

## Supporting Information

### Novel four dimensional approach for the structural characterization of neutral nitrogen compounds in vacuum gas oils using UHPLC-IM-QqToF analysis

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**Table S1: Macroscopic properties of the samples**

<b>Sample</b>	<b>Type</b>	<b>Nitrogen content (ppm)</b>	<b>Basic nitrogen (ppm)</b>	<b>% HDN conversion</b>
Feed	SRVGO	1335	347	-
HDT 3	HDT	534	79	62
HDT 2	HDT	825	70	41
HDT 1	HDT	1100	310	21

**Table S2: UHPLC elution conditions**

**Column:** Acquity UPLC CSH Phenyl-Hexyl (Waters, Milford, MA, USA) of dimensions 100 mm × 2.1 mm × 1.7 μm

**Flow rate:** 0.6 mL/min

**Injection volume:** 5 μL

**Mobile phases:** (A) H<sub>2</sub>O + 0.5 mM ammonium acetate

(B) (50% MeOH + 50% ACN) + 0.5 mM ammonium acetate

Retention time (min)	% A	%B
0	45	55
0.5	45	55
15	20	80
20	0	100
25	0	100
25.3	45	55
30	45	55

Figure S1: Possible reaction pathway of benzocarbazoles hydrogenation

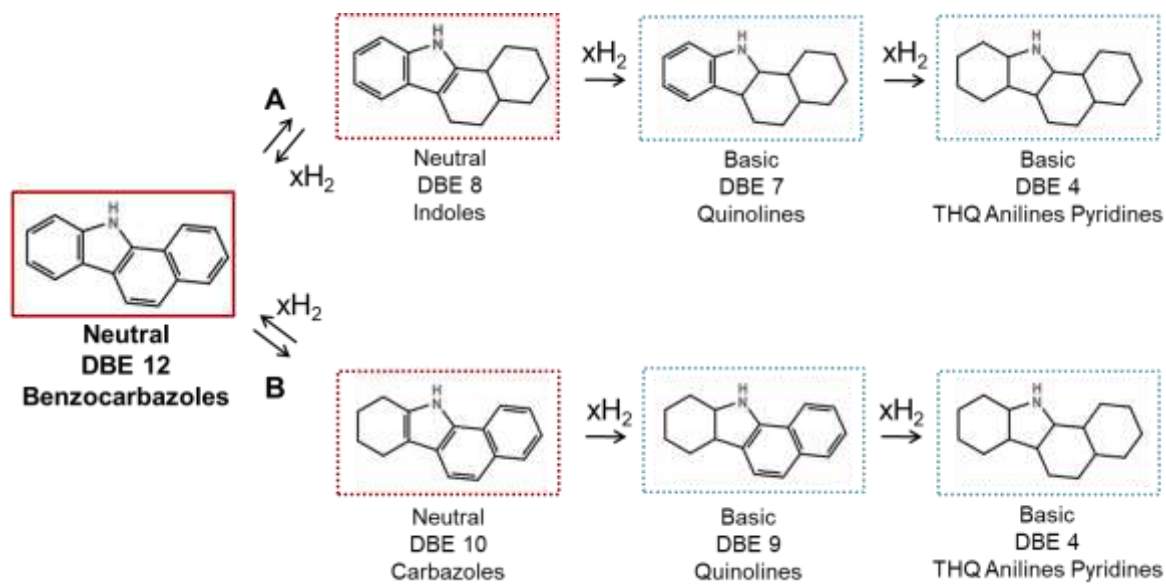
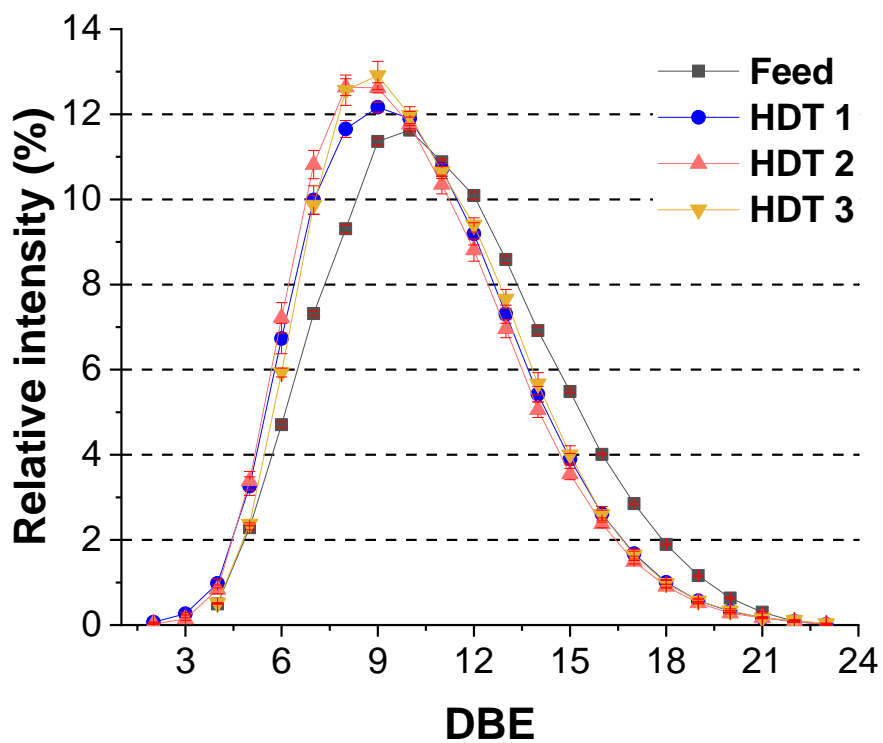
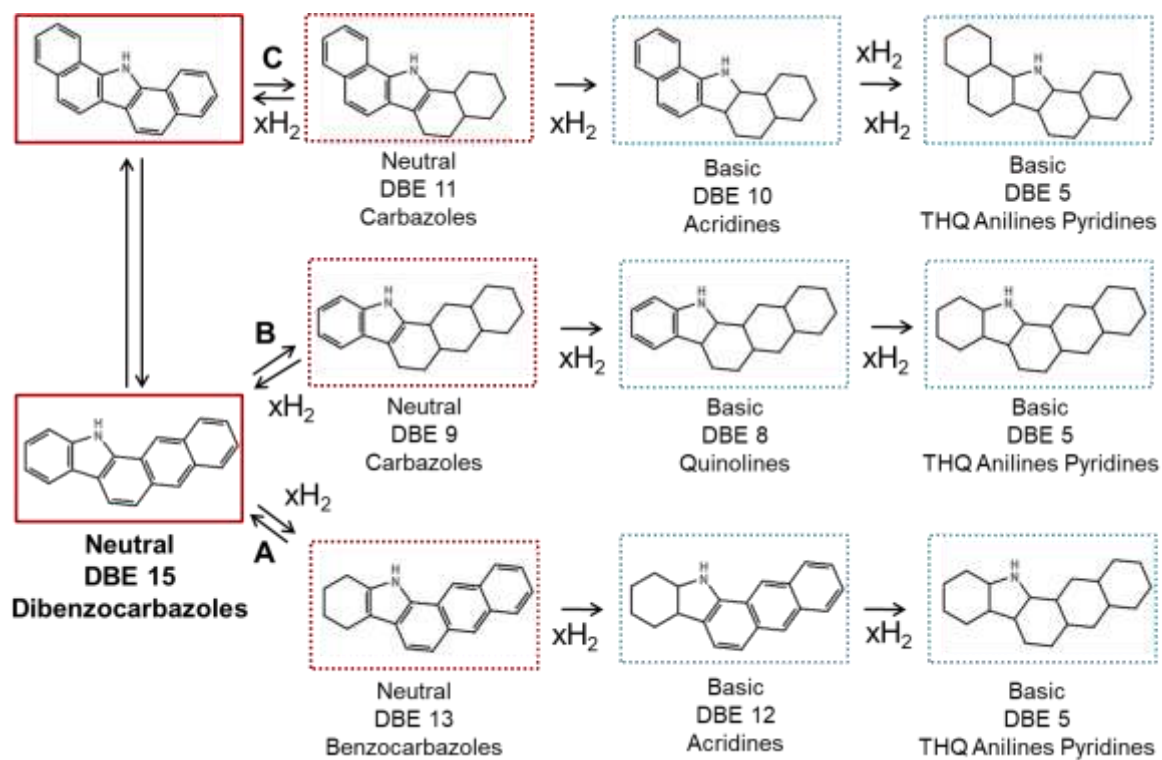


Figure S2: Evolution of the relative intensities of basic compounds as a function of DBE



**Figure S3: Possible reaction pathway of dibenzocarbazoles hydrogenation**



**Figure S4: Possible hydrogenation mechanisms of N1O1 and N1S1 species leading to N1 products**

