

Synthesis and structural characterization of new spiropyran containing conjugated vinyl-3*H*-indolium moiety and its hydrolysis product

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SUPPLEMENTARY INFORMATION

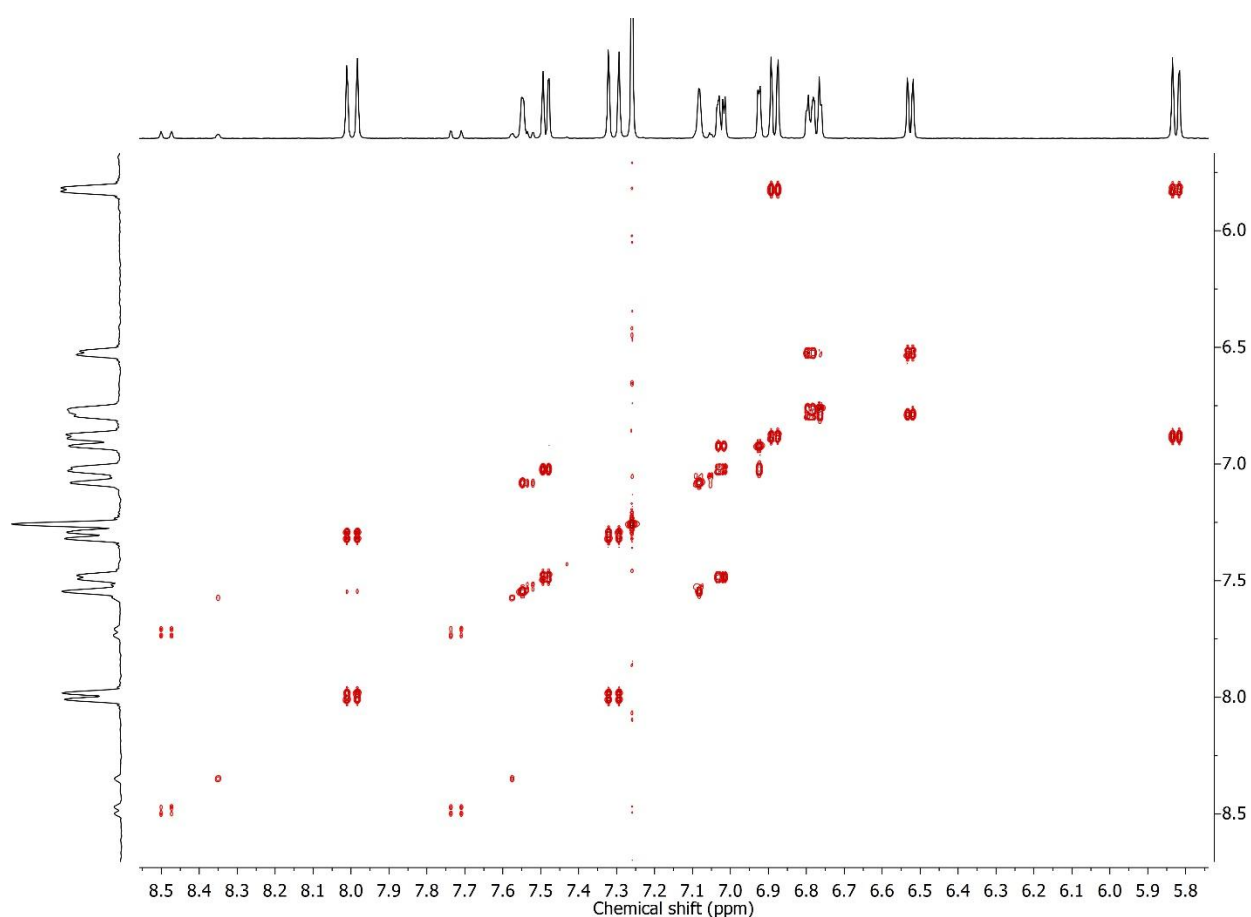


Figure S1. NMR COSY ¹H-¹H spectrum of compound **3**, aromatic protons' region, CDCl₃

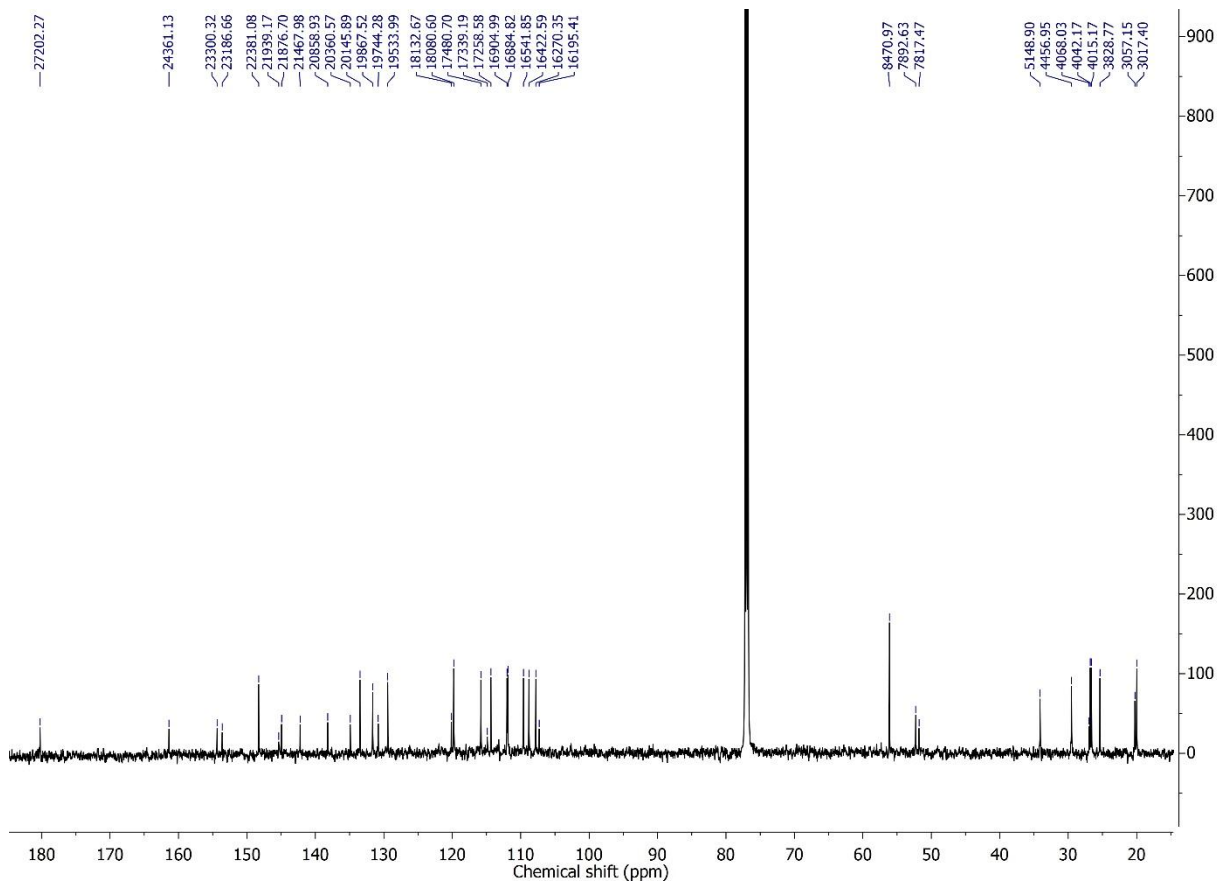


Figure S2. NMR ^{13}C spectrum of compound **3**, general view, CDCl_3

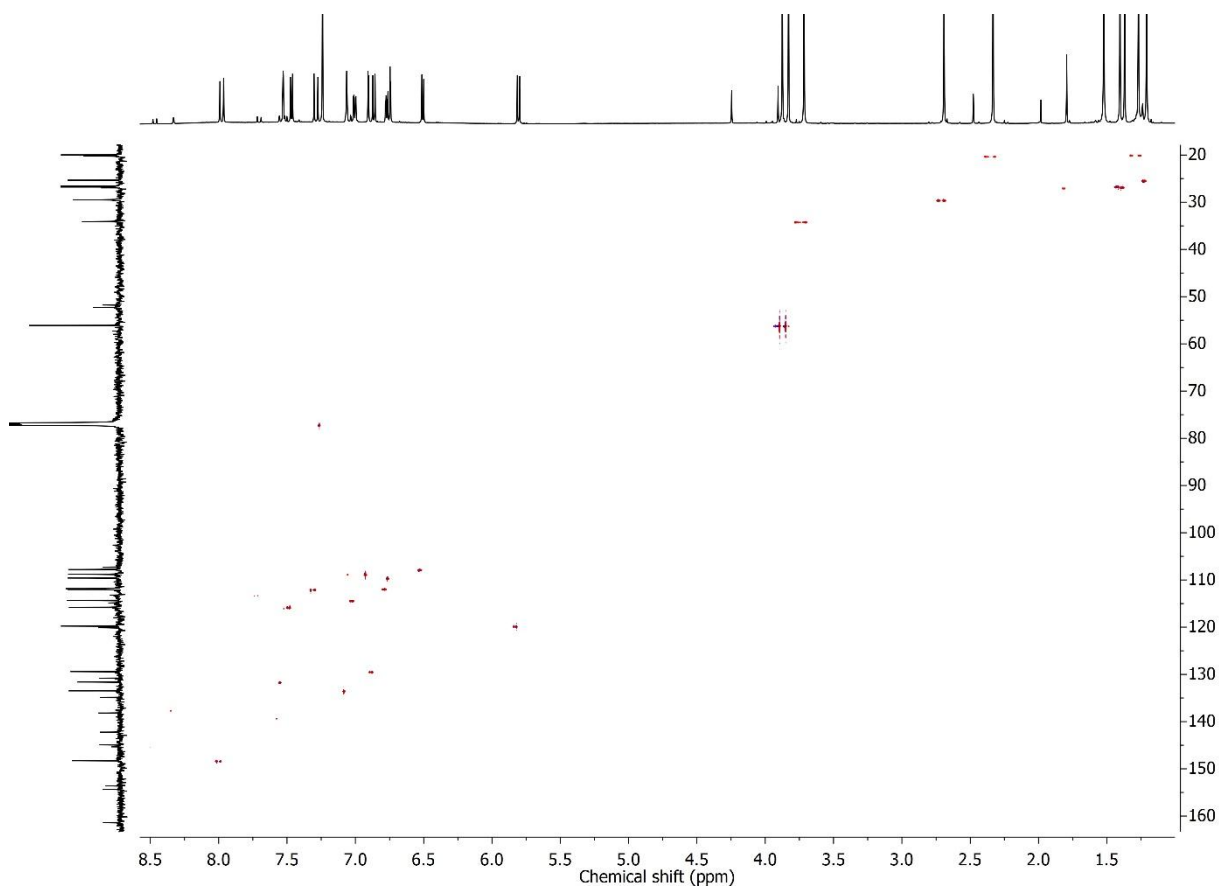


Figure S3. NMR HSQC ^1H - ^{13}C spectrum of compound **3**, general view, CDCl_3

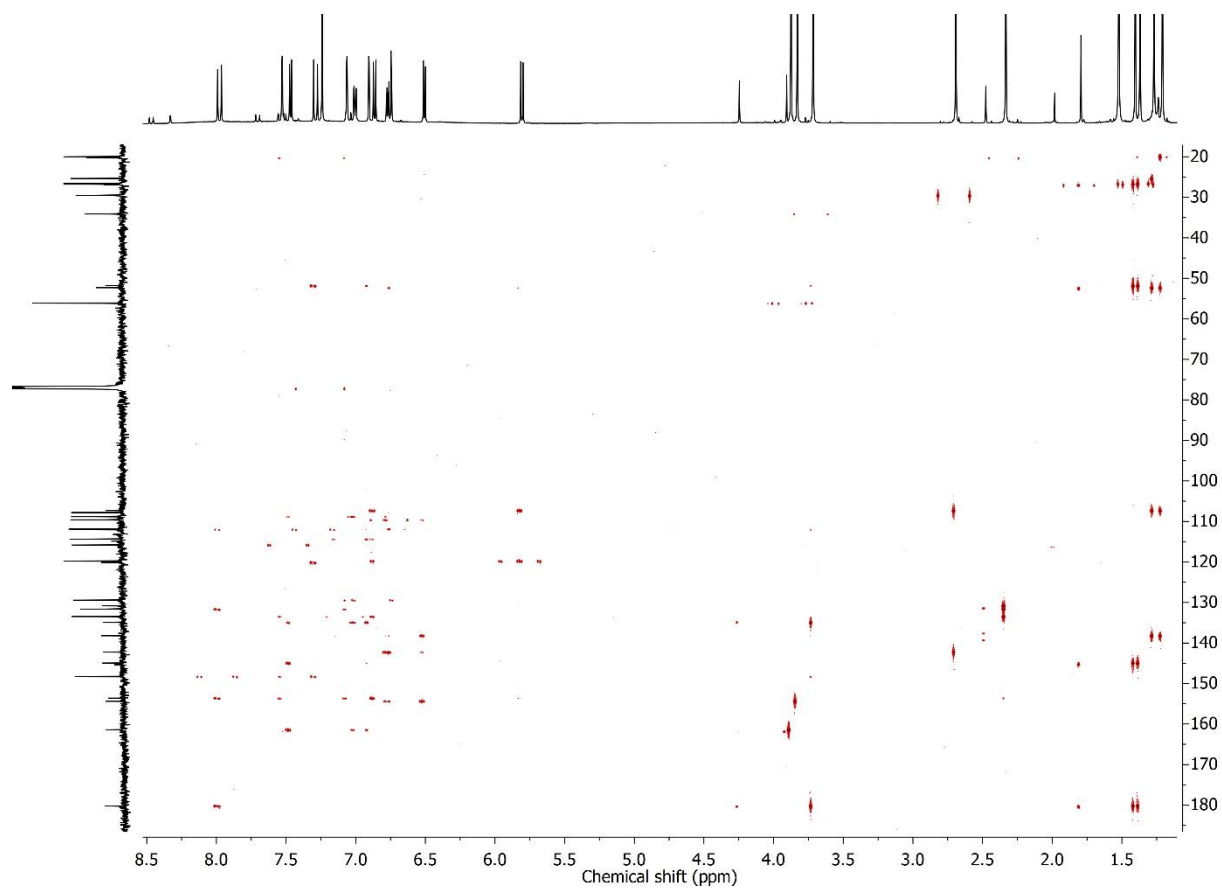


Figure S4. NMR HMBC ^1H - ^{13}C spectrum of compound **3**, general view, CDCl_3

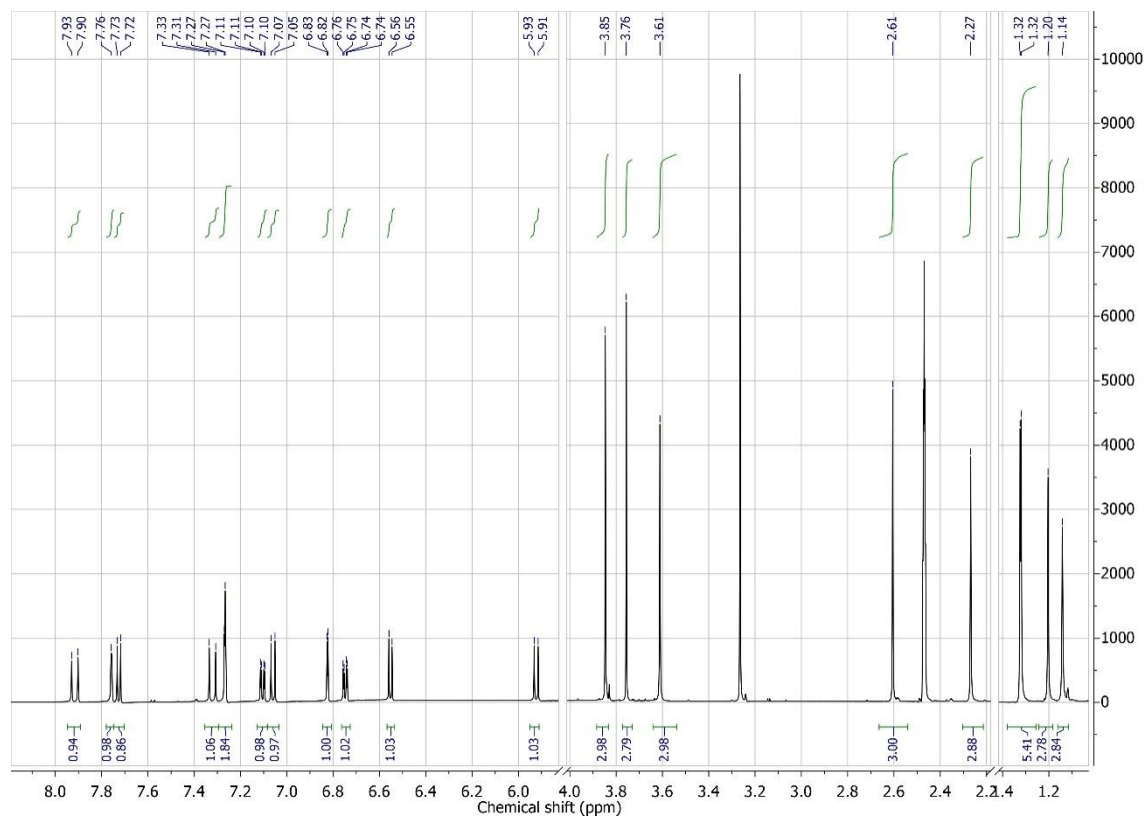


Figure S5. NMR ^1H spectrum of compound **3**, general view, $\text{DMSO}-d_6$

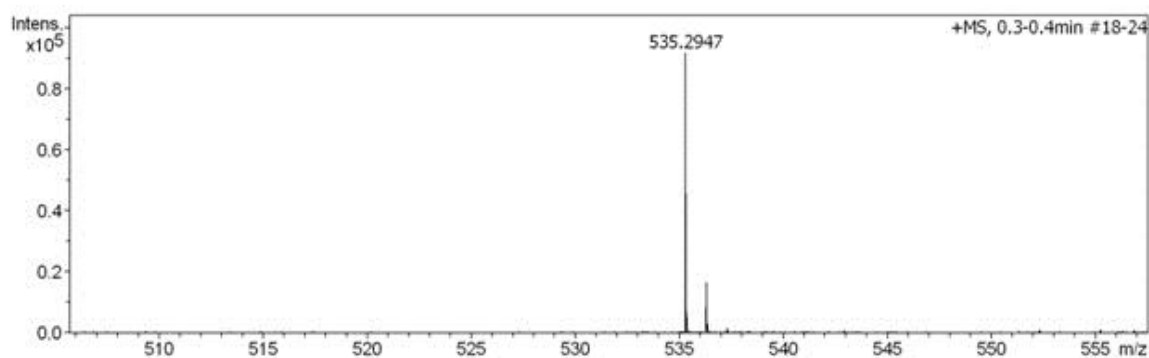


Figure S6. HRMS spectrum of compound **3**.

Table S7. The optimized cartesian coordinates (Å) of the compound **3 TTC-TTT** calculated by B3LYP/6-311G(d,p) method.

8	1.139301000	9.127133000	1.794551000
8	-6.196666000	2.499352000	1.733389000
7	-0.833835000	3.233080000	2.799002000
6	2.705267000	11.512293000	1.606301000
6	3.397663000	9.296673000	2.566397000
6	-2.806467000	1.641752000	2.715180000
6	-4.162669000	1.569036000	2.418137000
6	-2.881247000	4.007417000	2.159017000
6	4.426206000	7.278358000	3.550877000
6	2.134909000	8.584266000	2.322484000
6	3.236854000	6.582982000	3.325839000
6	0.890735000	6.471831000	2.527226000
6	0.625685000	5.150467000	2.804595000
6	2.108636000	7.172956000	2.741645000
6	-2.184862000	2.878632000	2.573197000
6	4.474678000	8.615341000	3.168350000
6	-4.877207000	2.701324000	1.992317000
6	0.159647000	2.258910000	3.249075000
6	-4.232334000	3.940981000	1.858890000
6	-1.930312000	5.187652000	2.112095000
6	3.601141000	10.655943000	2.213012000
6	-1.822841000	5.718365000	0.664537000
6	-2.399353000	6.288471000	3.088039000
6	-6.983240000	3.618963000	1.315068000
6	-0.620158000	4.538931000	2.582093000
6	5.617565000	6.586765000	4.167836000
1	-2.272966000	0.761391000	3.048630000
1	-4.697025000	0.631892000	2.513390000
1	3.188599000	5.542866000	3.626523000
1	1.404224000	4.535876000	3.237559000
1	5.391001000	9.175149000	3.337645000
1	-1.461856000	4.936623000	-0.006812000
1	-4.765919000	4.823652000	1.534470000
1	4.588038000	11.030840000	2.458275000
1	-2.813960000	6.031875000	0.330204000
1	0.118260000	7.089359000	2.089218000
1	-6.988690000	4.402045000	2.079138000

1	-1.726034000	7.145629000	3.075075000
1	-0.103407000	1.284227000	2.843363000
1	-6.612658000	4.029111000	0.370784000
1	5.303634000	5.904270000	4.960253000
1	-2.453547000	5.902046000	4.107868000
1	-1.151883000	6.574648000	0.597135000
1	0.180198000	2.221838000	4.338812000
1	6.319501000	7.311052000	4.586916000
1	-3.394606000	6.625840000	2.791117000
1	6.158682000	5.994122000	3.421584000
1	-7.991783000	3.234932000	1.176934000
1	1.145102000	2.540540000	2.889930000
1	1.726027000	11.121107000	1.377264000
1	3.801179000	14.266850000	3.461811000
1	0.207812000	12.836714000	1.266949000
6	4.641078000	13.833889000	2.914723000
1	5.492474000	14.513633000	2.990798000
6	0.699141000	13.193833000	0.361200000
6	1.942902000	15.990452000	-0.230402000
1	0.916859000	15.949538000	-0.571553000
6	2.688100000	17.151785000	-0.399366000
6	2.569110000	14.908775000	0.380500000
1	2.248999000	18.022352000	-0.870666000
7	2.061857000	13.620000000	0.672627000
6	4.023195000	17.230538000	0.029978000
1	0.144397000	14.038526000	-0.035828000
1	6.096135000	18.433749000	1.306134000
6	2.985906000	12.841901000	1.257115000
6	3.890369000	14.973735000	0.808747000
8	4.643130000	18.419137000	-0.196107000
6	4.637992000	16.128683000	0.644776000
6	4.281807000	13.643567000	1.424018000
1	0.718841000	12.393141000	-0.380332000
6	6.003170000	18.563880000	0.223777000
1	5.664797000	16.167615000	0.981635000
1	6.289140000	19.577546000	-0.048996000
6	5.449349000	13.012107000	0.634230000
1	6.651296000	17.847615000	-0.290031000
1	6.308877000	13.684523000	0.671383000
1	5.171142000	12.861863000	-0.410876000
1	5.744117000	12.052438000	1.058251000
1	4.912808000	12.888441000	3.384412000
17	2.968035000	3.366191000	5.733212000
8	3.716108000	4.506013000	6.345322000
8	3.213705000	3.350894000	4.253644000
8	3.435471000	2.075553000	6.318613000
8	1.506711000	3.541383000	5.994036000

Table S8. The optimized cartesian coordinates (Å) of the compound **3 TTT-TTT** calculated by B3LYP/6-311G(d,p) method.

8	2.277686000	9.733904000	4.714678000
8	-1.103798000	4.942113000	12.797560000
7	0.909253000	4.314530000	7.699529000

6	3.672559000	11.057053000	1.031757000
6	2.981724000	9.153989000	2.510332000
6	0.109009000	3.215565000	9.842167000
6	-0.395794000	3.489090000	11.107880000
6	0.219533000	5.611362000	9.443022000
6	2.988556000	6.775375000	1.887710000
6	2.487817000	8.845027000	3.863046000
6	2.519126000	6.456741000	3.167064000
6	1.783703000	7.090990000	5.449542000
6	1.582820000	5.830763000	5.961657000
6	2.265369000	7.417901000	4.150751000
6	0.405240000	4.299570000	9.021495000
6	3.210976000	8.114407000	1.589784000
6	-0.598029000	4.809818000	11.542693000
6	1.223453000	3.097275000	6.951513000
6	-0.283875000	5.890487000	10.703524000
6	0.644927000	6.554859000	8.334269000
6	3.206030000	10.519193000	2.213847000
6	-0.552595000	7.414522000	7.873385000
6	1.825803000	7.431429000	8.808759000
6	-1.337904000	6.262028000	13.298015000
6	1.079664000	5.564837000	7.247179000
6	3.221102000	5.686833000	0.868822000
1	0.260899000	2.191438000	9.527654000
1	-0.644611000	2.682339000	11.786127000
1	2.340082000	5.412765000	3.393190000
1	1.837904000	4.973220000	5.354447000
1	3.576922000	8.363999000	0.598906000
1	-1.369200000	6.781204000	7.520771000
1	-0.428731000	6.914003000	11.020625000
1	2.972107000	11.179478000	3.038587000
1	-0.911537000	8.005823000	8.718264000
1	1.577543000	7.959360000	6.061318000
1	-0.406641000	6.834041000	13.348799000
1	2.159474000	8.111610000	8.025315000
1	2.302397000	2.939898000	6.928816000
1	-2.063815000	6.794624000	12.676436000
1	3.766270000	4.846684000	1.305904000
1	2.669378000	6.809165000	9.114416000
1	-0.267906000	8.095711000	7.071438000
1	0.851998000	3.182329000	5.932496000
1	3.787216000	6.063734000	0.014610000
1	1.503990000	8.025283000	9.666796000
1	2.271543000	5.289845000	0.493524000
1	-1.741073000	6.129429000	14.299803000
1	0.740563000	2.252828000	7.434789000
1	3.904655000	10.393245000	0.208446000
1	1.546931000	13.802809000	1.308362000
1	3.781954000	11.469747000	-1.799518000
6	2.188798000	13.743474000	2.189685000
1	2.070782000	14.662902000	2.766861000
6	4.650349000	12.068514000	-1.522318000
6	4.924362000	15.165651000	-1.336390000

1	5.232951000	14.812317000	-2.311469000
6	4.967227000	16.523608000	-1.041554000
6	4.478528000	14.304524000	-0.338600000
1	5.307147000	17.236073000	-1.782974000
7	4.332638000	12.897019000	-0.361519000
6	4.575151000	17.009223000	0.216691000
1	4.916745000	12.711438000	-2.355613000
1	3.228885000	18.708594000	1.858777000
6	3.879850000	12.424778000	0.812023000
6	4.091157000	14.772271000	0.912338000
8	4.662236000	18.356767000	0.378805000
6	4.130521000	16.124771000	1.211821000
6	3.669890000	13.598475000	1.776669000
1	5.489747000	11.409301000	-1.293290000
6	4.281545000	18.912541000	1.640896000
1	3.827115000	16.478791000	2.187420000
1	4.434971000	19.985672000	1.548299000
6	4.596047000	13.491310000	3.008791000
1	4.906632000	18.519782000	2.448417000
1	4.510382000	14.406997000	3.597337000
1	5.636520000	13.373963000	2.698889000
1	4.324210000	12.647073000	3.642535000
1	1.859931000	12.906502000	2.805743000
17	3.081860000	2.588161000	3.796922000
8	3.833745000	3.499817000	4.712706000
8	3.803621000	2.481569000	2.494173000
8	2.957292000	1.238823000	4.422789000
8	1.712395000	3.153352000	3.561828000

Таблица 1. Кристаллографические данные для кристалла **5**.

Параметр	Кристалл 5
Брутто-формула	$C_{22}H_{24}NO_3$, ClO_4
Цвет кристалла	Темно-бордовый
Молекулярный вес, г/моль	449.89
Номер CCDC	2182739
Симметрия кристалла	Моноклинная
Пространственная группа	$P2_1/a$
Параметры элементарной ячейки	$a = 7.0274(5) \text{ \AA};$ $b = 28.9818(14) \text{ \AA};$ $c = 10.6208(6) \text{ \AA}$ $\beta = 104.789(6)^\circ$
Объем ячейки (V), \AA^3	2091.4(2)
Z	4
Выч. плотность(ρ), г/см ³	1.429
$F(000)$	944
$\mu(\text{MoK}\alpha)$, мм ⁻¹	0.228
Размеры кристалла, мм	0.41×0.33×0.25
Диапазон Θ , град	2.81< Θ <29.0
Измеренные рефлексы	10781
Независимые рефлексы	5558
Рефлексы с $F > 4\sigma(F)$	3479
	-9< h <7
Диапазон индексов	-32< k <39
	-14< l <14
Количество уточненных параметров	280
Добротность	0.958
R_{int}	0.0969
wR_2	0.0887
R_1 с $I > 2\sigma(I)$	0.0537