Summary of data/files

Compound identification (= NAME)

L1 = (±)-*Tris*-(*N*-ethyl-isonicotinoyl)cyclotriguaiacylene.3PF_6 = **ETHYL**

L2 = (±)-*Tris*-(*N*-propyl-isonicotinoyl)cyclotriguaiacylene.3PF_6 = **PROPYL**

L3 = (±)-*Tris*-(*N*-butyl-isonicotinoyl)cyclotriguaiacylene.3PF_6 = **BUTYL**

L4 =(±)-*Tris*-(*N*-octyl-isonicotinoyl)cyclotriguaiacylene.3PF_6 = **OCTYL**

DMP = dimethoxy-pillar[5]arene

NMR.zip

Images (*.TIFF) and MestReNova (*.mnova) for Nuclear Magnetic Resonance Data

File.*	**Content**
NAME Proton Shifts	^{1}H NMR spectra for **NAME**.3PF6 (lower) and {$(DMP)_3$·**NAME**} (upper)
NAME NOESY Processing	^{1}H NOESY spectra for {$(DMP)_3$·**NAME**}
NAME PF6 COSY	^{1}H COSY spectra for {$(DMP)_3$·**NAME**}
NAME Carbon	13C NMR for **NAME**

Crystal.zip

X-Ray crystal structure data and refinement files, all readable as text files.

Crystallographic Information Files (prefix.CIF)

Final refinement files (prefix.RES)

Datafiles: Observed and calculated structure factors (prefix.FCF)

Original hkl data before use of SQUEEZE procedure (complex#_presqueeze.hkl)

Compound	**Filename prefix**
(**PROPYL**·2(CH_3CN)·2(H_2O)	propylnicoCTG
ETHYL	ethylnicoCTG

Analysis.zip

Electrospray ionisation mass spectrometry, Infrared spectroscopy and CHN elemental analysis

File name	**Content**
NAME Hi-Res.png	Mass spectrum **NAME**
NAME PR.pdf	Mass spectrum for {$(DMP)_3$·**NAME**}
IRs.doc	Infrared spectra for L1-L4 (**ETHYL-OCTYL)**
NAME PF6 CHN.pdf	Elemental Analysis results for L1-L4 (**ETHYL-OCTYL)**

PR2.pdb

Protein Data base file for modelling of {$(DMP)_3$·(**PROPYL**)}.