NMR-ESPY

23:35:27 09-06-22
Andrographolide dataset

Experiment Information

Parameter	F1
Nucleus	^{1}H
Transmitter Frequency (MHz)	500.13
Sweep Width (Hz)	5000
Sweep Width (ppm)	9.9974
Transmitter Offset (Hz)	2000.5
Transmitter Offset (ppm)	4

6.665 - 6.590 ppm

Osc.	a	ϕ (°)	f(Hz)	f(ppm)	η(s^{-1})	$\int$
1	37.191 ±0.206 68	2.0261 ±0.318 41	3.3073×10^{3} $\pm 3.0833 \times 10^{-3}$	6.6128 $\pm 6.165 \times 10^{-6}$	4.8784 $\pm 1.9373 \times 10^{-2}$	1.6722
2	63.456 ±0.272 45	1.9139 ±0.246	3.309×10^{3} $\pm 3.3199 \times 10^{-3}$	6.6162 $\pm 6.6381 \times 10^{-6}$	6.6805 $\pm 2.086 \times 10^{-2}$	2.7541
3	94.14 ±0.244 48	1.2418 ±0.1488	3.3141×10^{3} $\pm 1.443 \times 10^{-3}$	6.6264 $\pm 2.8852 \times 10^{-6}$	5.0848 $\pm 9.0664 \times 10^{-3}$	4.2135
4	117.72 ±0.273 18	0.8198 ±0.132 96	3.3158×10^{3} $\pm 1.5008 \times 10^{-3}$	6.6299 $\pm 3.0009 \times 10^{-6}$	5.8845 $\pm 9.4301 \times 10^{-3}$	5.1836

5	58.877 ±0.303 98	0.159 39 ±0.295 82	3.3209×10^{3} $\pm 3.6855 \times 10^{-3}$	6.6401 $\pm 7.3691 \times 10^{-6}$	6.5374 $\pm 2.3157 \times 10^{-2}$	2.5618
6	46.45 ±0.254 39	0.184 52 ±0.313 78	3.3227×10^{3} $\pm 3.4428 \times 10^{-3}$	6.6436 $\pm 6.8837 \times 10^{-6}$	5.7537 $\pm 2.1632 \times 10^{-2}$	2.0505

2.380 - 2.280 ppm

Osc.	a	ϕ (°)	f(Hz)	f(ppm)	$\eta(s^{-1})$	$\int$
1	51.184 ±0.470 98	1.1676 ±0.527 23	1.1533×10^{3} $\pm 6.3549 \times 10^{-3}$	2.306 $\pm 1.2707 \times 10^{-5}$	7.6739 $\pm 3.9929 \times 10^{-2}$	2.1863
2	69.706 ±1.5469	0.886 73 ±1.2715	1.1556×10^{3} $\pm 1.298 \times 10^{-2}$	2.3106 $\pm 2.5953 \times 10^{-5}$	7.9588 $\pm 8.1556 \times 10^{-2}$	2.9649
3	68.13 ±1.568	0.488 38 ±1.3187	1.1574×10^{3} $\pm 1.3249 \times 10^{-2}$	2.3143 $\pm 2.6491 \times 10^{-5}$	7.8995 $\pm 8.3246 \times 10^{-2}$	2.9004
4	53.452 ±0.501 69	-4.0107×10^{-2} ±0.537 76	1.1598×10^{3} $\pm 5.7548 \times 10^{-3}$	2.319 $\pm 1.1506 \times 10^{-5}$	6.9911 $\pm 3.6158 \times 10^{-2}$	2.3079
5	46.805 ±0.395 98	1.0755 ±0.484 73	1.166×10^{3} $\pm 5.2471 \times 10^{-3}$	2.3314 $\pm 1.0491 \times 10^{-5}$	6.6178 $\pm 3.2969 \times 10^{-2}$	2.0336
6	64.016 ±1.4015	0.3593 ±1.2544	1.1685×10^{3} $\pm 1.2481 \times 10^{-2}$	2.3364 $\pm 2.4955 \times 10^{-5}$	7.7368 $\pm 7.8419 \times 10^{-2}$	2.7319
7	55.995 ±1.4453	0.128 28 ±1.4789	1.1703×10^{3} $\pm 1.4689 \times 10^{-2}$	2.34 $\pm 2.937 \times 10^{-5}$	7.69 $\pm 9.2292 \times 10^{-2}$	2.3912
8	44.148 ±0.442 18	−0.171 26 ±0.573 87	1.1726×10^{3} $\pm 6.884 \times 10^{-3}$	2.3446 $\pm 1.3764 \times 10^{-5}$	7.5003 $\pm 4.3253 \times 10^{-2}$	1.8908

1.430 - 1.290 ppm

Osc.	a	ϕ (°)	f(Hz)	f(ppm)	$\eta(s^{-1})$	$\int$
1	29.779 ±0.109 86	0.400 49 ±0.211 38	657.12 $\pm 4.8573 \times 10^{-3}$	1.3139 $\pm 9.7119 \times 10^{-6}$	8.4864 $\pm 3.0519 \times 10^{-2}$	1.2572
2	33.191 ±0.119 99	0.332 46 ±0.207 13	661.28 $\pm 4.3471 \times 10^{-3}$	1.3222 $\pm 8.6919 \times 10^{-6}$	8.1158 $\pm 2.7314 \times 10^{-2}$	1.4085

3	86.337 ±0.1284	−0.201 01 $\pm 8.5209 \times 10^{-2}$	670.12 $\pm 1.7721 \times 10^{-3}$	1.3399 $\pm 3.5433 \times 10^{-6}$	8.2588 $\pm 1.1134 \times 10^{-2}$	3.6565
4	85.676 ±0.125 97	−0.563 65 $\pm 8.4239 \times 10^{-2}$	674.31 $\pm 1.68 \times 10^{-3}$	1.3483 $\pm 3.3591 \times 10^{-6}$	7.9341 $\pm 1.0556 \times 10^{-2}$	3.6455
5	82.459 ±0.132 49	3.4106×10^{-2} $\pm 9.2058 \times 10^{-2}$	683.14 $\pm 1.8853 \times 10^{-3}$	1.3659 $\pm 3.7696 \times 10^{-6}$	8.2456 $\pm 1.1846 \times 10^{-2}$	3.4929
6	79.721 ±0.132 26	−0.961 47 $\pm 9.5056 \times 10^{-2}$	687.31 $\pm 1.9808 \times 10^{-3}$	1.3743 $\pm 3.9605 \times 10^{-6}$	8.3566 $\pm 1.2446 \times 10^{-2}$	3.3716
7	27.021 ±0.115 68	−0.321 33 ±0.2453	696.16 $\pm 5.1493 \times 10^{-3}$	1.392 $\pm 1.0296 \times 10^{-5}$	8.0118 $\pm 3.2354 \times 10^{-2}$	1.1484
8	23.519 ±0.102 87	−0.829 78 ±0.250 59	700.29 $\pm 5.4969 \times 10^{-3}$	1.4002 $\pm 1.0991 \times 10^{-5}$	7.9849 $\pm 3.4538 \times 10^{-2}$	1

Estimation performed using NMR-EsPy.
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For more information:


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


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


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If used in a publication, please cite:

Simon G. Hulse, Mohammadali Foroozandeh. *"Newton meets Ockham: Parameter estimation and model selection of NMR data with NMR-EsPy"*. J. Magn. Reson. 338 (2022) 107173.
https://doi.org/10.1016/j.jmr.2022.107173