

*Supplementary material for manuscript DE5027*

**Table S1.** List of CSD refcodes for compounds corresponding to the scheme **2.Ib**

ACCITR10	GUKYAM	LIZBUR	RAVRIP	DHXBZP10	LIKDEO
BAGPAA	HUFYAI	NARBAJ	SAPTOS	HMXBZP	POVGAI
BOYKIJ	JIFVEZ	NIDZAB	SIWVID	HMXCBP10	SILFOI
CDAGLN	JUBMIC	PEKBAI	VOGXOE	NOZTEB	SOGFEZ
CUFYOR	KAWXIP	PEKBEM	VOXPED	POVLAN	SUVYUD
DACHQO	KIXLOS	PEKNEY	XEGJOI	POVLER	YIVPOI
DAUSNA	KOGSUU	QAMNUN	XEGXOW	QALBOU	YIVPUO
DHXBHP10	LIQQIL	QEKWIM	CAGDEU	FAQFOS	YIVRAW
DOVXIV	LIQQOR	QQQGT01	CHBCOU	KUMZOH	

**Table S2.** List of CSD refcodes for compounds corresponding to the scheme **2.IIa**

BAKBEU	DAXYIK	HIKXII	LOMYER	QEYBEB	XAGVEG
BEDZIT01	DEPSIA	JADSUC	MAMTEZ	QEYBIF	YEJCEV
BELQOY	DUFBEL	KOKBIV	PESNUW	RERROV	YIJSAL
BEQXOK	ETACIM	KOKBIV01	PICFOW	RIMHIE	ZIZVIN
CAVDUY	FAGQEJ	KONWIT	PICGEN	SIRZIC	ZORDIT
CICGOK	FUBHIT	KUXJUI	PNCQUX	SOJYOF	ZUWQOX
CIMCAC	GOKXIN	KUXJUI01	QENXEM	VUBJUX	ZUWQUD