SUPPORTING INFORMATION

Playing with Isomerism: Cocrystallization of Isomeric *N*-Salicylideneaminopyridines with Perfluorinated Compounds as Halogen Bond Donors and Its Impact on Photochromism

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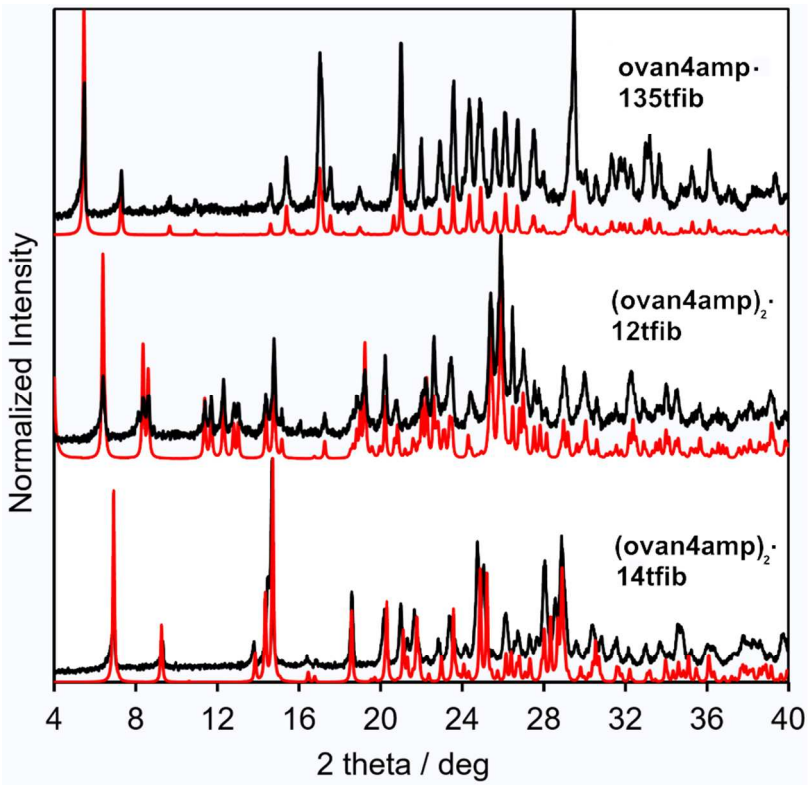

Figure S1**.** PXRD patterns of **ovan4amp** cocrystals mechanosyntheses (red = simulated pattern; black = experimental pattern)

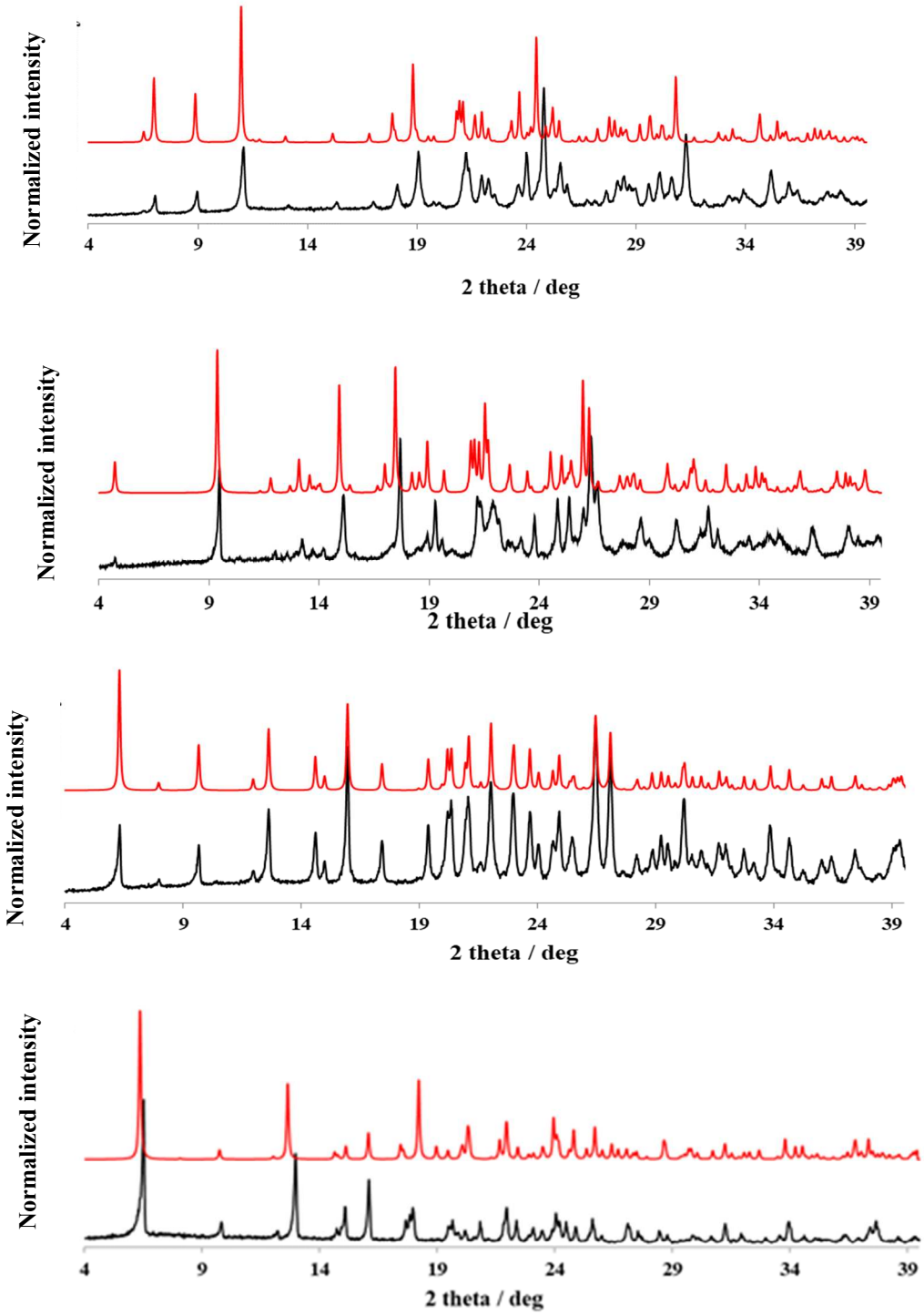

Figure S2. PXRD patterns of **ovan3amp** cocrystals (from top to bottom: **ovan3amp·12tfib, ovan3amp·13tfib, (ovan3amp)$_2$·14tfib, (ovan3amp)$_2$·ofib)** mechanosyntheses.

Table S1. Crystallographic parameters of **ovan3amp and ovan4amp** cocrystals.

	ovan3amp·12tfib	**ovan3amp·13tfib**	**(ovan3amp)$_2$·14tfib**	**(ovan3amp)$_2$·135tfib**
Chemical formula	$C_{13}H_{12}N_2O_2\cdot C_6F_4I_2$	$C_{13}H_{12}N_2O_2\cdot$ C6F4I$_2$	$C_{13}H_{12}N_2O_2\cdot 0.5(C_6F_4I_2)$	$2(C_{13}H_{12}N_2O_2)\cdot C_6F_3I_3$
M$_r$	630.11	630.11	429.18	966.25
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Triclinic
Space group	$P2_12_12_1$	$P2_1/c$	$P2_1/n$	$P\overline{1}$
***T* (K)**	295	298	115	293
***a*, *b*, *c* (Å)**	4.9559 (1), 15.9467 (5), 25.0955 (7)	19.597 (2), 7.1629 (7), 15.5499 (18)	4.6036 (3), 27.982 (2), 12.0308 (6)	4.9424 (4), 14.3285 (10), 23.8841 (18)
***α*, *β*, *γ* (°)**	90, 90, 90	90, 107.431 (12), 90	90, 96.165 (5), 90	82.468 (6), 89.490 (7), 84.574 (6)
***V* (Å^3)**	1983.30 (9)	2082.5 (4)	1540.81 (18)	1669.3 (2)
Z	4	4	4	2
CSD REFCODE	1850125	1547940	SEDFIT01	1850126
	(ovan3amp)$_2$·ofib	**(ovan4amp)$_2$·12tfib**	**(ovan4amp)$_2$·14tfib**	**ovan4amp·135tfib**
Chemical formula	$C_{13}H_{12}N_2O_2\cdot 0.5\ (C_4F_8I_2)$	$(C_{13}H_{12}N_2O_2)_2\cdot C_6F_4I_2$	$C_{13}H_{12}N_2O_2\cdot 0.5(C_6F_4I_2)$	$C_{13}H_{12}N_2O_2\cdot C_6F_3I_3$
M$_r$	455.17	858.35	429.18	738.01
Crystal system	Monoclinic	Triclinic	Monoclinic	Orthorhombic
Space group	$P2_1/n$	$P\overline{1}$	$P2_1/n$	*Pbca*
***T* (K)**	100(2)	293	150	298
***a*, *b*, *c* (Å)**	4.89023(7), 27.7231(5), 11.86723(20)	4.7846 (3), 14.4237 (8), 23.5788 (12)	16.6673 (6), 4.6723 (2), 19.0963 (9)	18.2946 (6), 7.3264 (3), 32.3563 (14)
***α*, *β*, *γ* (°)**	90, 92.9167(13) 90	73.922 (5), 89.176 (4), 85.918 (4)	90 92.004 (4), 90	90, 90, 90
***V* (Å^3)**	1606.78(5)	1559.57 (16)	1486.21 (12)	4336.8 (3)
Z	4	2	4	8
CSD REFCODE	1582770	1552262	1548172	1548140

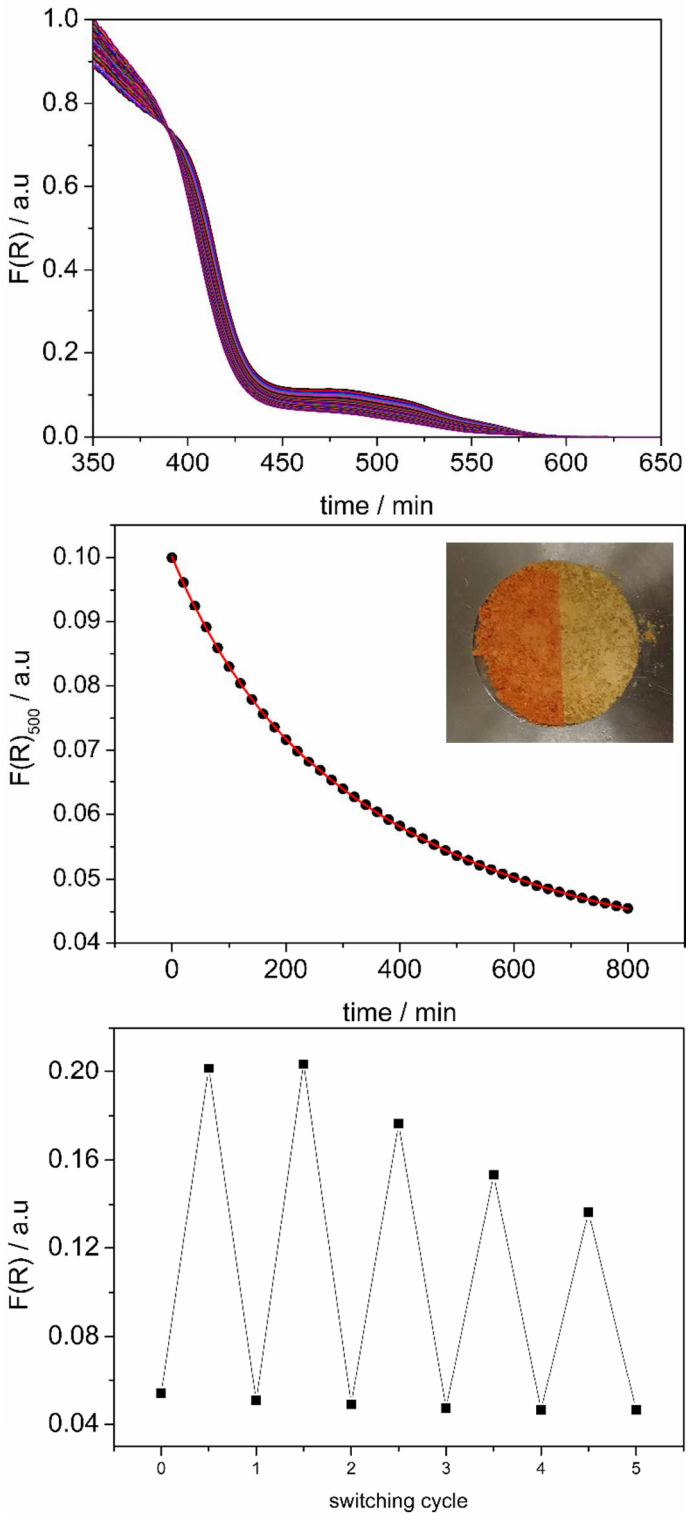

Figure S3. Diffuse reflectance spectra of **(ovan3amp)$_2$·ofib** (top) showing thermal fading of the orange-red coloration. Points at 500 nm were plotted over the time and fitted by a bi-exponential curve (middle). Repeating photochemical recovery over 5 switching cycles (bottom).

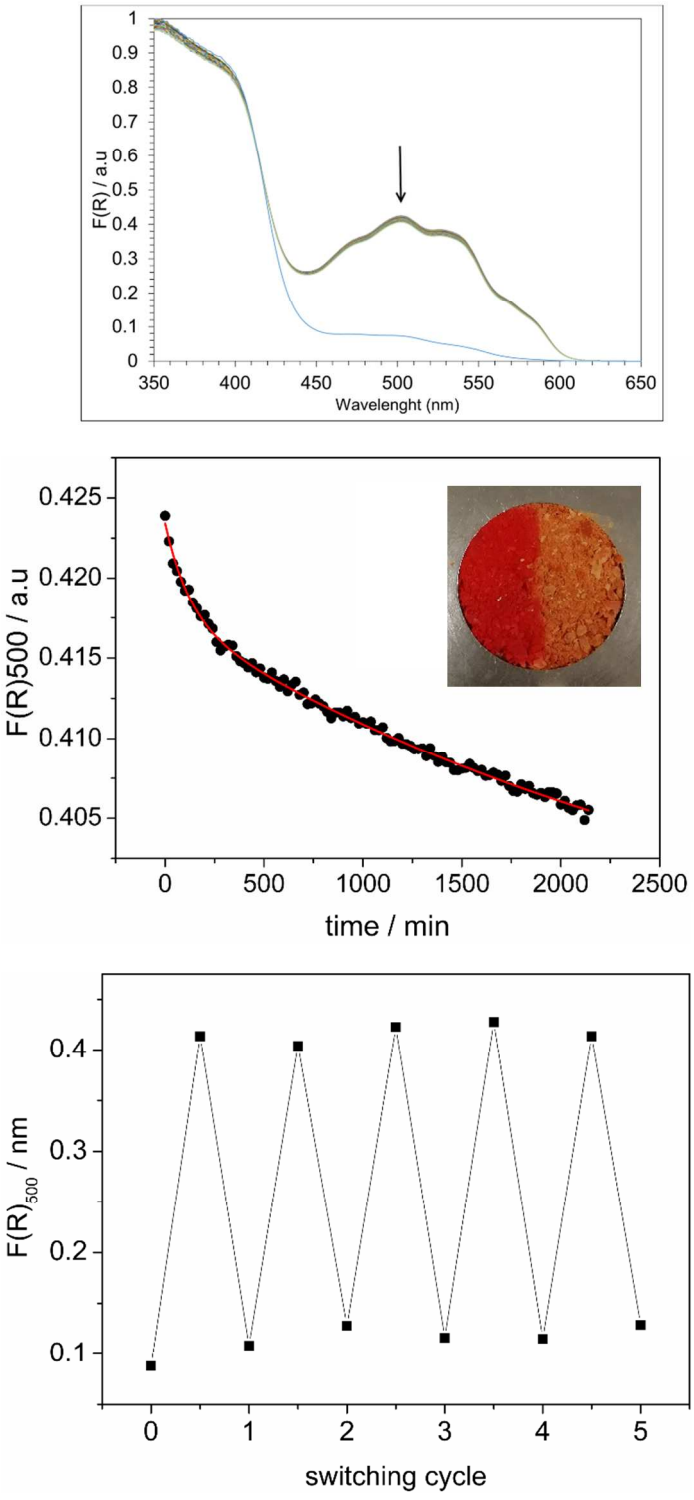

Figure S4. Diffuse reflectance spectra of **ovan3amp·12tfib** (top) showing thermal fading of the orange-red coloration. Points at 500 nm were plotted over the time and fitted by a bi-exponential curve (middle). Repeating photochemical recovery over 5 switching cycles (bottom).

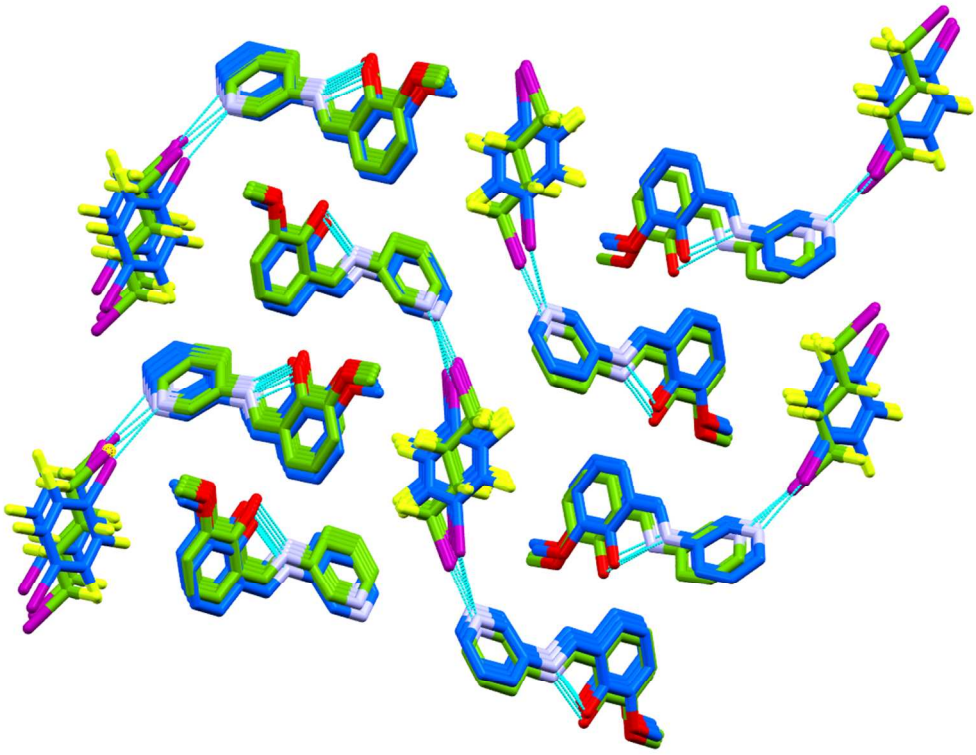

Figure S5. Superimposition of **(ovan3amp)$_2$·14tfib** (blue sticks) **and (ovan3amp)$_2$·ofib** (green sticks).

Table S2. The results of TG analysis.

Cocrystal	t_1 / °C	t_2 / °C	**%**
ovan3amp·12tfib	119	367	62.3
ovan3amp·13tfib	113	365	61.6
(ovan3amp)$_2$·14tfib	117	381	59.8
(ovan3amp)$_2$·135tfib	150	358	55.1
(ovan4amp)$_2$·12tfib	107	239	12.8
	239	390	10.2
(ovan4amp)$_2$·14tfib	118	255	20.5
	255	469	20.8
ovan4amp·135tfib	161	404	50.8

Table S3. The results of DSC analysis.

Cocrystal	t_e / °C	**ΔH / kJmol^{-1}**
ovan3amp·12tfib	92	34.09
ovan3amp·13tfib	99	0.46
	104	20.92
(ovan3amp)$_2$·14tfib	110	65.69
(ovan3amp)$_2$·135tfib	112	46.52
(ovan4amp)$_2$·12tfib	96	45.14
(ovan4amp)$_2$·14tfib	150	58.74
ovan4amp·135tfib	136	33.37

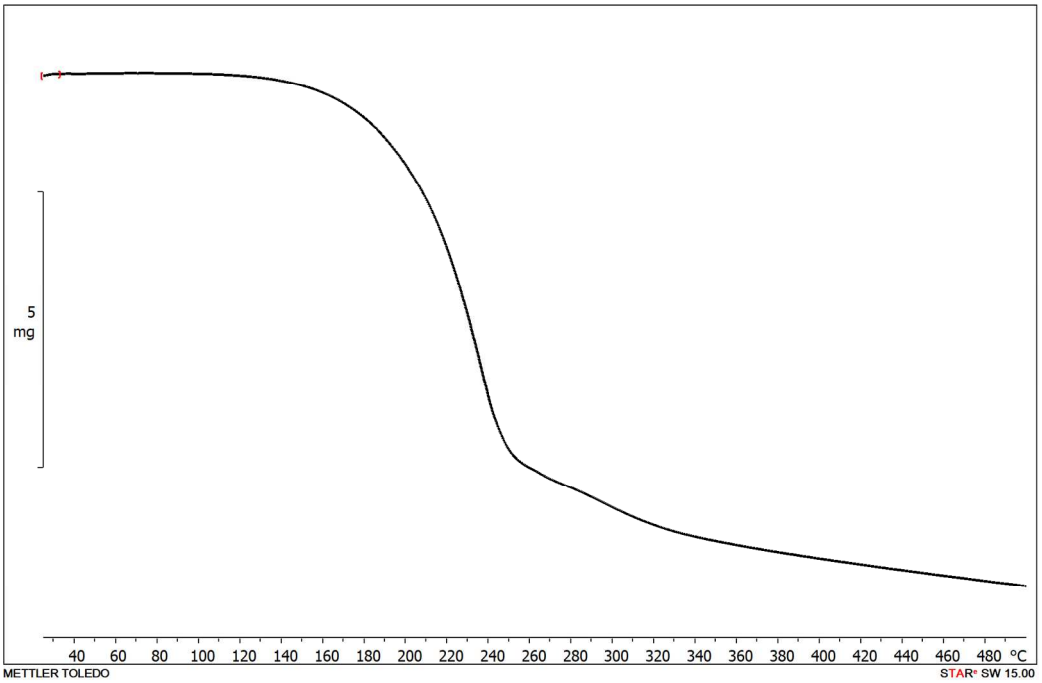

Figure S6. TG curve of the powder product of neat grinding of **ovan**, **3amp** and **12tfib** (1:1:1).

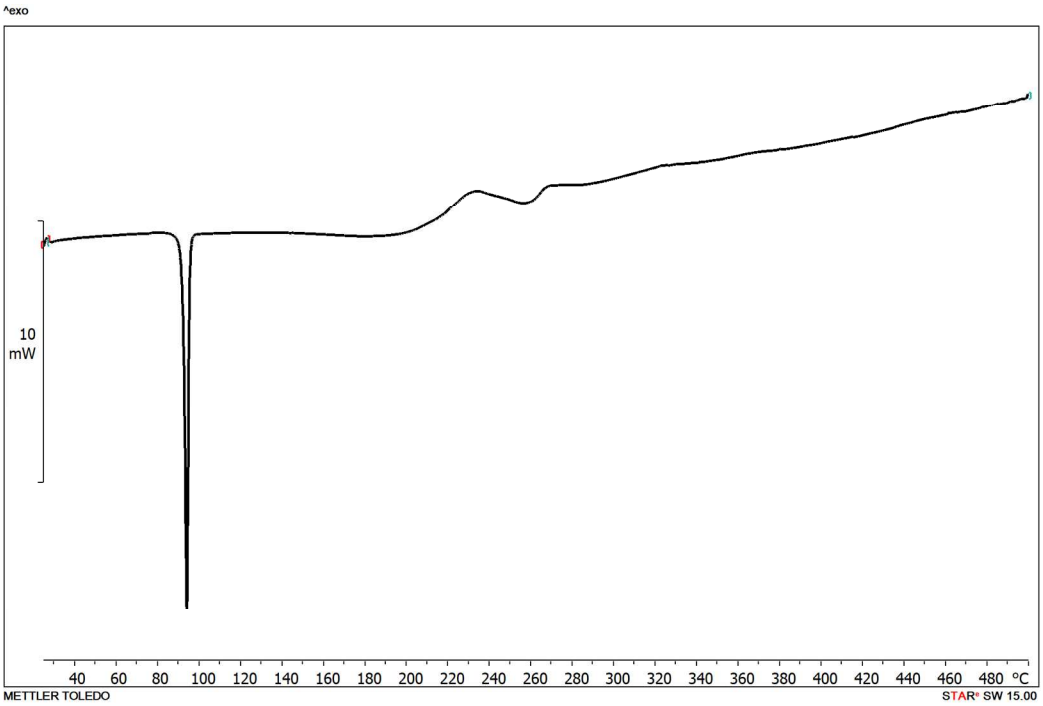

Figure S7. DSC curve of the powder product of neat grinding of **ovan**, **3amp** and **12tfib** (1:1:1).

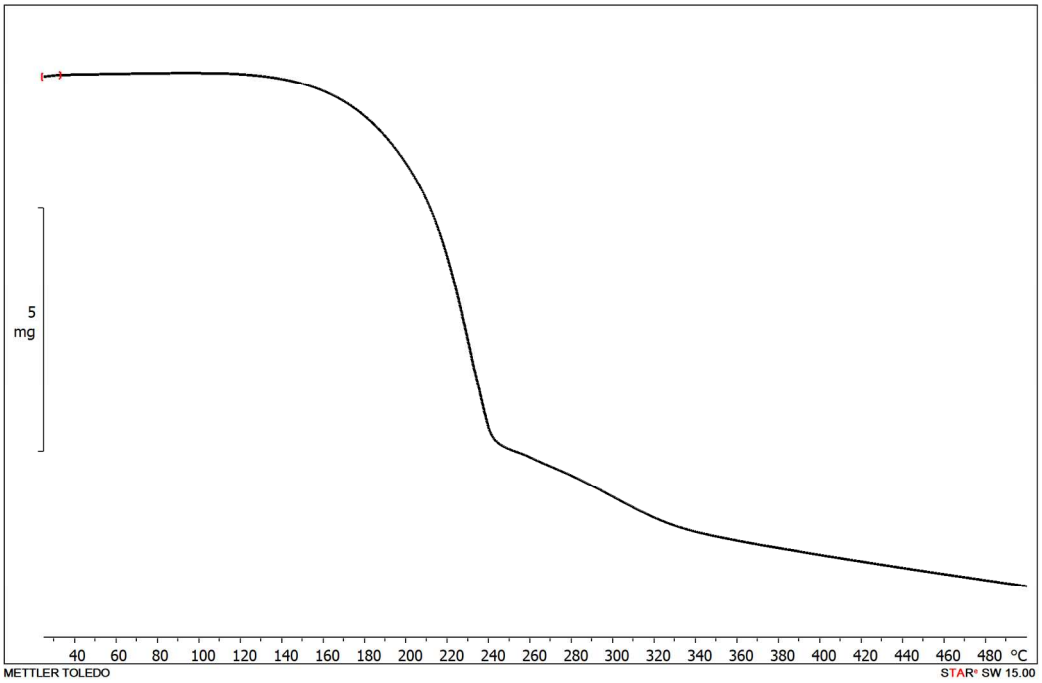

Figure S8. TG curve of the powder product of neat grinding of **ovan**, **3amp** and **13tfib** (1:1:1).

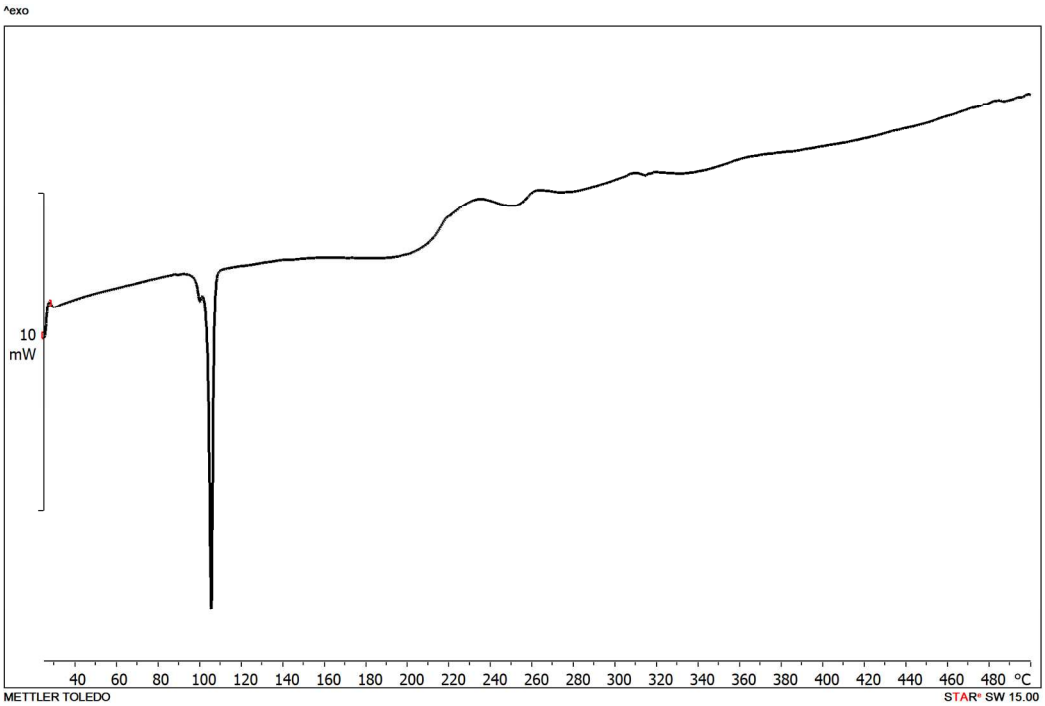

Figure S9. DSC curve of the powder product of neat grinding of **ovan**, **3amp** and **13tfib** (1:1:1).

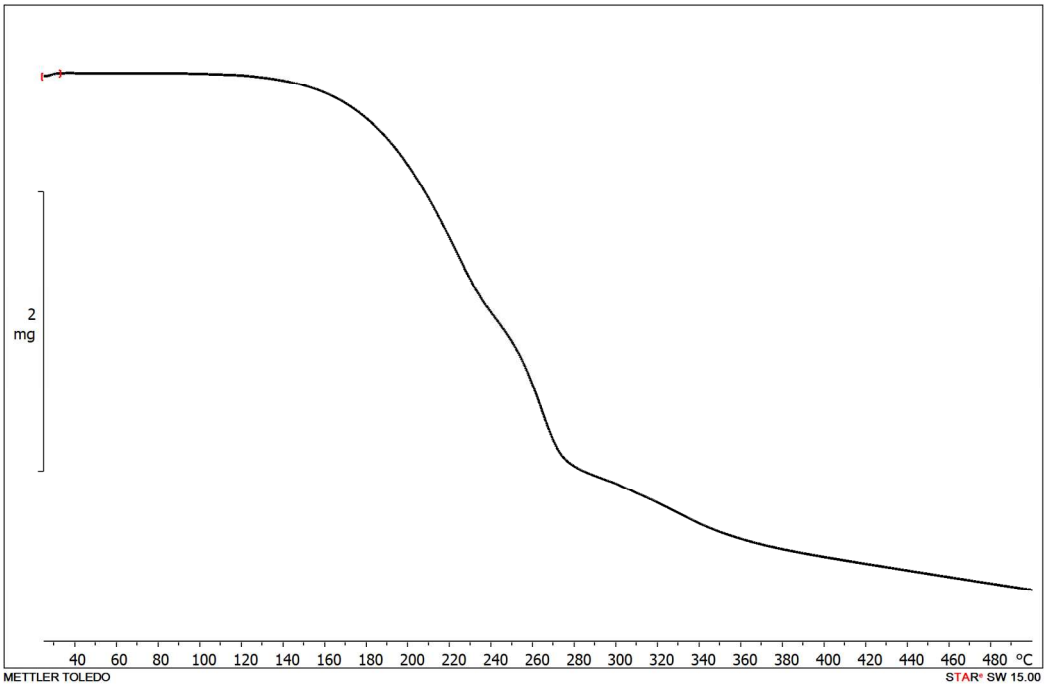

Figure S10. TG curve of the powder product of neat grinding of **ovan**, **3amp** and **14tfib** (2:2:1).

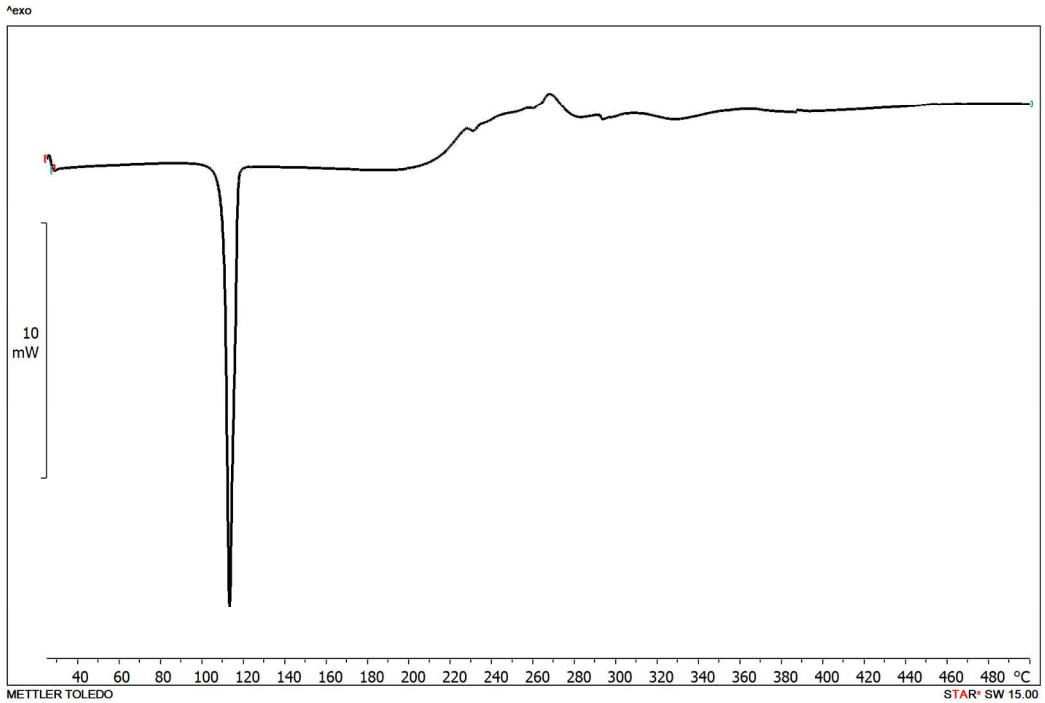

Figure S11. DSC curve of the powder product of neat grinding of **ovan**, **3amp** and **14tfib** (2:2:1).

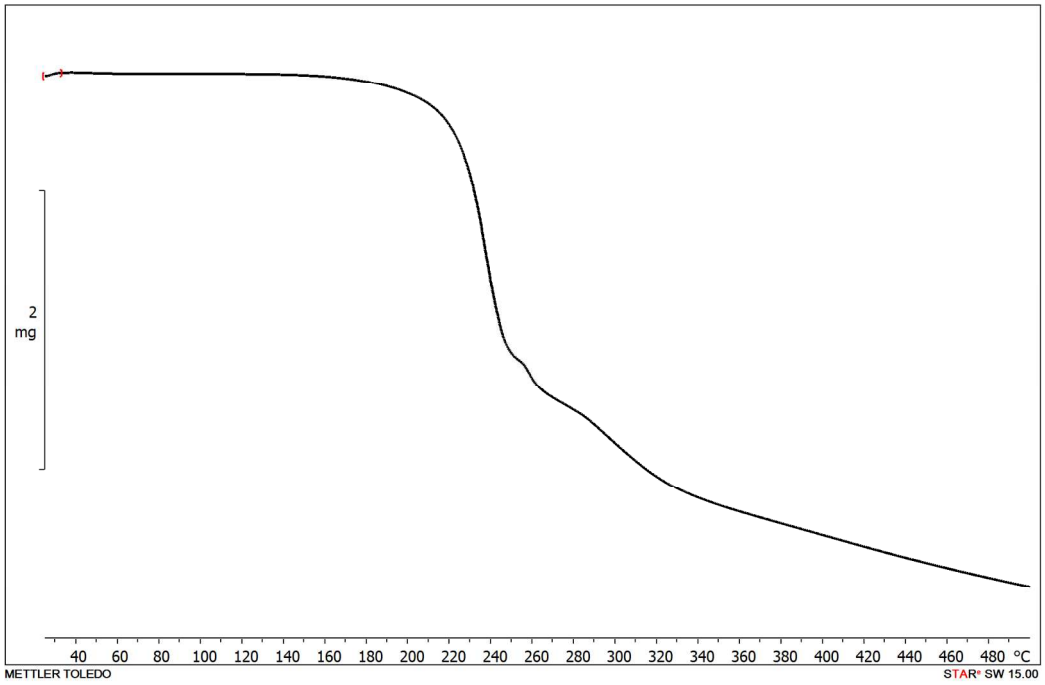

Figure S12. TG curve of the powder product of neat grinding of **ovan**, **3amp** and **135tfib** (2:2:1).

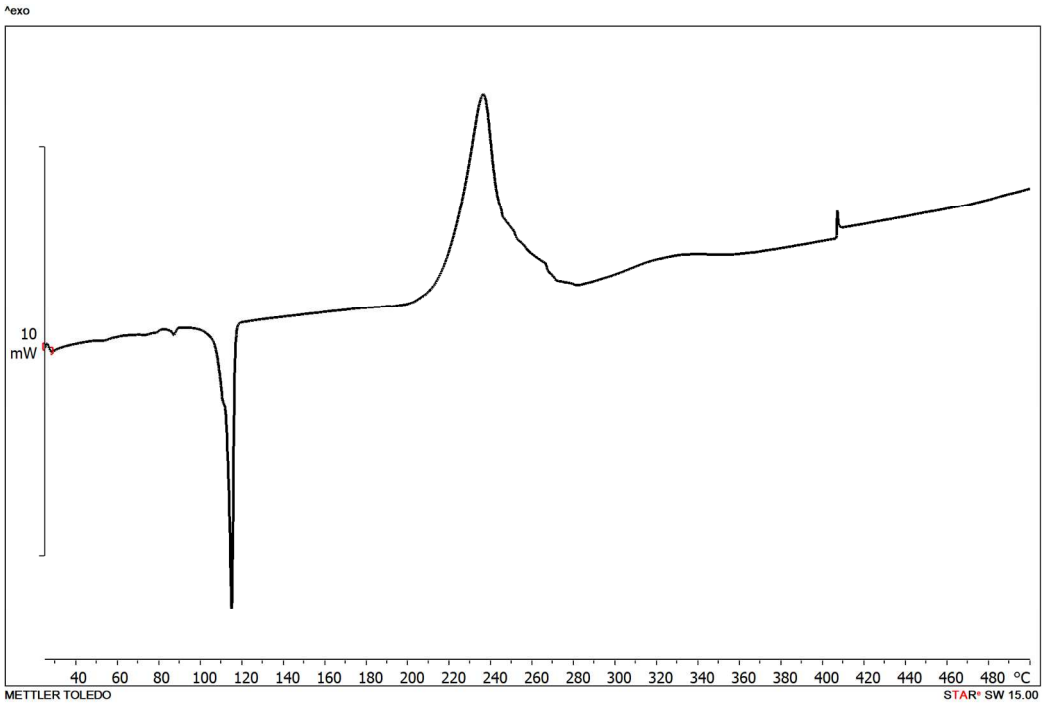

Figure S13. DSC curve of the powder product of neat grinding of **ovan**, **3amp** and **135tfib** (2:2:1).

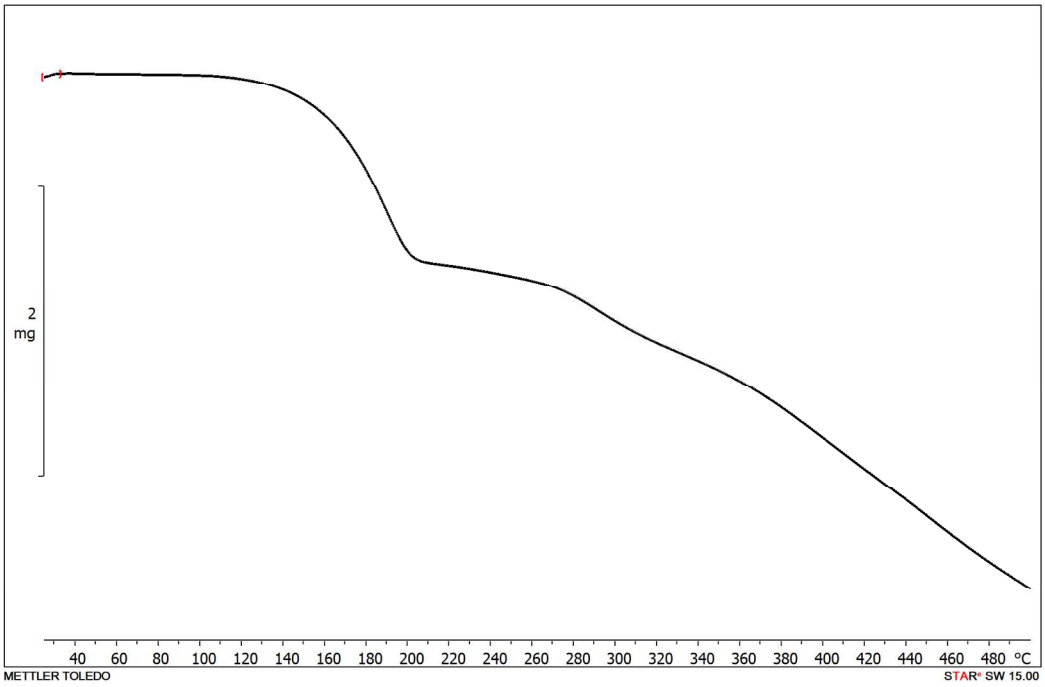

Figure S14. TG curve of the powder product of neat grinding of **ovan**, **4amp** and **12tfib** (2:2:1).

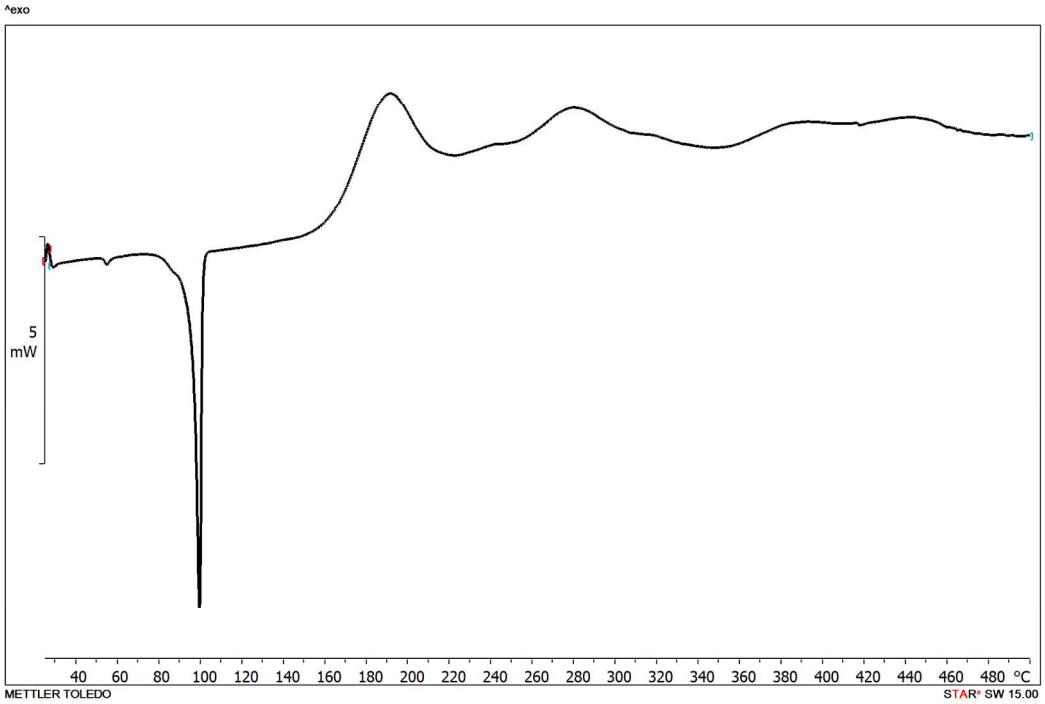

Figure S15. DSC curve of the powder product of neat grinding of **ovan**, **4amp** and **12tfib** (2:2:1).

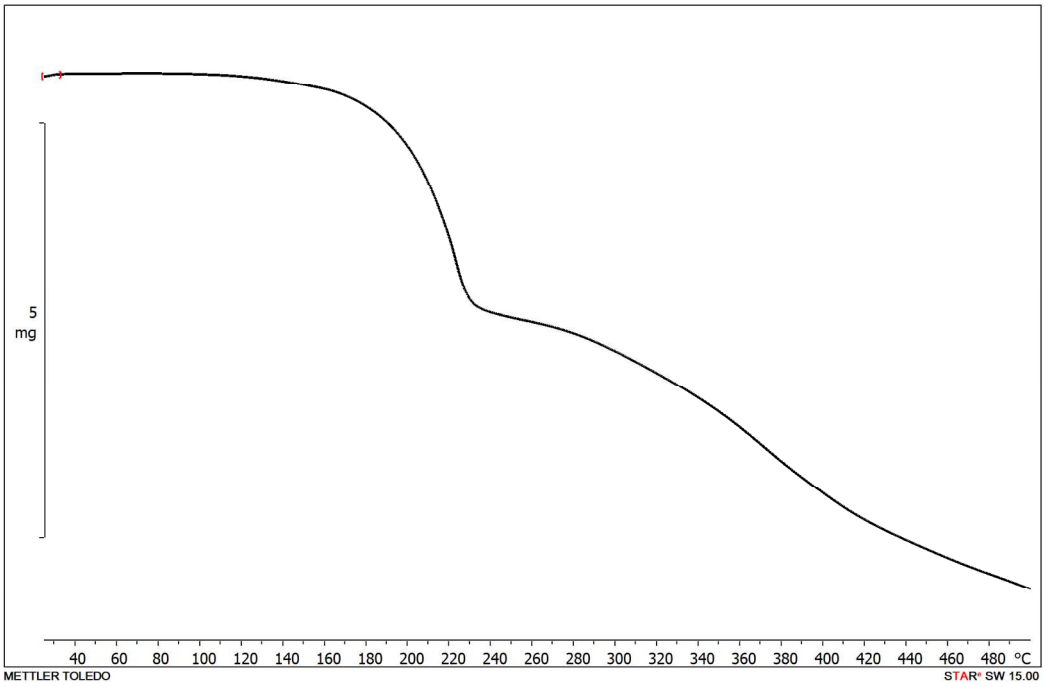

Figure S16. TG curve of the powder product of neat grinding of **ovan**, **4amp** and **14tfib** (2:2:1).

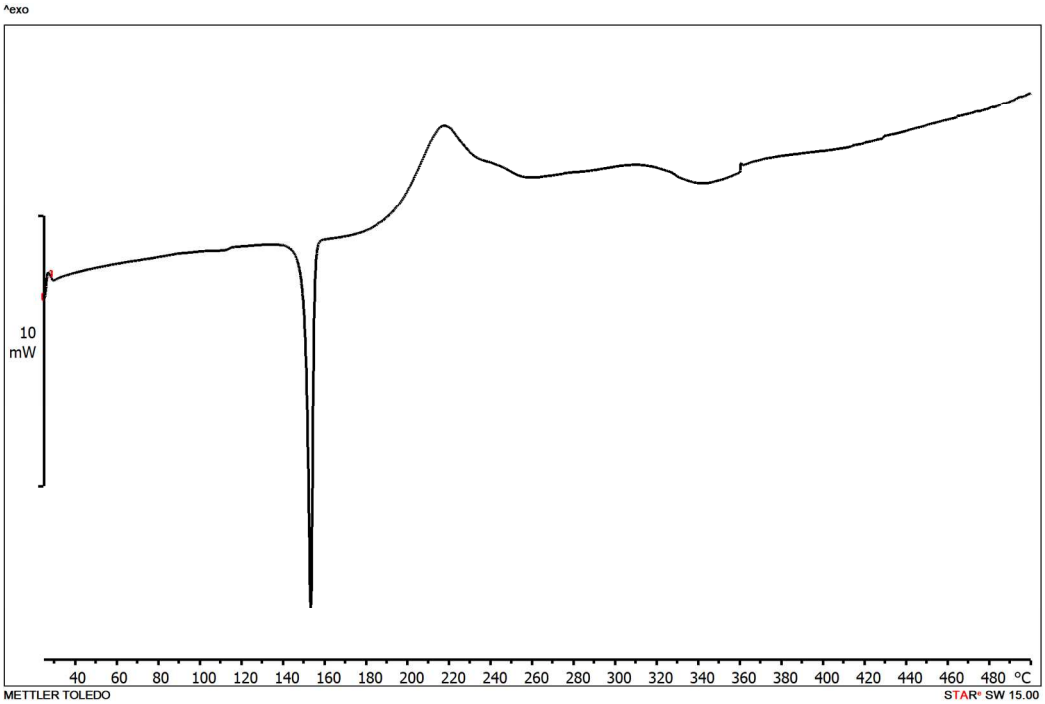

Figure S17. DSC curve of the powder product of neat grinding of **ovan**, **4amp** and **14tfib** (2:2:1).

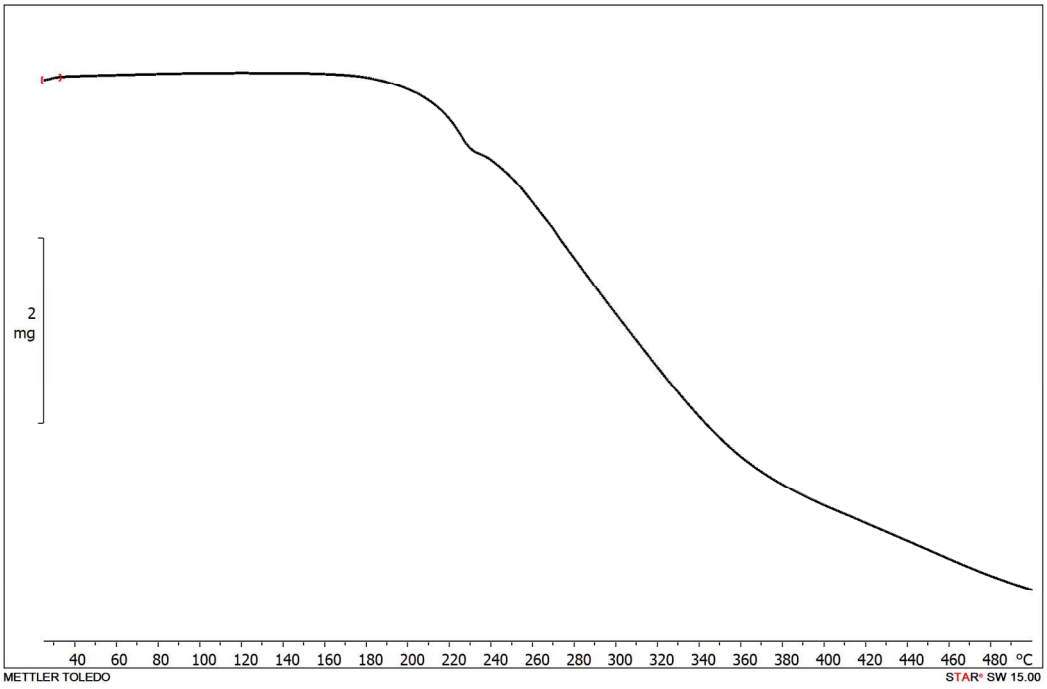

Figure S18. TG curve of the powder product of neat grinding of **ovan**, **4amp** and **135tfib** (1:1:1).

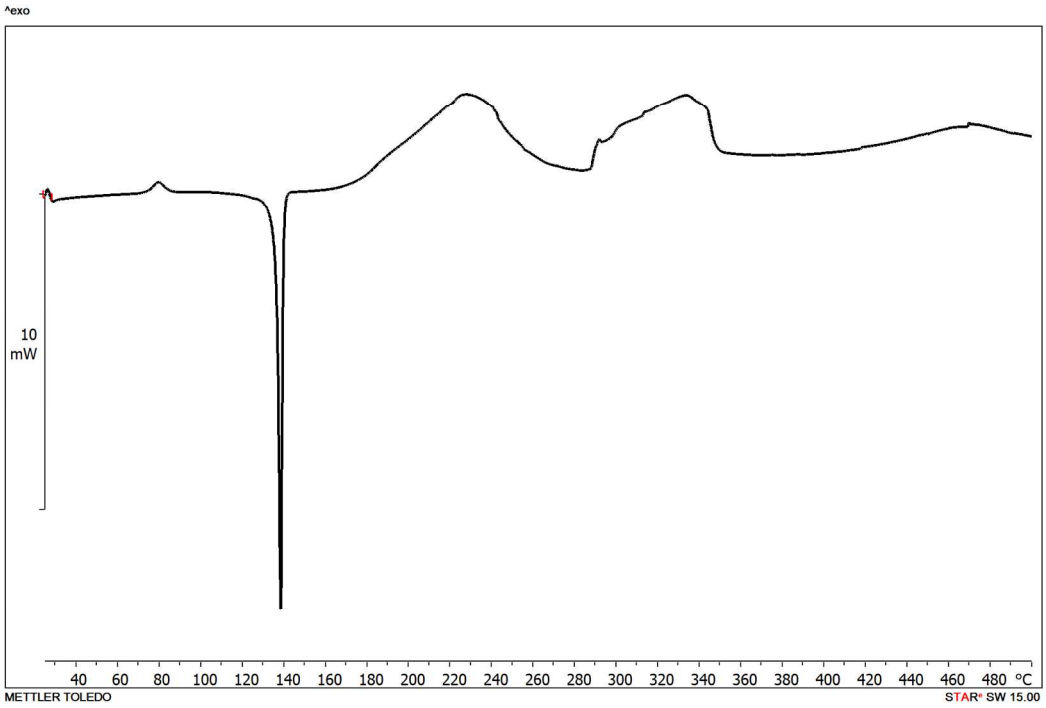

Figure S19. DSC curve of the powder product of neat grinding of **ovan**, **4amp** and **135tfib** (1:1:1).

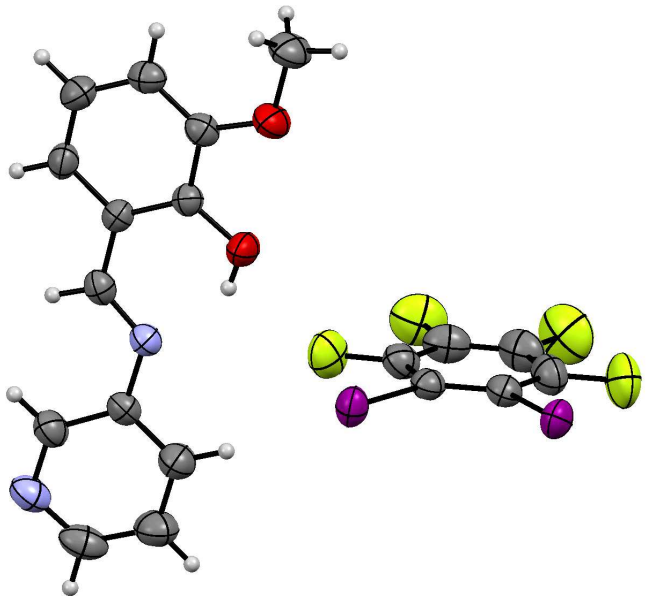

Figure S20. ORTEP diagram of **ovan3amp·12tfib**

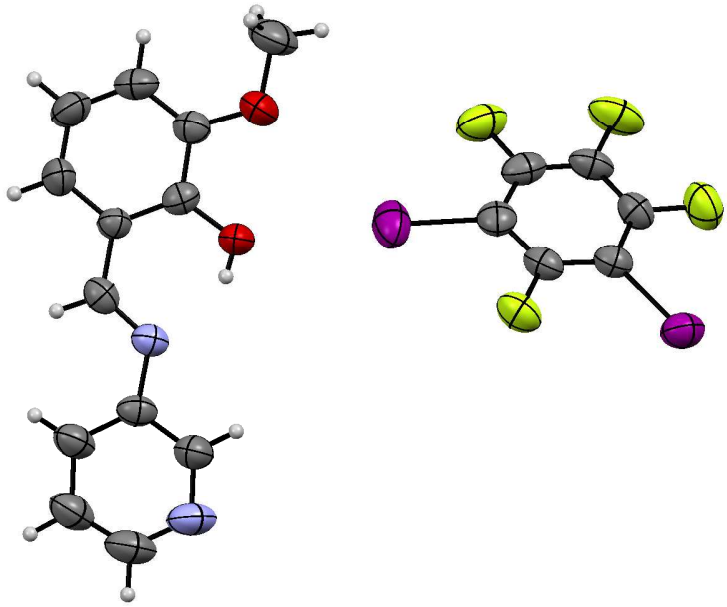

Figure S21. ORTEP diagram of **ovan3amp·13tfib**

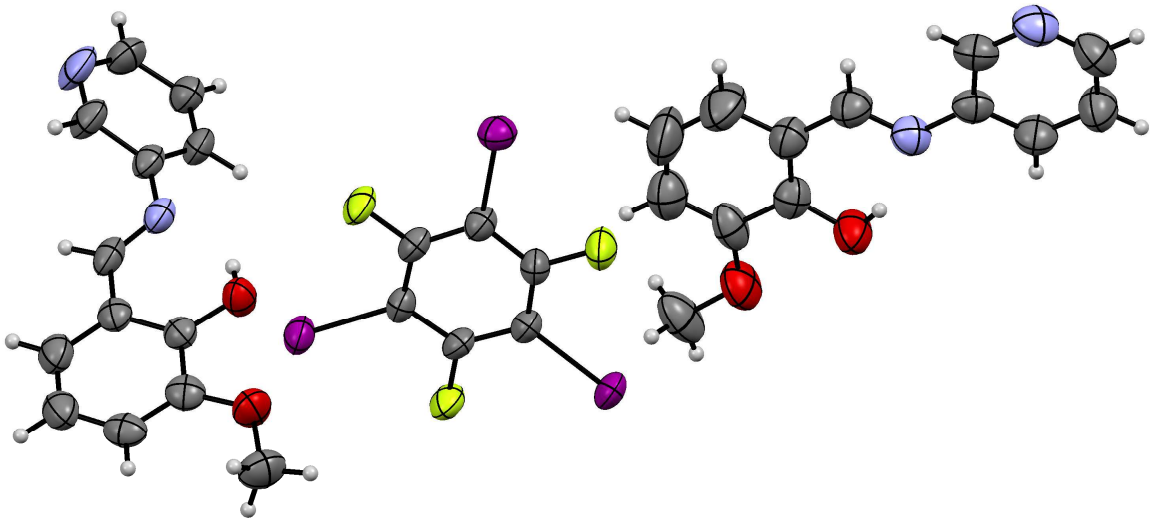

Figure S22. ORTEP diagram of **(ovan3amp)$_2$·135tfib**

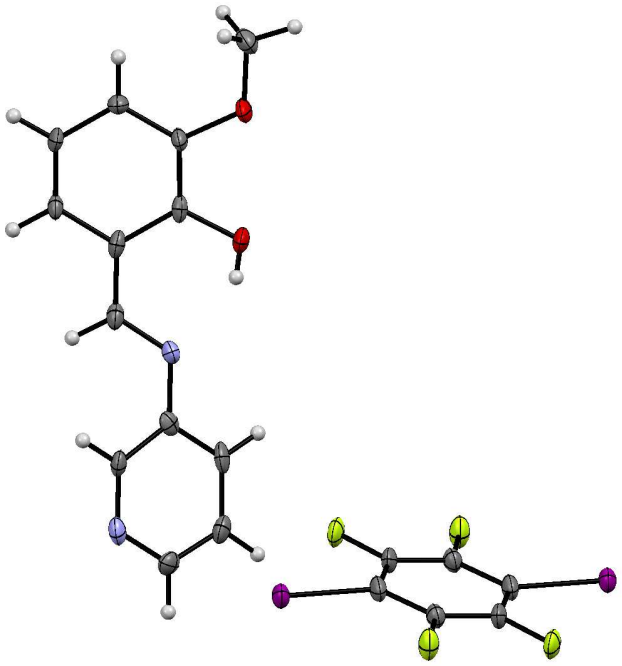

Figure S23. ORTEP diagram of **(ovan3amp)$_2$·14tfib**

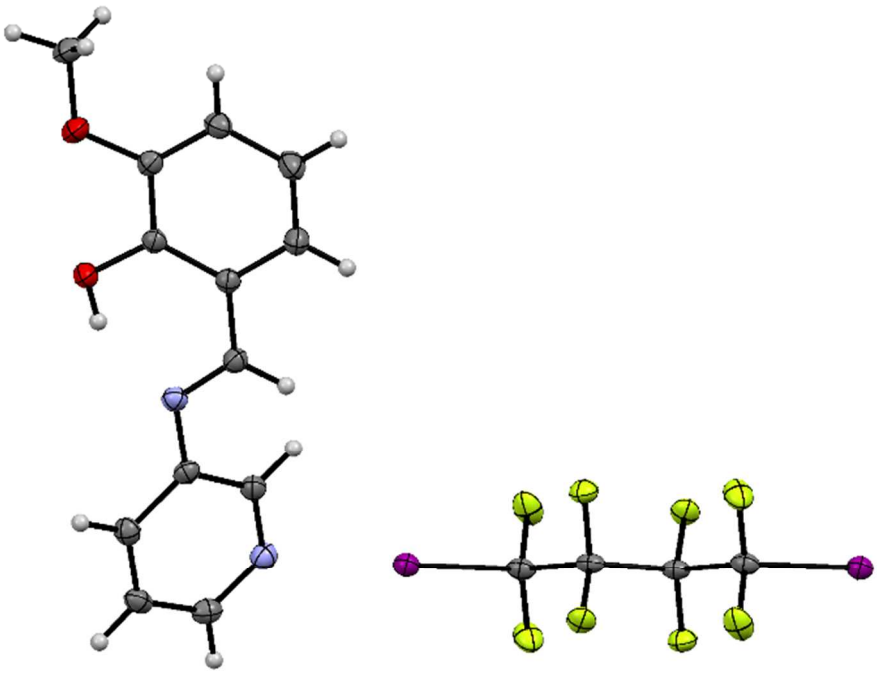

Figure S24. ORTEP diagram of **(ovan3amp)$_2$·ofib**

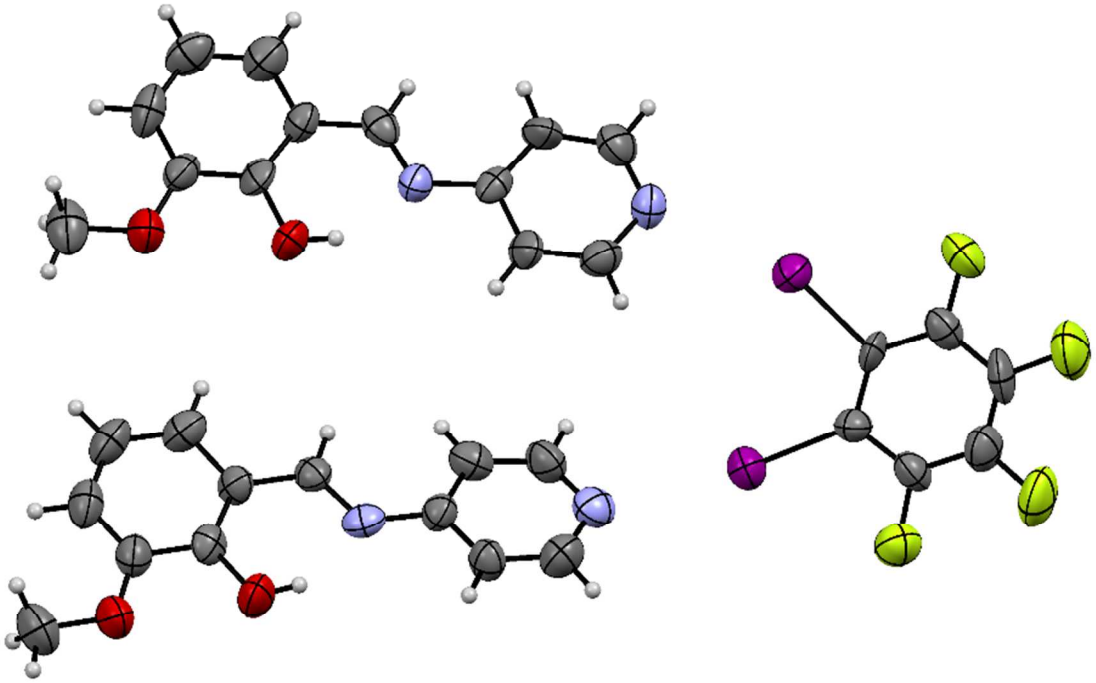

Figure S25. ORTEP diagram of **(ovan4amp)$_2$·12tfib**

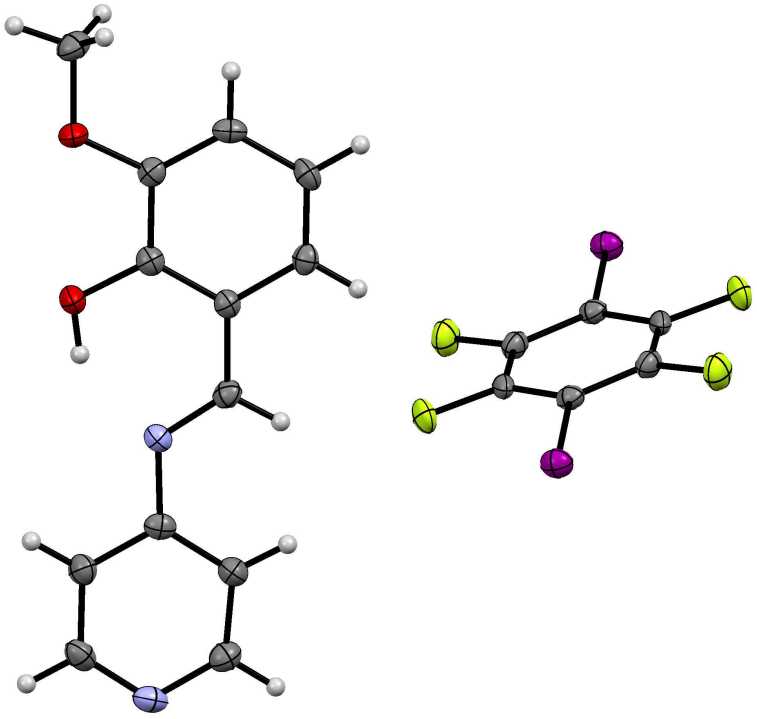

Figure S26. ORTEP diagram of **(ovan4amp)$_2$·14tfib**

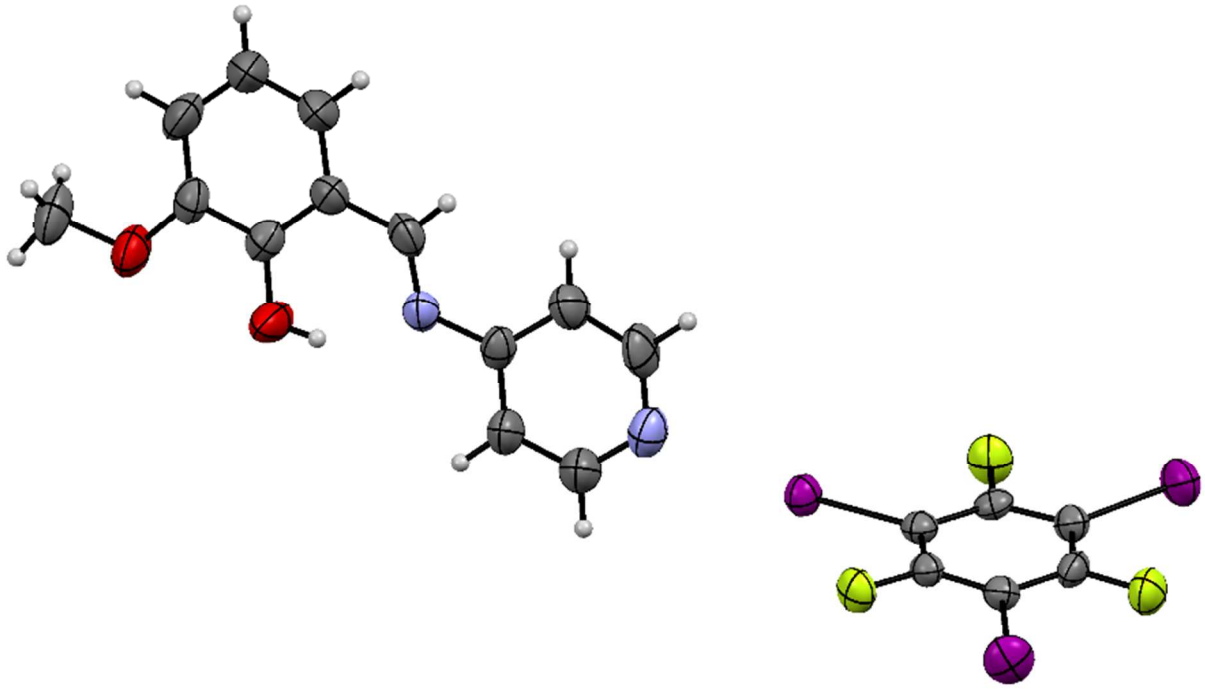

Figure S27. ORTEP diagram of **ovan4amp·135tfib**