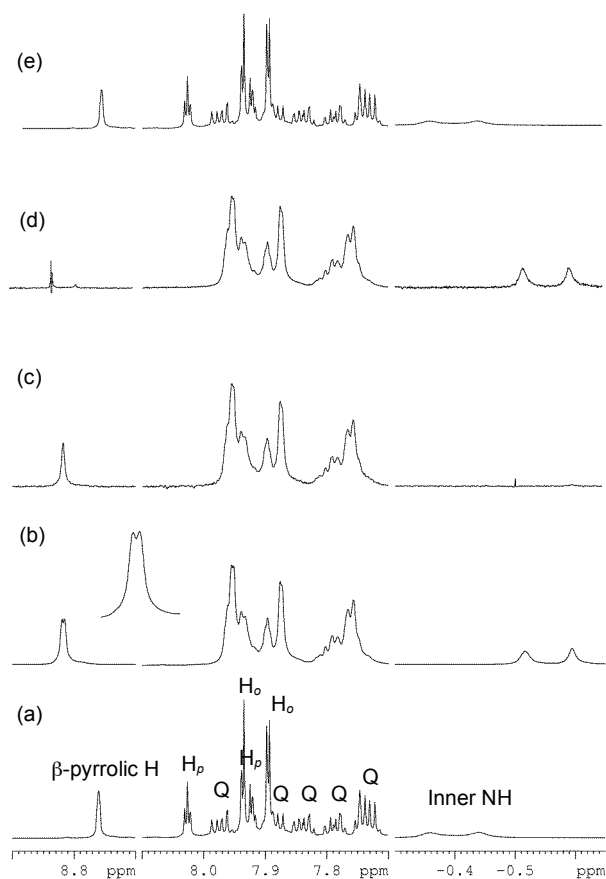
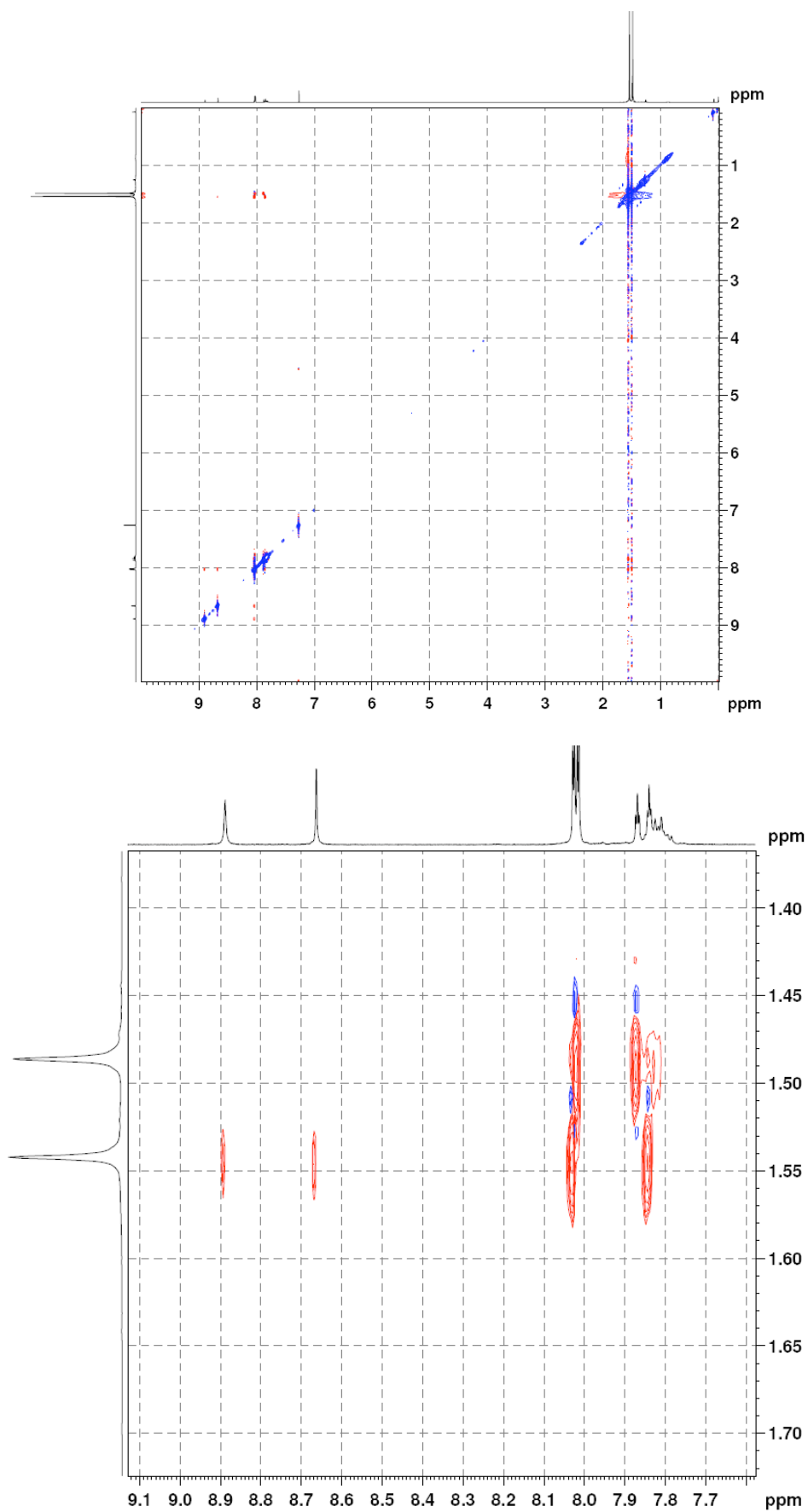


## Expansion of the porphyrin $\pi$ -system: stepwise annelation of porphyrin $\beta, \beta'$ -pyrrolic faces leading to trisquinoxalinoporphyrin

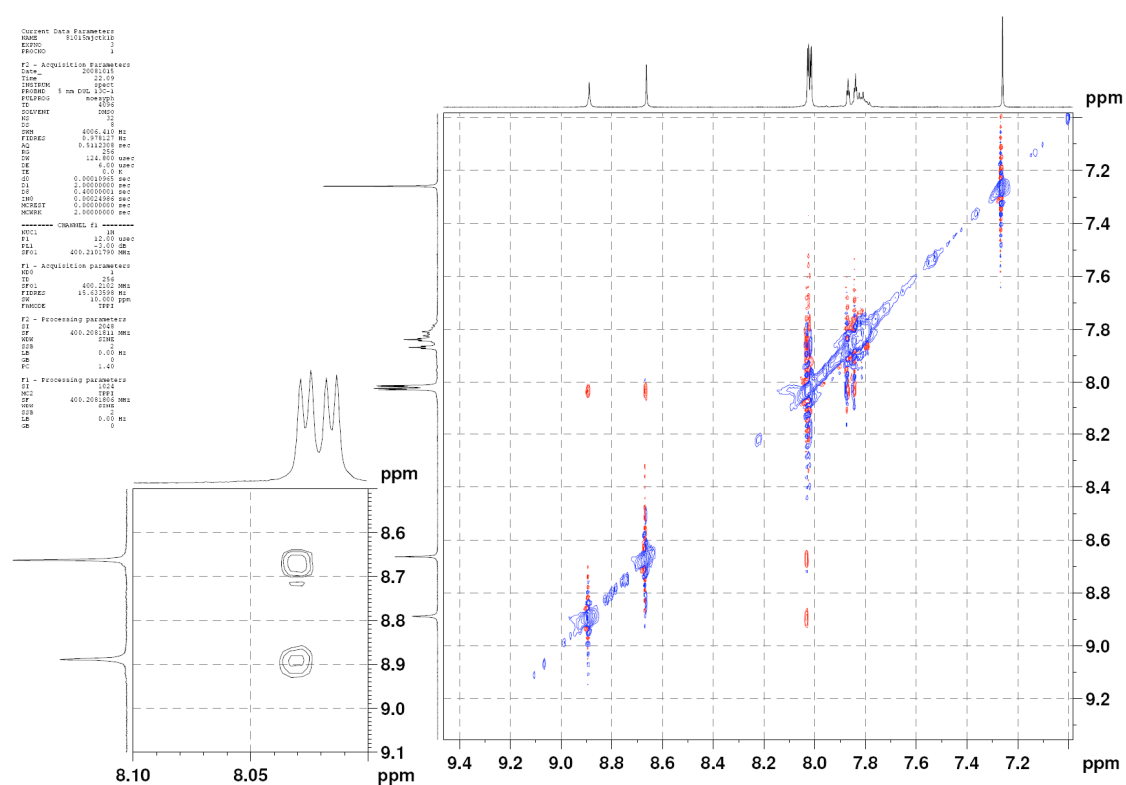
Tony Khoury and Maxwell J. Crossley\*



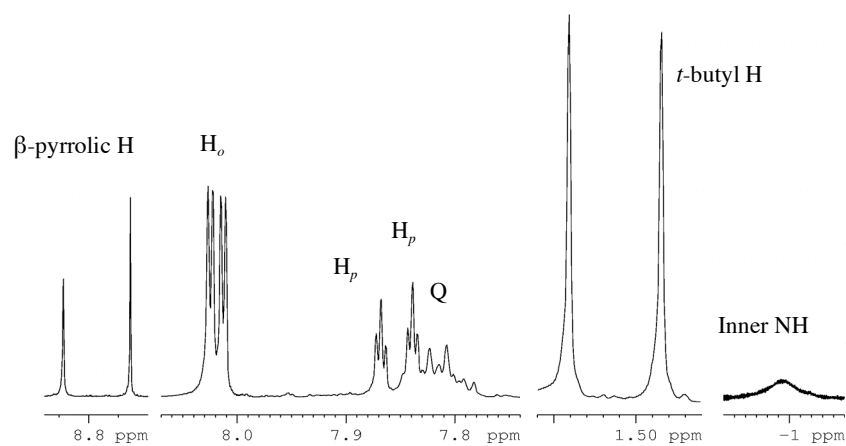
**Figure S1**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of Trisquinoxalinoporphyrin **1**: (a) at  $T = 300$  K, (b) at  $T = 230$  K, (c) at  $T = 230$  K with irradiation at  $-0.55$  ppm, (d) at  $T = 230$  K with irradiation at  $8.8$  ppm, (e) back to  $T = 300$  K.



**Figure S2**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) NOESY spectra of 7,18-dinitro-quinoxalinoporphyryn **24a**.



**Figure S3**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) NOESY spectra of 7,18-dinitro-quinoxalino porphyrin **24a**.



**Figure S4**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of 7,18-dinitro-quinoxalino porphyrin **24a**.

**The full Infra-Red Characterisation of Synthesised Products:**

**{12- and 13-Nitro-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:7,8-*b''*]porphyrinato}zinc(II) 11.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3066w, 3034w, 3022s, 3011w, 2963s, 2867m, 1595s, 1523m, 1503m, 1477m, 1392w, 1363s, 1344m, 1297m, 1248m, 1229s, 1222s, 1201s, 1195m, 1171w, 1115m, 1012w, 956m.

**{12- and 13-Nitro-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:7,8-*b''*]porphyrinato}copper(II) 13.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3058w, 3036w, 3017s, 2964s, 2904m, 2866m, 1594s, 1527m, 1511w, 1477m, 1430w, 1393w, 1363s, 1348m, 1298m, 1247w, 1232m, 1206s, 1194w, 1163w, 1117w, 1000w.

**13-Nitro-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:7,8-*b''*]porphyrin 14a.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3325w, 3060w, 3028w, 3021s, 3008w, 2964s, 2928m, 2865m, 1595m, 1507m, 1476m, 1427w, 1393w, 1362s, 1352s, 1298m, 1248m, 1234w, 1220m, 1205m, 1170w, 1132w, 1106m, 1016w.

**12-Nitro-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:7,8-*b''*]porphyrin 14b.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3326w, 3064w, 3026s, 3014w, 2864s, 2866m, 1595m, 1549w, 1524w, 1476m, 1393w, 1363m, 1351m, 1298w, 1248m, 1237s, 1212s, 1204m, 1170w, 1111m, 1098w, 1006m.

**5,10,15,20-Tetrakis(3,5-di-*tert*-butylphenyl)trisquinoxalino[2,3-*b'*:7,8-*b''*:12,13-*b'''*]porphyrin 1.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3346w, 3059w, 2962s, 2926s, 2856s, 1595s, 1576w, 1558w, 1545w, 1516w, 1506w, 1495w, 1487w, 1475m, 1466m, 1431w, 1393w, 1362s, 1352m, 1300m, 1248m, 1236m, 1204w, 1190w, 1173w, 1153m, 1136w, 1111s.

**12,13-Dioxo-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:7,8-*b''*]porphyrin 16.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3354w, 3059w, 3013w, 2964s, 2903m, 2866m, 1724s, 1595m, 1568w, 1545w, 1475m, 1462w, 1427w, 1393w, 1379w, 1364m, 1352w, 1300w, 1265w, 1248m, 1240w, 1227s, 1186w, 1136w, 1115w, 1095w, 1068w, 1001w.

**{7-Nitro-5,10,15,20-Tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:12,13-*b''*]porphyrinato}zinc(II) 18.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3059w, 3020m, 2964s, 2903m, 2866m, 1595s, 1556w, 1526m, 1487w, 1477m, 1468w, 1431w, 1402w, 1393m, 1362s, 1337w, 1300m, 1285w, 1248m, 1227s, 1207s, 1192w, 1159m, 1140w, 1111s, 1078w.

**7-Nitro-5,10,15,20-Tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:12,13-*b''*]porphyrin 20.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3369w, 3059w, 2964s, 2905m, 2866m, 1595s, 1533m, 1497w, 1477m, 1460w, 1452w, 1431w, 1393w, 1364m, 1346m, 1298m, 1248w, 1225s, 1153m, 1138w, 1107s, 1007w.

**{7-Nitro-5,10,15,20-Tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:12,13-*b''*]porphyrinato}copper(II) 19.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3059w, 3024m, 2964s, 2903m, 2866m, 1595s, 1522w, 1493w, 1477m, 1466w, 1431w, 1418w, 1393w, 1362s, 1339m, 1300w, 1290w, 1248m, 1231w, 1198s, 1163w, 1138w, 1113m, 1036w.

**Dinitro-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-phenyl)quinoxalino[2,3-*b'*]porphyrinato}copper(II) Isomers 23.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3135w, 3060w, 3020m, 2985s, 2905s, 2868s, 1593s, 1530s, 1496w, 1477m, 1427w, 1394w, 1363s, 1342s, 1297m, 1248m, 1229m, 1205m, 1168w, 1113m, 1015w, 1000w.

**Dinitro-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)quinoxalino[2,3-*b'*]porphyrin Isomers 24.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3369w, 3038w, 3006s, 3000s, 2965s, 2868m, 1593s, 1533m, 1477s, 1426w, 1394w, 1363s, 1347s, 1296w, 1248m, 1233s, 1209s, 1168w, 1105m, 1000w.

**7,18-Dinitro-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)quinoxalino[2,3-*b'*]porphyrin 24a.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3323w, 3059w, 3028m, 3016s, 2965s, 2905m, 2868m, 1593m, 1526m, 1476m, 1427w, 1394w, 1363s, 1293m, 1265w, 1246m, 1224s, 1210s, 1202w, 1161w, 1121w, 1087w.

**Linear 7-amino-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:12,13-*b''*]porphyrin 21.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3492w, 3376w, 3058w, 3032w, 3024m, 2960s, 2927s, 2871s, 1609w, 1594m, 1549m, 1463s, 1361m, 1248w, 1210s, 1152m, 1108s, 1010m.

**7,8-Dioxo-5,10,15,20-tetrakis(3,5-di-*tert*-butylphenyl)bisquinoxalino[2,3-*b'*:12,13-*b''*]chlorin 22.**  $\nu_{\max}(\text{CHCl}_3)/\text{cm}^{-1}$  3400w, 3059w, 3039w, 3028m, 3024s, 3017s, 3012w, 3004w, 2961s, 2929s, 2858m, 1725s, 1598s, 1547m, 1476m, 1363m, 1299w, 1262w, 1248w, 1226m, 1220s, 1206s, 1204m, 1143m, 1106s, 1009w.