1.9512	−0.001
47.091	1.9283	3	4	1	2	47.085	1.9295	0.006
47.885	1.8981	2	4	4	7	47.886	1.8990	−0.001
49.797	1.8296	2	−2	4	2	49.770	1.8314	0.027
50.703	1.79906	1	4	4	9	50.726	1.7992	−0.023
54.301	1.68805	4	2	7	3	54.297	1.6889	0.004
56.499	1.62746	0.8	2	−5	9	56.509	1.6280	−0.010
58.069	1.58715	1	1	5	9	58.078	1.5876	−0.009

TABLE VII. Powder diffraction data for 2-(4-chloro-3,5-dimethylphenoxy)-*N*-pyridin-2-ylacetamide $C_{15}H_{15}ClN_2O_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
6.603	13.3762	3	0	0	1	6.618	13.3520	−0.015
7.294	12.1104	65	0	1	0	7.240	12.2063	0.054
8.544	10.3403	13	1	0	0	8.508	10.3897	0.036
9.258	9.5448	1	0	1	1	9.250	9.5579	0.008

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TABLE VII. (*Continued.*)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
9.922	8.9079	4	1	1	1	9.928	8.9066	−0.006
11.901	7.4302	2	1	0	1	11.868	7.4547	0.033
13.339	6.6324	100	0	0	2	13.354	6.6283	−0.015
13.993	6.3239	3	−1	−1	2	14.043	6.3046	−0.050
15.636	5.6629	38	1	1	2	15.643	5.6632	−0.007
16.230	5.4570	17	2	3	0	16.307	5.4341	−0.077
17.224	5.1442	6	1	3	0	17.230	5.1450	−0.006
18.013	4.9206	5	2	3	1	17.984	4.9309	0.029
18.591	4.7688	1	0	2	2	18.575	4.7754	0.016
18.827	4.7095	1	−1	−3	1	18.784	4.7227	0.043
19.238	4.6100	3	3	2	0	19.258	4.6075	−0.020
20.043	4.4265	3	0	0	3	20.089	4.4187	−0.046
20.288	4.3736	2	−1	−1	3	20.265	4.3808	0.023
20.694	4.2888	1	2	1	2	20.728	4.2839	−0.034
21.630	4.1052	9	2	4	0	21.675	4.0989	−0.045
22.637	3.9249	3	−1	1	3	22.627	3.9285	0.010
23.475	3.7866	1	0	2	3	23.432	3.7953	0.043
23.699	3.7513	1	−2	0	3	23.698	3.7533	0.001
24.287	3.6618	4	0	3	2	24.292	3.6629	−0.005
25.588	3.4785	49	2	4	2	25.586	3.4805	0.002
26.608	3.3474	14	−3	0	2	26.635	3.3458	−0.027
27.093	3.2886	1	3	4	2	27.125	3.2864	−0.032
27.774	3.2095	7	−4	−4	2	27.813	3.2067	−0.039
28.454	3.1343	4	−1	3	0	28.463	3.1349	−0.009
29.288	3.0469	3	0	4	0	29.257	3.0516	0.031
30.250	2.9522	9	4	5	1	30.242	2.9544	0.008
31.238	2.8610	2	−3	−3	4	31.187	2.8670	0.051
32.277	2.7713	1	4	1	1	32.248	2.7751	0.029
33.147	2.7005	2	−1	0	5	33.135	2.7028	0.012
34.309	2.6117	2	−4	−2	4	34.343	2.6104	−0.034
35.591	2.5204	2	4	1	2	35.590	2.5218	0.001
36.359	2.4690	2	−5	−5	3	36.355	2.4704	0.004
36.770	2.4423	3	5	6	1	36.773	2.4433	−0.003
37.885	2.3729	1	−4	−6	3	37.866	2.3752	0.019
39.347	2.2881	2	1	−1	5	39.356	2.2887	−0.009
40.127	2.2454	1	−1	−6	1	40.153	2.2451	−0.026
40.659	2.2172	2	−5	−7	2	40.650	2.2188	0.009
41.026	2.1982	1	−2	0	6	41.049	2.1981	−0.023
41.547	2.1718	1	−2	3	4	41.572	2.1717	−0.025
42.054	2.1468	1	5	3	3	42.066	2.1473	−0.012
42.221	2.1388	1	2	7	1	42.235	2.1391	−0.014
42.376	2.1313	0.9	1	2	6	42.398	2.1312	−0.022
43.005	2.1016	2	−4	−7	3	43.003	2.1026	0.002
43.411	2.0828	3	−1	−4	5	43.424	2.0832	−0.013
43.645	2.0722	2	−1	5	2	43.674	2.0719	−0.029
44.239	2.0457	2	0	6	1	44.235	2.0469	0.004
44.985	2.0135	2	−6	−7	3	44.985	2.0135	0.000
46.181	1.9641	1	4	4	5	46.176	1.9653	0.005
46.432	1.9541	1	4	3	5	46.447	1.9544	−0.015
47.533	1.9114	2	1	−5	2	47.539	1.9121	−0.006
48.432	1.8780	1	−5	1	1	48.458	1.8779	−0.026
49.182	1.8511	2	2	7	4	49.164	1.8526	0.018
49.804	1.8294	1	0	6	4	49.771	1.8314	0.033
50.005	1.82253	2	−1	−6	4	50.009	1.8232	−0.004
51.062	1.78725	0.9	−5	−1	6	51.046	1.7886	0.016
51.597	1.76996	1	0	−6	3	51.585	1.7712	0.012
52.505	1.74146	2	5	0	3	52.503	1.7424	0.002
53.281	1.71793	1	2	7	5	53.269	1.7191	0.012
54.161	1.69205	2	5	−1	2	54.177	1.6924	−0.016

TABLE VII. (*Continued.*)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I/I_o (0.1–100)	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
54.454	1.68366	2	−3	4	4	54.443	1.6848	0.011
54.838	1.67277	2	4	−2	3	54.845	1.6734	−0.007
55.333	1.65898	1	−3	−2	8	55.390	1.6582	−0.057
55.995	1.64092	1	−2	1	8	55.996	1.6417	−0.001
56.470	1.62825	2	−3	−3	8	56.463	1.6292	0.007
57.623	1.59836	1	1	3	8	57.621	1.5992	0.002
59.973	1.54123	1	−5	−4	8	59.974	1.5419	−0.001
61.001	1.51769	0.8	3	−5	1	60.999	1.5184	0.002

TABLE VIII. Powder diffraction data for 1-[(4-chloro-3,5-dimethylphenoxy)acetyl]-4-methylpiperazine $C_{15}H_{21}ClN_2O_2$.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
6.643	13.2941	16	0	1	0	6.643	13.3018	0.000
7.540	11.7149	100	0	1	1	7.547	11.7104	−0.007
12.098	7.3099	7	1	0	1	12.121	7.2997	−0.023
13.581	6.5148	21	−1	0	1	13.600	6.5090	−0.019
15.133	5.8499	45	0	2	2	15.148	5.8471	−0.015
15.535	5.6993	12	−1	2	1	15.481	5.7221	0.054
16.699	5.3045	2	−1	0	2	16.678	5.3140	0.021
17.055	5.1948	4	−1	−1	1	17.072	5.1922	−0017
17.997	4.9250	3	0	−2	2	17.959	4.9377	0.038
19.116	4.6391	2	1	1	3	19.150	4.6332	−0.034
19.490	4.5510	3	−1	1	3	19.517	4.5469	−0.027
20.122	4.4093	2	1	2	1	20.078	4.4211	0.044
20.567	4.3149	23	−1	0	3	20.534	4.3240	0.033
21.492	4.1314	11	1	0	4	21.484	4.1349	0.008
21.948	4.0466	3	0	2	4	21.937	4.0505	0.011
23.434	3.7931	3	−2	2	0	23.420	3.7973	0.014
24.391	3.6464	7	2	0	2	24.379	3.6500	0.012
24.833	3.5825	2	−1	0	4	24.832	3.5844	0.001
25.846	3.4444	5	1	0	5	25.852	3.4453	−0.006
26.469	3.3647	2	−2	3	1	26.498	3.3627	−0.029
26.990	3.3009	1	2	−2	3	27.015	3.2995	−.025
28.188	3.1632	4	2	1	3	28.189	3.1647	−.001
28.580	3.1208	0.5	1	−4	2	28.565	3.1239	0.015
29.335	3.0421	5	1	−3	4	29.329	3.0443	0.006
29.930	2.9830	2	2	−2	4	29.876	2.9898	0.054
30.328	2.9448	2	2	1	4	30.362	2.9430	−0.034
30.936	2.8883	1	1	1	6	30.898	2.8932	0.038
31.242	2.8607	1	−2	4	2	31.251	2.8613	−0.009
31.878	2.8051	1	−2	2	4	31.889	2.8055	−0.011
32.251	2.7734	0.7	1	4	2	32.250	2.7749	0.001
32.957	2.7156	1	1	−5	1	32.971	2.7158	−0.014
33.914	2.6412	1	2	−4	3	33.893	2.6440	0.021
34.312	2.6115	1	3	−1	1	34.299	2.6137	0.013
34.624	2.5886	3	−3	1	0	34.617	2.5904	0.007
35.695	2.5134	1	−3	1	1	35.672	2.5161	0.023
36.126	2.4844	1	0	5	4	36.141	2.4846	−0.015
36.752	2.4434	0.5	2	−5	2	36.760	2.4441	−0.008
38.060	2.3624	1	1	−4	5	38.019	2.3660	0.041
38.479	2.3376	1	0	5	5	38.478	2.3389	0.001
39.423	2.2838	0.7	0	−5	3	39.423	2.2849	0.000
39.991	2.2527	0.6	1	4	6	39.991	2.2538	0.000
40.176	2.2427	0.6	−2	6	1	40.155	2.2450	0.021
40.891	2.2052	0.6	0	6	3	40.864	2.2076	0.027
41.671	2.1657	3	−3	0	3	41.613	2.1696	0.058

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TABLE VIII. (*Continued.*)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
42.322	2.1339	1	2	2	7	42.310	2.1355	0.012
42.937	2.1047	2	−1	1	8	42.919	2.1066	0.018
43.463	2.0805	4	2	−4	6	43.455	2.0818	0.008
44.250	2.0453	0.6	2	−1	8	44.231	2.0471	0.019
44.842	2.0196	0.5	1	5	6	44.876	2.0191	−0.034
45.161	2.0061	2	−2	−3	4	45.174	2.0065	−0.013
45.502	1.9919	0.5	3	−3	6	45.495	1.9931	0.007
45.929	1.9743	0.6	−3	1	5	45.925	1.9754	0.004
46.235	1.9620	0.7	−2	0	7	46.235	1.9629	0.000
46.436	1.9539	0.9	−3	4	5	46.435	1.9549	0.001
46.761	1.9411	2	3	0	7	46.760	1.9421	0.001
47.838	1.8999	1	4	−4	1	47.837	1.9008	0.001
48.254	1.8845	0.9	3	−4	6	48.228	1.8863	0.026
48.550	1.8737	0.4	−4	4	1	48.531	1.8753	0.019
49.206	1.8502	3	−1	6	7	49.214	1.8508	−0.008
49.649	1.8347	0.4	−1	−2	8	49.642	1.8359	0.007
50.330	1.81152	0.5	1	1	10	50.321	1.8127	0.009
51.335	1.77839	1	−1	7	6	51.338	1.7791	−0.003
51.813	1.76307	0.6	1	−3	9	51.816	1.7638	−0.003
52.686	1.73592	0.6	2	3	9	52.699	1.7363	−0.013
52.955	1.72774	0.8	2	−3	9	52.958	1.7284	−0.003
53.358	1.71564	0.8	−2	8	3	53.361	1.7163	−0.003
55.201	1.66264	2	−1	4	10	55.211	1.6631	−0.010
56.673	1.62288	2	−1	6	9	56.675	1.6236	−0.002
57.644	1.59784	0.6	−1	5	10	57.645	1.5985	−0.001
58.458	1.57751	0.5	−2	2	10	58.460	1.5782	−0.002
61.347	1.50996	0.5	1	8	5	61.340	1.5108	0.007
61.651	1.50326	1	−2	−4	7	61.652	1.5039	−0.001

TABLE IX. Powder diffraction data for 1-benzyl-4-[(4-chloro-3,5-dimethylphenoxy)acetyl]-piperazine C_{21} H_{25} Cl N_2 O_2.

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
4.262	20.7133	100	0	0	1	4.222	20.9225	0.040
8.379	10.5438	4	0	1	0	8.368	10.5632	0.011
9.691	9.1193	5	1	0	1	9.700	9.1155	−0.009
10.174	8.6873	0.8	−1	0	1	10.163	8.7012	0.011
11.028	8.0165	3	1	1	1	11.013	8.0315	0.015
12.590	7.0255	11	−1	0	2	12.604	7.0210	−0.014
12.922	6.8457	3	−1	1	0	12.907	6.8569	0.015
13.881	6.3747	2	1	1	3	13.808	6.4114	0.073
15.092	5.8659	22	0	1	4	15.025	5.8947	0.067
16.025	5.5261	2	0	2	3	16.015	5.5325	0.010
16.848	5.2581	9	0	2	0	16.851	5.2598	−0.003
17.246	5.1378	6	1	2	3	17.289	5.1276	−0.043
17.776	4.9858	2	0	2	4	17.810	4.9787	−0.034
18.069	4.9055	4	2	0	0	18.104	4.8985	−0.035
18.814	4.7129	4	−1	2	1	18.821	4.7135	−0.007
19.515	4.5452	7	2	0	2	19.524	4.5453	−0.009
20.381	4.3539	16	−2	0	2	20.359	4.3607	0.022
20.874	4.2522	6	0	0	5	20.853	4.2585	0.021
21.590	4.1128	29	2	−1	1	21.625	4.1082	−0.035
22.225	3.9968	6	2	1	4	22.267	3.9912	−0.042
22.735	3.9082	2	−2	1	3	22.757	3.9064	−0.022
23.739	3.7450	4	1	3	2	23.693	3.7541	0.046
24.605	3.6152	13	1	3	1	24.620	3.6148	−0.015
25.427	3.5001	2	0	3	0	25.393	3.5065	0.034

TABLE IX. (*Continued.*)

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$ (°)
25.969	3.4284	0.5	−2	2	0	25.941	3.4337	0.028
26.479	3.3634	3	−1	3	1	26.440	3.3700	0.039
27.455	3.2461	1	−1	−1	5	27.470	3.2459	−0.015
28.141	3.1685	0.9	3	0	2	28.132	3.1710	0.009
28.831	3.0942	2	2	3	5	28.799	3.0991	0.032
29.443	3.0313	0.6	3	0	3	29.470	3.0300	−0.027
29.765	2.9992	0.5	3	1	4	29.760	3.0012	0.005
30.398	2.9382	1	2	3	6	30.393	2.9401	0.005
30.890	2.8925	3	3	2	0	30.893	2.8936	−0.003
31.449	2.8423	2	1	1	8	31.441	2.8444	0.008
32.777	2.7301	2	−3	1	4	32.781	2.7311	−0.004
33.651	2.6612	0.6	3	0	5	33.651	2.6625	0.000
34.210	2.6190	0.4	−2	2	7	34.225	2.6191	−0.015
34.464	2.6002	1	2	4	2	34.482	2.6002	−0.018
35.025	2.5599	0.5	3	−1	4	35.044	2.5598	−0.019
36.575	2.4549	0.4	4	1	2	36.557	2.4572	0.018
36.957	2.4304	0.3	4	1	0	36.914	2.4343	0.043
37.425	2.4010	1	−3	1	6	37.452	2.4005	−0.027
37.838	2.3758	0.4	−4	−1	1	37.830	2.3774	0.008
38.241	2.3517	1	1	2	10	38.245	2.3526	−0.004
39.472	2.2811	3	3	4	2	39.470	2.2823	0.002
40.264	2.2381	0.4	−3	1	7	40.312	2.2366	−0.048
40.661	2.2171	0.5	2	2	10	40.658	2.2183	0.003
41.223	2.1882	0.9	0	5	1	41.226	2.1891	−0.003
41.655	2.1665	0.4	−3	0	7	41.654	2.1676	0.001
42.009	2.1490	0.3	−1	−4	3	41.985	2.1512	0.024
42.213	2.1391	0.9	2	1	10	42.227	2.1395	−0.014
42.664	2.1176	0.7	0	−1	9	42.655	2.1190	0.009
44.052	2.0540	1	−3	−4	1	44.043	2.0554	0.009
44.918	2.0164	0.5	−1	5	0	44.857	2.0199	0.061
45.402	1.9960	0.5	−1	−2	8	45.389	1.9975	0.013
46.020	1.9706	0.6	1	−4	4	46.033	1.9710	−0.013
46.218	1.9626	0.3	−3	4	0	46.214	1.9637	0.004
46.459	1.9530	0.5	4	1	8	46.475	1.9533	−0.016
46.699	1.9436	0.6	−2	5	7	46.694	1.9447	0.005
48.693	1.8685	0.3	1	6	2	48.715	1.8686	−0.022
48.932	1.8599	0.5	−1	6	6	48.934	1.8608	−0.002
49.515	1.8394	0.5	5	3	2	49.567	1.8385	−0.052
50.110	1.81896	0.3	5	−1	3	50.108	1.8199	0.002
50.706	1.79894	0.4	−5	−2	2	50.708	1.7997	−0.002
52.722	1.73480	0.5	−5	−3	1	52.732	1.7353	−0.010
53.213	1.71995	0.4	−2	1	12	53.218	1.7206	−0.005
53.716	1.70503	0.3	−2	4	12	53.730	1.7054	−0.014
55.711	1.64861	0.5	3	4	13	55.715	1.6493	−0.004
57.316	1.60619	0.3	−3	3	12	57.323	1.6068	−0.007
59.511	1.55209	0.3	−3	−6	1	59.514	1.5527	−0.003
59.875	1.54351	0.9	3	−5	3	59.876	1.5442	−0.001

confirms that diffraction analysis can be an effective instrument in identification of organic compounds.

The melting temperatures for investigated materials are presented in column 6 in Table I. For samples synthesised by procedure I, melting point is greater than for samples obtained by procedure II. In addition, samples 1–5 are not soluble in water.

In order to determine the correlation between biological activity and the crystal structure for the derivatives of 4-chloro-3,5-dimethylphenoxyacetamide (new compounds

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TABLE X. Unit cell parameters for investigated samples.

No sample	Sample	Crystal system	Unit-cell data (Å)	Unit-cell data (°)	Volume (Å^3)	M_{30}	F_{30}
1	$C_{16}H_{15}ClFNO_2$	triclinic	$a=12.503$	$\alpha=98.511$	1730.56	3	6.(0.015598, 353)
			$b=10.514$	$\beta=131.432$			
			$c=18.068$	$\gamma=92.258$			
2	$C_{16}H_{14}Cl_2FNO_2$	triclinic	$a=7.7112$	$\alpha=137.843$	1583.64	2	4.(0.022957, 398)
			$b=13.9550$	$\beta=104.584$			
			$c=23.8484$	$\gamma=90.923$			
3	$C_{17}H_{14}Cl_2F_3NO_2$	triclinic	$a=7.7856$	$\alpha=129.490$	1727.58	3	6.(0.016042, 343)
			$b=15.0341$	$\beta=117.635$			
			$c=21.8462$	$\gamma=66.432$			
4	$C_{17}H_{17}Cl_2NO_2$	monoclinic	$a=18.3353$	$\alpha=90.000$	1560.61	3	5.(0.023448, 265)
			$b=7.6296$	$\beta=124.257$			
			$c=13.4972$	$\gamma=90.000$			
5	$C_{16}H_{13}Br_3ClNO_2$	triclinic	$a=8.7696$	$\alpha=85.965$	1724.84	3	9.(0.019205, 177)
			$b=12.1208$	$\beta=51.131$			
			$c=21.1939$	$\gamma=79.952$			
6	$C_{15}H_{15}ClN_2O_2$	triclinic	$a=14.1633$	$\alpha=91.524$	2305.15	3	7.(0.025666, 188)
			$b=16.4937$	$\beta=99.669$			
			$c=13.5325$	$\gamma=48.138$			
7	$C_{15}H_{21}ClN_2O_2$	triclinic	$a=7.8889$	$\alpha=82.385$	1902.64	3	8.(0.020329, 185)
			$b=14.1336$	$\beta=83.501$			
			$c=18.2575$	$\gamma=107.178$			
8	$C_{21}H_{25}ClN_2O_2$	triclinic	$a=9.8864$	$\alpha=63.722$	2457.32	2	7.(0.025990, 182)
			$b=11.7740$	$\beta=83.999$			
			$c=23.7699$	$\gamma=82.729$			

belonging to a group of potential pesticides), research on more samples of this derivatives group will be needed in future.

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