**14N-1H HMQC solid-state NMR as a powerful tool to study amorphous formulations – an exemplary study of paclitaxel loaded polymer micelles**

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1. **PXRD experiments: raw files as recorded under ambient conditions. All experiments were recorded by Marvin Grüne supported by Dominik Heuler.**
2. POL-4-PTX (FormulationPOL-4-PTX), recorded on 24.04.2019:
	1. P2\_4\_PTX.brml
	2. P2\_4\_PTX.raw
	3. P2\_4\_PTX\_exported.xye
3. Crystalline PTX (PTXCrystalline), recorded on 01.02.2019
	1. ACP-PTX-krist.brml
	2. ACP-PTX-krist.raw
	3. ACP-PTX-krist.txt
	4. ACP-PTX-krist\_bg\_subtracted.xye (background subtracted)
	5. ACP-PTX-krist\_exported.xye
4. Amorphous PTX (PTXAmorphous), recorded on 23.01.2019
	1. ACP-PTX-amorph.brml
	2. ACP-PTX-amorph.raw
	3. ACP-PTX-amorph\_bg\_subtracted.xye
	4. ACP-PTX-amorph\_exported
5. Polymer POL (PolymerPOL), recorded on 13.12.2019
	1. Polymer-POL.brml
	2. Polymer-POL.txt
6. **NMR experiments: raw files as recorded for the compounds by Marvin Grüne supported by Ann-Christin Pöppler and Dinu Iuga. If the record date is not stated within the experimental title, it is mentioned separately.**
7. **Dipeptide β-Asp-Ala,**

**Figure S5:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_AspAla\_20180813-1

**14N-1H HMQC MAS (L6=4, 850 MHz):** 1.3mm\_AspAla\_20180813-5

**14N-1H HMQC MAS (L6=12, 850 MHz):** 1.3mm\_AspAla\_20180813-8

1. **Polymer POL**

**Figure 1a: 13CCP MAS (600 MHz):** 600b00886-126 (recorded on 24.01.2019)

**Figure 1b: 15N CP MAS (400 MHz):** MG\_BuOx (recorded on 10.12.2019, supported by R. Bertermann)

**Figure 2b:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_BuOxTg\_20190328-7

**14N-1H HMQC MAS (266.7 µs, 50 MHz):** 1.3mm\_BuOxTg\_20190328-8

**Figure S3a: 1H (D2O, 600 MHz):** 600a00746-12 (recorded on 17.08.2018)

**Figure S3b: 13C (D2O, 600 MHz):** 600a00746-11 (recorded on 16.08.2018)

**Figure S7:**

**1H-1H NOESY MAS (20 ms, 850 MHz) + extracted Row (623):** 1.3mm\_BuOxTg\_20190328-201

**1H-1H NOESY MAS (50 ms, 850 MHz) + extracted Row (623):** 1.3mm\_BuOxTg\_20190328-601

**1H-1H NOESY MAS (100 ms, 850 MHz) + extracted Row (624):** 1.3mm\_BuOxTg\_20190328-401

1. **Crystalline PTX**

**Figure 1a: 13C CP MAS (600 MHz):** 600b00555-13 (recorded on 17.05.2017)

**Figure 1b: 15N CP MAS (400 MHz):** MGr13112019-2-2 (recorded on 18.11.2019, supported by R. Bertermann)

**Figure 2a:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_PTX\_20180813-2

**14N-1H HMQC MAS (133.3 µs, 850 MHz):** 1.3mm\_PTX\_20180813-8

**14N-1H HMQC MAS (400 µs, 850 MHz):** 1.3mm\_PTX\_20180813-5

**Figure S2a: 1H (CDCl3, 600 MHz):** 600b00929-12 (recorded on 12.04.2019)

**Figure S2b: 13C (CDCl3, 600 MHz):** 600b00929-11 (recorded on 12.04.2019)

1. **Amorphous PTX**

**Figure S6:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_PTXamo\_20190327-4

**14N-1H HMQC MAS (133.3 µs, 850 MHz):** 1.3mm\_PTXamo\_20190327-3

**14N-1H HMQC MAS (266.7 µs, 850 MHz):** 1.3mm\_PTXamo\_20190327-5

1. **Formulation POL-2-PTX**

**Figure 3a:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_P2-2-PTXKIS\_20190329-8

**14N-1H HMQC MAS (133.3 µs, 850 MHz):** 1.3mm\_P2-2-PTXKIS\_20190329-9

**14N-1H HMQC MAS (266.7 µs, 850 MHz):** 1.3mm\_P2-2-PTXKIS\_20190329-11

1. **Formulation POL-4-PTX**

**Figure 3b:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_P2-4-PTX-20181023-1

**14N-1H HMQC (850 MHz):** 1.3mm-P2-4-PTX-20181023-40

1. **Formulation POL-9-PTX**

**Figure 1a: 13C CP MAS (600 MHz):** 600b0586-13 (recorded on 30.06.2017)

**Figure 1b: 15N CP MAS (850 MHz):** 4mm\_HX\_old\_sample1\_20190924-4 (recorded by. D. Iuga)

**Figure 4:**

**1H one-pulse MAS (850 MHz):** 1.3mm\_P2-9-PTX\_20180814-2

**14N-1H HMQC (850 MHz):** 1.3mm\_sample1\_20190808 (recorded by. D. Iuga)

**Figure S3a: 1H (D2O, 600 MHz):** 600a00732-20 (recorded on 03.07.2018)

**Figure S3b: 13C (D2O, 600 MHz):** 600a00732-21 (recorded on 03.07.2018)