

Overview of qNMR Standard Certified Reference Materials



1,3,5-Trimethoxybenzene

Article number: 690321

Solvent	Solubility (mg/ml)	Chemical shift (ppm)*	T1 relaxation time (s)
CDCI ₃	250	6,1 3,7	2,9 1,6
DMSO-d ₆	250	6,1 3,7	2,4 1,2
CD3OD	250	6,1 3,7	3,1 1,9
CD₃CN	250	6,1 3,7	3,4 2,0
D ₂ O	-		

*1H-NMR (δ: 0 ppm, TMS, 26°C)

Solubility tests were performed at room temperature with commercially available NMR solvents.

Tests were performed with up to 250 mg/ml. T1 relaxation times were recorded for the single CRM solution (at 26°C). In mixtures, it is recommended to check the T1 delay prior to the qNMR experiment. Chemical shifts and T1 relaxation times were recorded on a Magritek 60 MHz spectrometer.



Dimethyl sulfone

Article number:

691165

Solvent	Solubility (mg/ml)	Chemical shift (ppm)*	T1 relaxation time (s)
CDCI ₃	80	3,0	2,8
DMSO-d ₆	250	3,0	2,3
CD ₃ OD	50	3,0	3,4
CD ₃ CN	250	2,9	3,6
D ₂ O	250	2,9	5,0

*1H-NMR (δ: 0 ppm, TMS, 26°C)

Solubility tests were performed at room temperature with commercially available NMR solvents.

Tests were performed with up to 250 mg/ml. T1 relaxation times were recorded for the single CRM solution (at 26°C). In mixtures, it is recommended to check the T1 delay prior to the qNMR experiment. Chemical shifts and T1 relaxation times were recorded on a Magritek 60 MHz spectrometer.

Dimethyl terephthalate

Article number:

691155

Solvent	Solubility (mg/ml)	Chemical shift (ppm)*	T1 relaxation time (s)
CDCI ₃	160	8,1 3,9	3,2 1,5
DMSO-d ₆	14	8,1 3,9	2,4 1,1
CD₃OD	4	8,1 4,8	3,0 2,0
CD₃CN	20	8,1 3,9	3,7 2,4
D ₂ O	-	-	-

*1H-NMR (δ: 0 ppm, TMS, 26°C)

Solubility tests were performed at room temperature with commercially available NMR solvents.

Tests were performed with up to 250 mg/ml. T1 relaxation times were recorded for the single CRM solution (at 26°C). In mixtures, it is recommended to check the T1 delay prior to the qNMR experiment. Chemical shifts and T1 relaxation times were recorded on a Magritek 60 MHz spectrometer.



Ethylene carbonate

Article	number:	
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Solubility (mg/ml)	Chemical shift (ppm)*	T1 relaxation time (s)
255	4,5	3,8
255	4,5	4,2
245	4,5	3,8
250	4,5	4,6
250		
	Solubility (mg/ml) 255 255 245 250	Solubility (mg/ml) Chemical shift (ppm)* 255 4,5 255 4,5 245 4,5 250 4,5

*1H-NMR (δ: 0 ppm, TMS, 26°C)

Solubility tests were performed at room temperature with commercially available NMR solvents. Tests were performed with up to 255 mg/ml. T1 relaxation times were recorded for the single CRM solution (at 26°C). In mixtures, it is recommended to check the T1 delay prior to the qNMR experiment. Chemical shifts and T1 relaxation times were recorded on a Magritek 60 MHz spectrometer.

Maleic acid

Article number:

691772

691573

Solvent	Solubility (mg/ml)	Chemical shift (ppm)*	T1 relaxation time (s)
CDCI ₃	-		
DMSO-d ₆	250	6,3	1,2
CD ₃ OD	10	6,3	2,9
CD ₃ CN	20	6,4	3,8
D ₂ O	250	6,4	3,8

*1H-NMR (δ: 0 ppm, TMS, 26°C)

Solubility tests were performed at room temperature with commercially available NMR solvents.

Tests were performed with up to 250 mg/ml. T1 relaxation times were recorded for the single CRM solution (at 26°C). In mixtures, it is recommended to check the T1 delay prior to the qNMR experiment. Chemical shifts and T1 relaxation times were recorded on a Magritek 60 MHz spectrometer.

Version	Reason for Change	Date
1	Initial Version	11 Mar 2024