

## Supplementary Information

### **Isolation, identification, spectral studies and *X-ray* crystal structures of two compounds from *Bixa orellana* and their DFT and DNA binding studies**

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**Table S1** The experimental parameters related to the monocrystalline *X-ray* examination of **1** and **2**.

<b>4,6-Diacetylresorcinol (1)</b>		<b>3-O-methyl ellagic acid dihydrate (2)</b>	
Bond precision: C-C = 0.0040 Å Wavelength=0.71073		Bond precision: C-C = 0.0018 Å Wavelength=0.71073	
Cell: a=7.095(12) b=11.374(19) c=11.66(2) alpha=90 beta=100.46(3) gamma=90		Cell: a=10.1687(6) b=6.9037(5) c=21.3367(13) alpha=90 beta=107.668(3) gamma=90	
Temperature: 293 K		Temperature: 293 K	
Volume	Calculated 925(3)	Volume	1427.22(16)
Space group	P 21/c	Space group	P 21/c
Hall group	-P 2ybc	Hall group	-P 2ybc
Moiety formula	C10 H10 O4	Moiety formula	C15 H8 O8, 2(H2 O)
Sum formula	C10 H10 O4	Sum formula	C15 H12 O10
Mr	194.18	Mr	352.25
Dx, g cm <sup>-3</sup>	1.394	Dx, g cm <sup>-3</sup>	1.639
Z	4	Z	4
Mu (mm <sup>-1</sup> )	0.109	Mu (mm <sup>-1</sup> )	0.142
F000	408.0	F000	728.0
F000'	408.26	F000'	728.55
h,k,lmax	9,14,15	h,k,lmax	13,9,28
Nref	2113	Nref	3466
Tmin,Tmax		Tmin,Tmax	0.955,0.969
Tmin'		Tmin'	0.921
Correction method=	Not given	Correction method=	# Reported T Limits: Tmin=0.849 Tmax=0.969
AbsCorr =		AbsCorr =	MULTI-SCAN
Data completeness=	1.001	Data completeness=	0.979
R(reflections)=	0.0519( 989)	R(reflections)=	0.0390( 2807)
S =	0.992 Npar= 131	S =	1.043 Npar= 230
Theta(max)=	27.461	Theta(max)=	28.020
wR2(reflections)=	0.1479( 2115)	wR2(reflections)=	0.1282( 3393)