3,3'-(4,11-bis(4-(trifluoromethyl)benzyl)-1,4,8,11-tetraazacyclotetradecane-1,8-diyl)dipropanenitrile

Inês M. Nunes [1,2], Elisabete R. Silva [2] and Luis G. Alves [3,*]

[1] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal

[2] BioISI - Biosystems & Integrative Sciences Institute, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal

[3] Centro de Química Estrutural – Institute of Molecular Sciences, Associação do Instituto Superior Técnico para a Investigação e Desenvolvimento, Av. António José de Almeida, 1000-043 Lisboa, Portugal

* Correspondence: luis.g.alves@tecnico.ulisboa.pt (L.G.A.)

Table S1. Relevant C-H$\cdots$N hydrogen bond distances (Å) and angles (°) of compound **2**.

C-H$\cdots$N	d(C-H)	d(H$\cdots$N)	d(C$\cdots$N)	(CĤN)	Symmetry operation
C(1)-H(1A)$\cdots$N(3)	0.989	2.520	3.444	155.39	½-x, ½-y, -z
C(11)-H(11)$\cdots$N(3)	0.949	2.731	3.473	135.57	½-x, -½-y, -z
C(15)-H(15A)$\cdots$N(3)	0.990	2.645	3.314	125.09	½-x, ½-y, -z

Table S2. Crystal data and details of structure refinement for compound **2**.

Empirical formula	$C_{32}H_{40}F_6N_6$
Formula weight	622.70
Temperature (K)	150(2)
Crystal system, space group	Monoclinic, C2/c
a, (Å)	25.328(2)
b, (Å)	5.7081(5)
c, (Å)	24.491(2)
α, (°)	90
β, (°)	118.384(4)
γ, (°)	90
Volume (Å^3)	3115.1(5)
Z	4
Calculated density (g / cm^3)	1.328
Absorption coefficient (mm^{-1})	0.105
F (000)	1312
Crystal size (mm)	0.060 x 0.100 x 0.180
θ range for data collection (°)	1.905 – 27.180
Limiting indices	-32 ≤ h ≤ 32, -7 ≤ k ≤ 7, -26 ≤ l ≤ 31
Reflections collected/unique	10078 / 3475 [R_{int} = 0.0579]
Completeness to θ = 25.242	99.9 %
Data / restraints / parameters	3457 / 0 / 199
Goodness-of-fit on F^2	1.050
Final R indices [I > 2σ(I)][a]	R_1 = 0.0642, wR_2 = 0.1533
Final R indices (all data)[a]	R_1 = 0.1257, wR_2 = 0.1729
Largest diff. peak and hole (e A^{-3})	0.674 and -0.397

[a] $R_1 = \Sigma\,||F_0|\,-|F_c||\,/\,\Sigma\,|F_0|$; $wR_2 = \{\Sigma[w(F^2_0 - F^2_c)^2]/\,\Sigma[w(F^2_0)^2]\}^{1/2}$
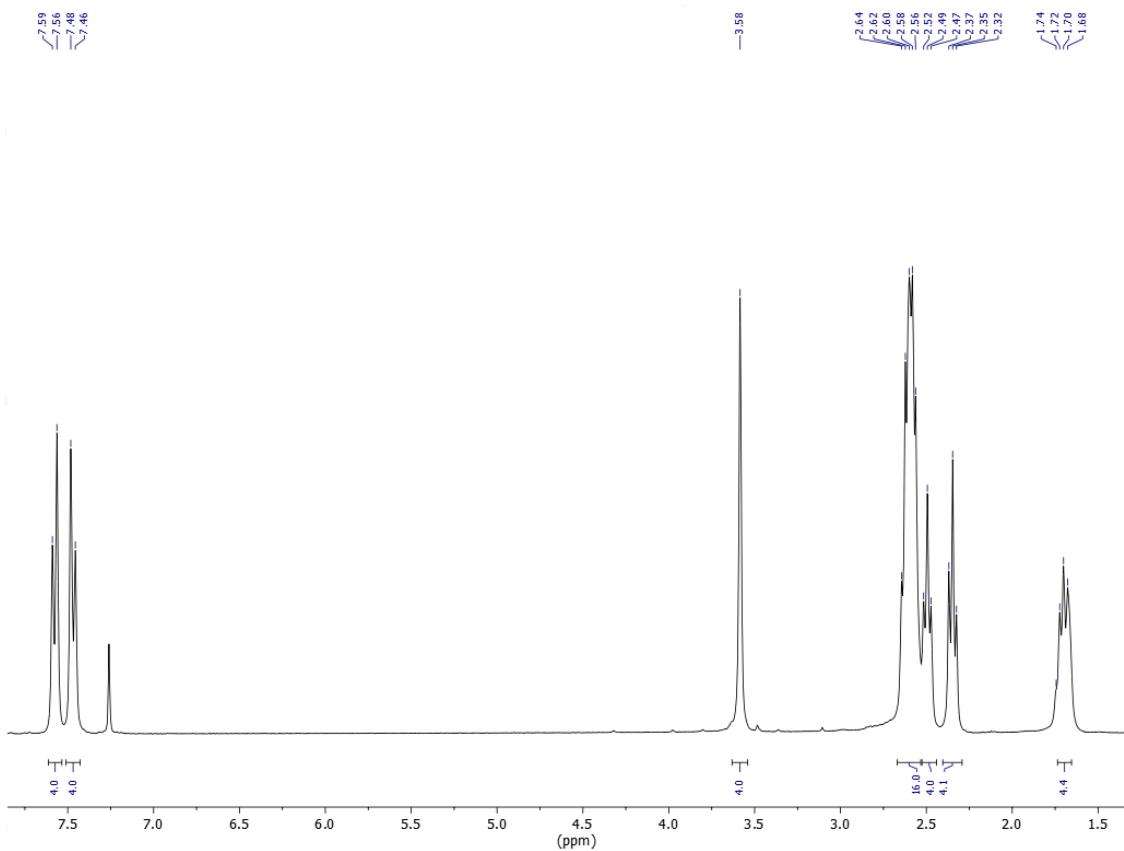
Figure S1. ^{1}H NMR spectrum of compound **2** in CHCl$_3$.
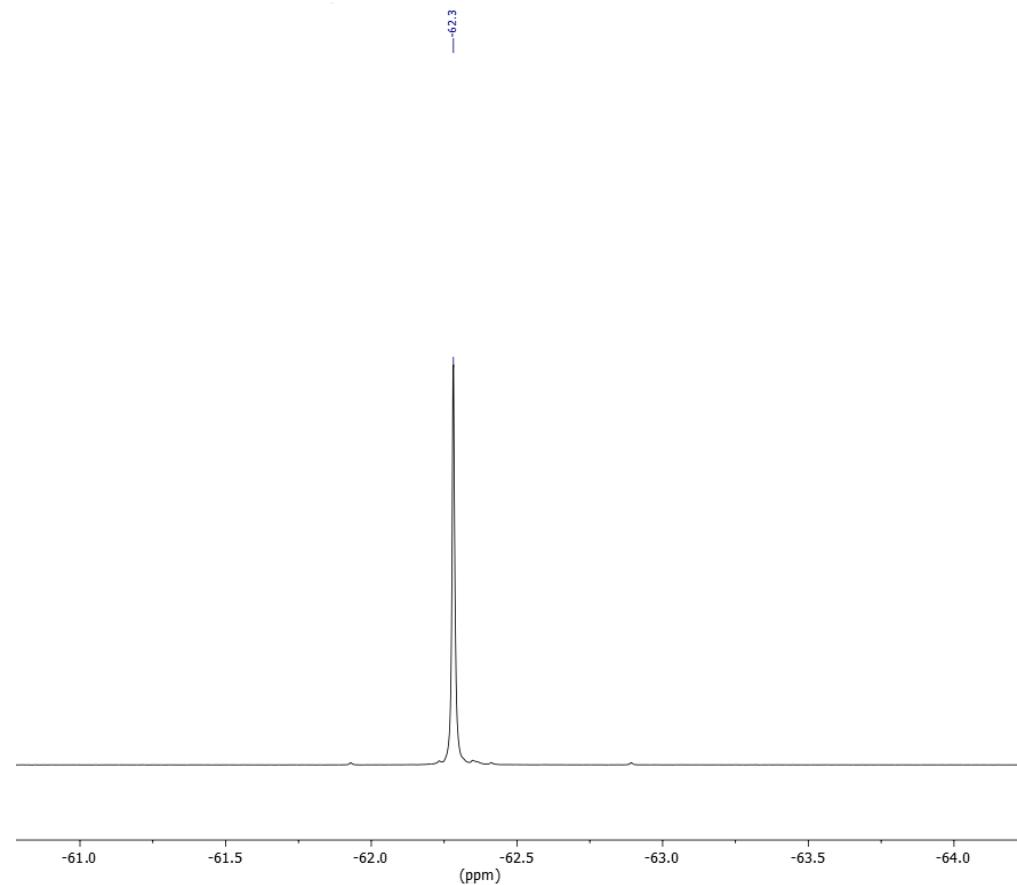
**Figure S2.** ^{19}F NMR spectrum of compound **2** in CHCl$_3$.
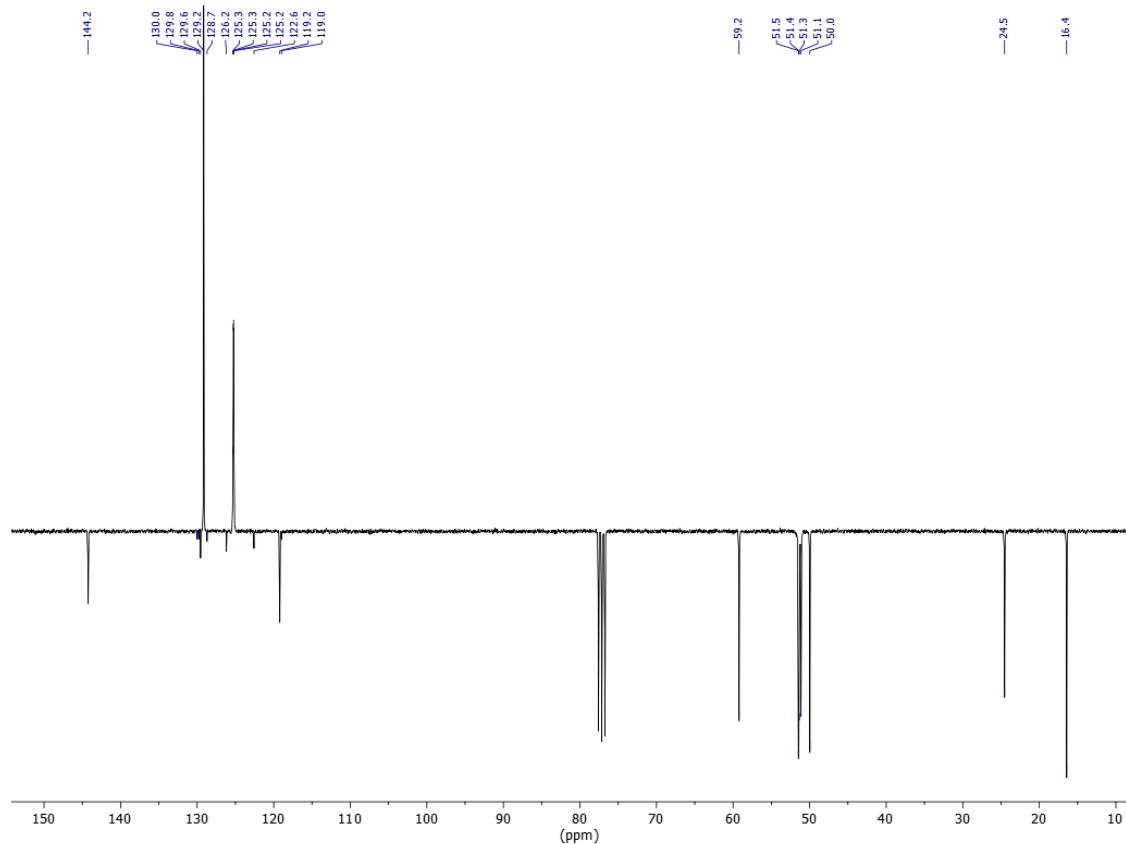
Figure S3. $^{13}C\{^1H\}$ NMR spectrum of compound **2** in $CHCl_3$.
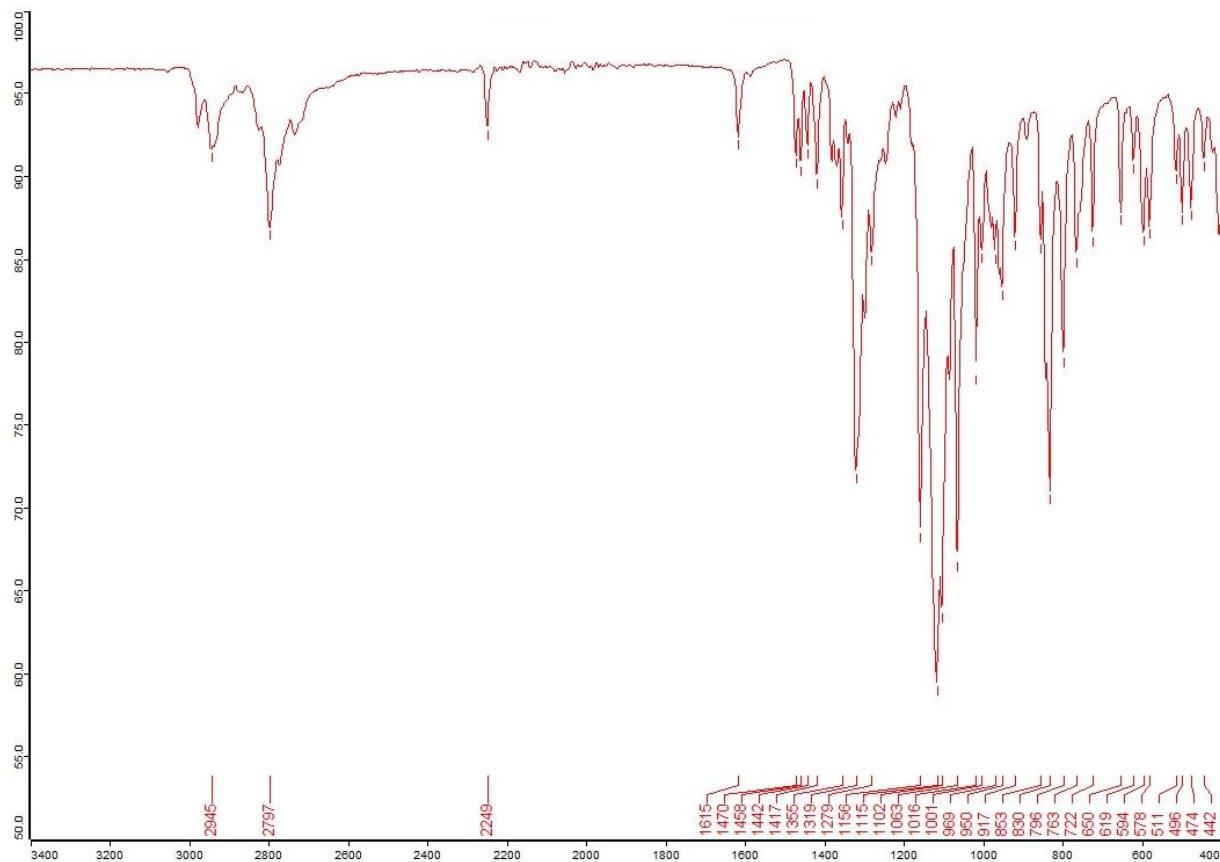
**Figure S4.** FT-IR spectrum of compound **2**.
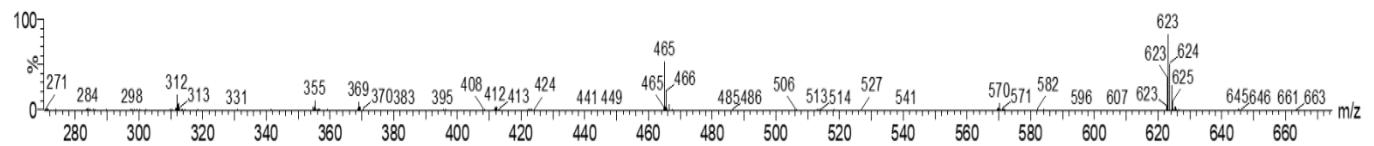
Figure S5. ESI-MS spectrum of compound **2** in positive ion mode.