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Supporting information for article:

Analysis of diffuse scattering in electron diffraction data for the crystal structure determination of Pigment Orange 13, C32H24Cl2N8O2

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1.

2. CSD search on the interplanar angle in pyrazolone pigments

The interplanar angle between the pyrazolone moiety and the terminal phenyl ring in pyrazolone hydrazone pigments was investigated by a search in the Cambridge Structural Database.

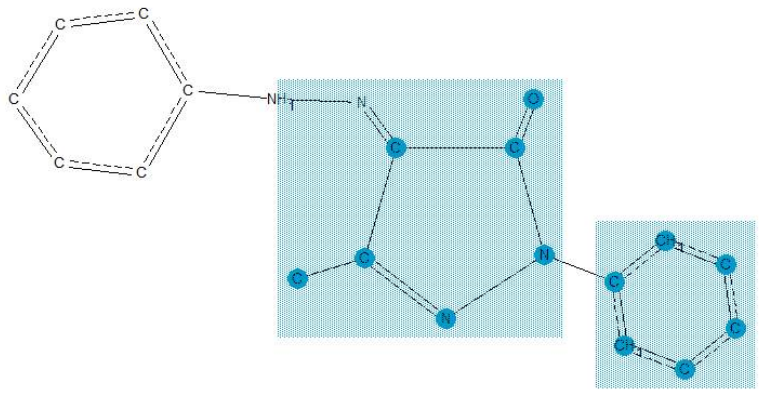

Figure S1 CSD search fragment. The interplanar angle between the two planes shown in blue is denoted as phi2 .

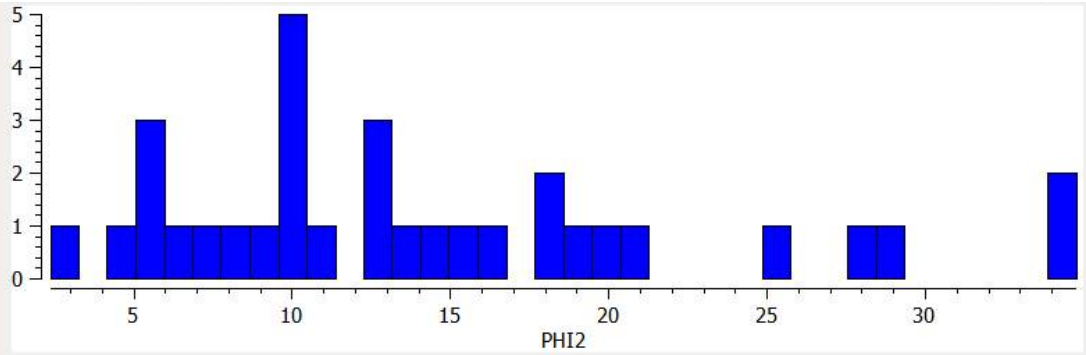

Figure S2 Histogram of the interplanar angle phi2.

Remark: The "outlier" with a phi2 angle of 34-35° (1 compound with two CSD entries) is not an unusual molecule, but a typical pyrazolone pigment (Figure S3). From this observation, we conclude that the interplanar angle between the pyrazolone fragment and the phenyl group can adopt all values between 0° and 35°.

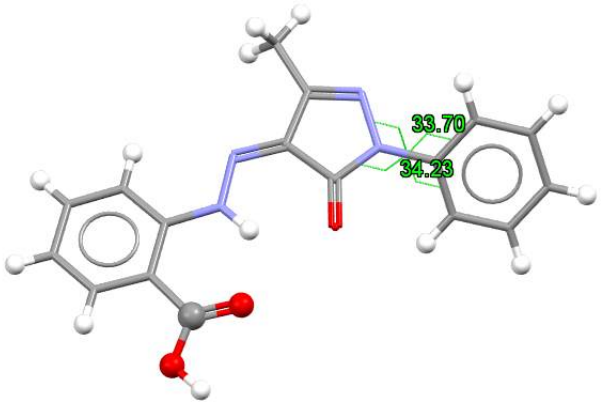

Figure S3 Pyrazolone compound with a phi2 angle of about 34°. (The values are the NNCC and CNCC torsion angles).