



16:59:22 28-05-2021

Description

50mM cyclosporin in Benzene-d6 (Example 1)

Experiment Information

Sweep Width (Hz)	5494.51
Sweep Width (ppm)	10.9861
Transmitter Offset (Hz)	2249.21
Transmitter Offset (ppm)	4.49722
Transmitter Frequency (MHz)	500.132
Basic Frequency (MHz)	500.13
Nucleus	^{1}H

Filter region (Hz): 2644.19 - 2593.21 Filter region (ppm): 5.28697 - 5.18505

Result

m	a _m	ϕ_m (rad)	f _m (Hz)	f _m (ppm)	$\eta_m~(\mathrm{s}^{-1})$	ſ	5/ 5
1	1.5945×10^{4}	0.029904	2.6019×10^{3}	5.2023	7.371	1.4467×10^{9}	0.274
	\pm 80.299	$\pm~9.0154 \times 10^{-3}$	$\pm~9.4141 \times 10^{-3}$	$\pm\ 1.8823 imes 10^{-5}$	$\pm \ 0.043436$	-	_
2	3.2978×10^4	6.343×10^{-3}	2.6093×10^{3}	5.2172	6.7376	3.023×10^{9}	0.57253
	$\pm \ 206.9$	$\pm 3.5484 \times 10^{-3}$	$\pm\ 2.1995 \times 10^{-3}$	$\pm 4.3979 \times 10^{-6}$	$\pm\ 0.034551$	-	-
3	1.5949×10^4	8.2753×10^{-3}	2.6116×10^{3}	5.2218	7.4847	1.4446×10^9	0.27359
	± 308.45	$\pm \ 0.012671$	$\pm~8.2016 \times 10^{-3}$	$\pm~1.6399 \times 10^{-5}$	± 0.093504	-	_

4	1.9198×10^{4}	8.7189×10^{-4}	2.6167×10^{3}	5.2319	8.4204	1.7155×10^{9}	0.32489
	± 199.66	$\pm~9.4538 \times 10^{-3}$	$\pm\ 0.011157$	$\pm\ 2.2309 \times 10^{-5}$	$\pm\ 0.070405$	-	-
5	2.9948×10^4	-3.8286×10^{-3}	2.619×10^{3}	5.2366	6.3228	2.765×10^{9}	0.52367
	± 205.49	$\pm~6.0139 \times 10^{-3}$	$\pm~4.5162 \times 10^{-3}$	$\pm~9.0299 \times 10^{-6}$	$\pm \ 0.034655$	-	-
6	708.57	3.7992×10^{-3}	2.6219×10^{3}	5.2424	5.6154	6.6293×10^{7}	0.012555
	\pm 122.71	$\pm 9.0038 \times 10^{-3}$	$\pm \ 0.074974$	$\pm~1.4991 \times 10^{-4}$	$\pm~0.82271$	-	-
7	2.1844×10^4	-9.6734×10^{-3}	2.6262×10^{3}	5.2509	8.6988	1.9445×10^9	0.36827
	$\pm\ 111.5$	$\pm\ 5.0574 imes 10^{-3}$	$\pm~6.8436 imes 10^{-3}$	$\pm~1.3684 imes 10^{-5}$	$\pm \ 0.050882$	-	-
8	673.59	3.4037×10^{-3}	2.6299×10^{3}	5.2584	5.2998	6.3426×10^7	0.012012
	± 76.526	$\pm 5.3405 \times 10^{-3}$	$\pm \ 0.068378$	$\pm 1.3672 \times 10^{-4}$	$\pm \ 0.63093$	-	-
9	4.6997×10^3	-2.8134×10^{-3}	2.6365×10^{3}	5.2715	7.0852	4.2836×10^{8}	0.081127
	\pm 59.003	$\pm 4.1243 \times 10^{-3}$	$\pm \ 0.014385$	$\pm 2.8763 \times 10^{-5}$	\pm 0.11783	-	-

Estimation performed using NMR-EsPy.

Author: Simon Hulse For more information:



https://nmr-espy.readthedocs.io/en/1.0.0rc1/



https://github.com/foroozandehgroup/NMR-EsPy



simon.hulse@chem.ox.ac.uk

If used in a publication, please cite:

No references yet...