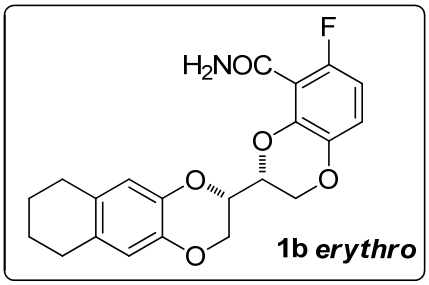
Supporting Information

6-Fluoro-3-(2,3,6,7,8,9-hexahydronaphtho[2,3-b][1,4]dioxin-2-yl)-2,3-dihydrobenzo[b][1,4]dioxine-5-carboxamide (*threo* and *erythro* isomers)

Valentina Straniero*, Lorenzo Suigo, Giulia Lodigiani, and Ermanno Valoti

Summary

6-Fluoro-3-(2,3,6,7,8,9-hexahydronaphtho[2,3-b][1,4]dioxin-2-yl)-2,3-dihydrobenzo[b][1,4]dioxine-5-carboxamide (1b *erythro*)



^{1}H in DMSO-d_6

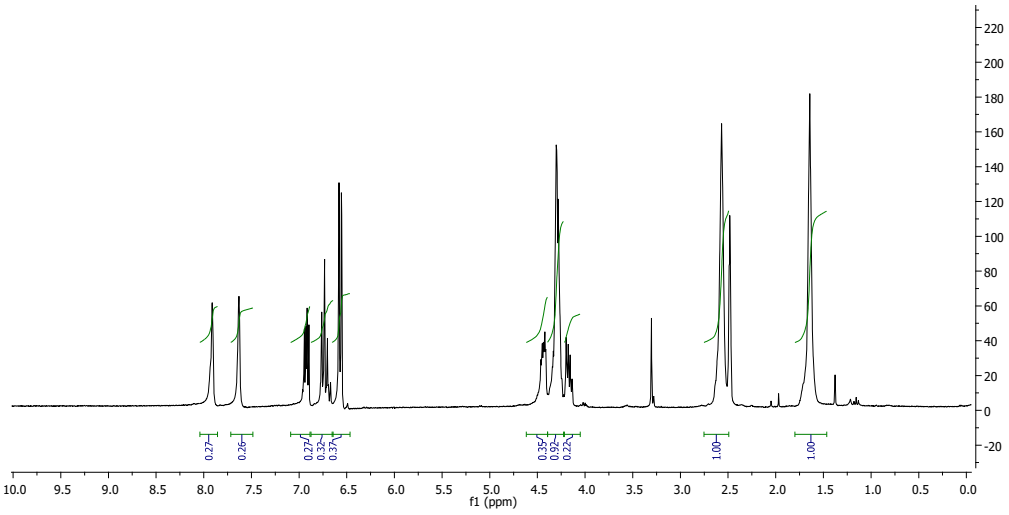


Figure S1. ^{1}H-NMR spectrum of Compound 1b erythro in DMSO-d6.

^{13}C in DMSO-d_6

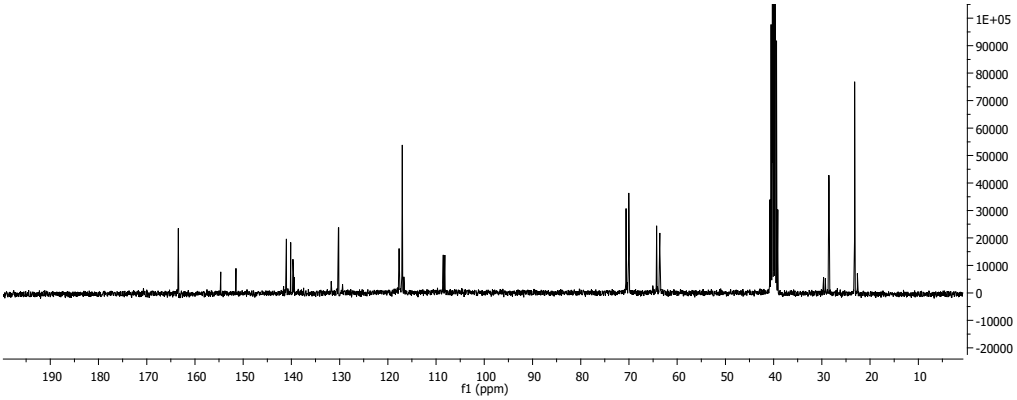


Figure S2. copy of ^{13}C-NMR spectrum of Compound 1b erythro in DMSO-d_6

HIGH-RESOLUTION MASS ANALYSIS

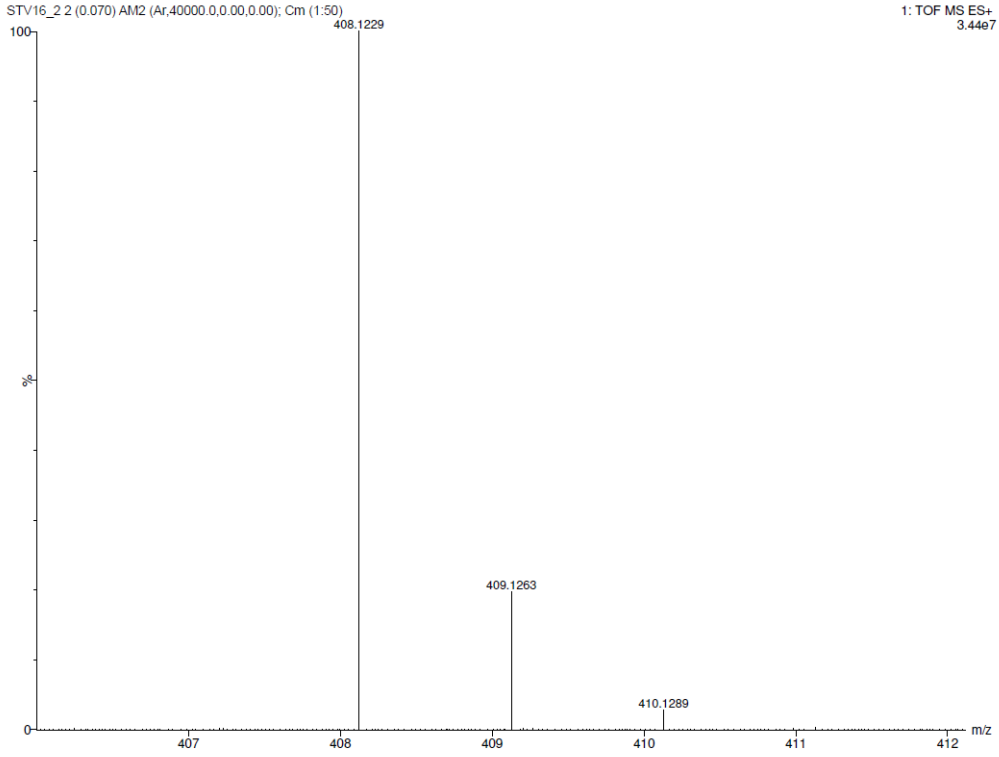
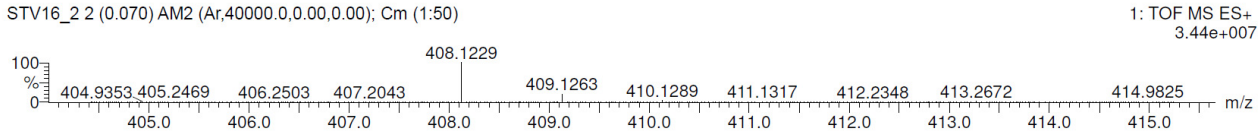


Figure S3. copy of HRMS spectrum of Compound 1b erythro

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

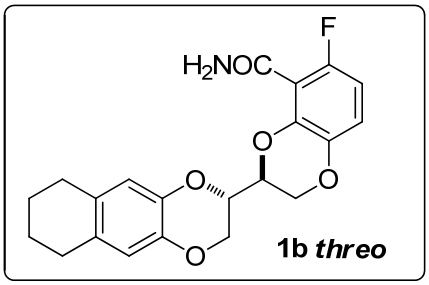
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 21-21 H: 20-21 N: 1-1 O: 5-5 Na: 0-4 F: 1-1



Minimum:				-5.0				
Maximum:		5.0	5.0	300.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.1229	408.1223	0.6	1.5	11.5	2502.2	n/a	n/a	C21 H20 N O5 Na F

Figure S4. copy of Elemental Composition Report of Compound 1b erythro

6-Fluoro-3-(2,3,6,7,8,9-hexahydronaphtho[2,3-b][1,4]dioxin-2-yl)-2,3-dihydrobenzo[b][1,4]dioxine-5-carboxamide (1b *threo*)



^{1}H in DMSO-d_6

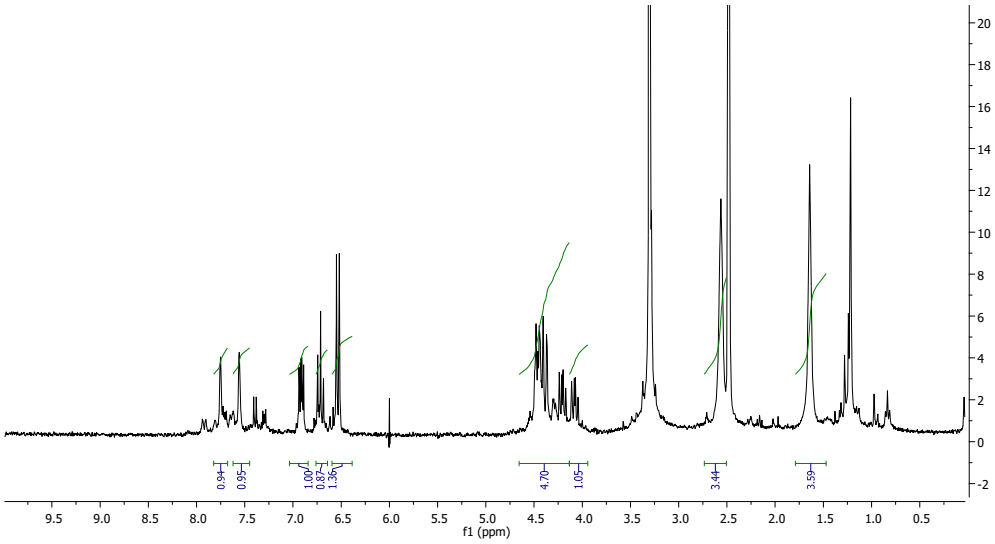


Figure S5. copy of ^{1}H-NMR spectrum of Compound 1b threo in DMSO-d_6

^{13}C in DMSO-*d*6

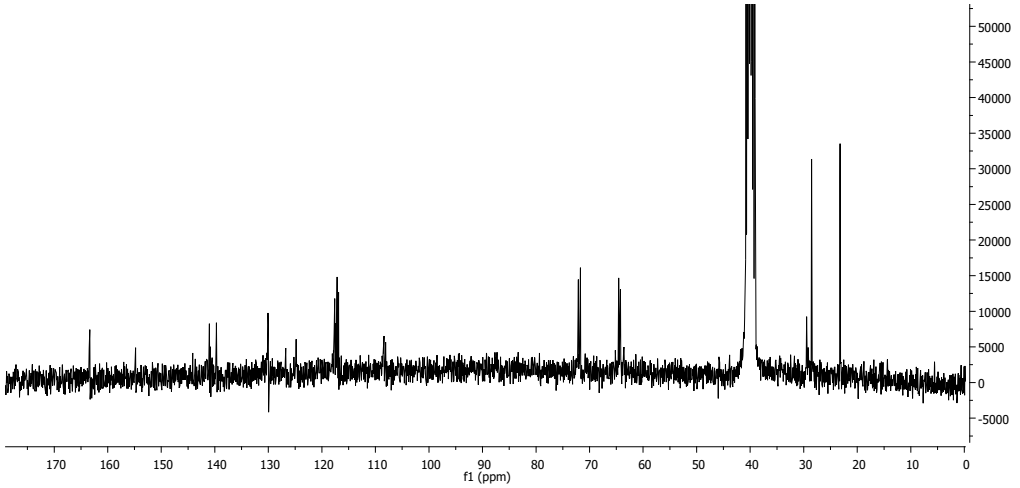


Figure S6. copy of ^{13}C-NMR spectrum of Compound 1b threo in DMSO-d_6

HIGH-RESOLUTION MASS ANALYSIS

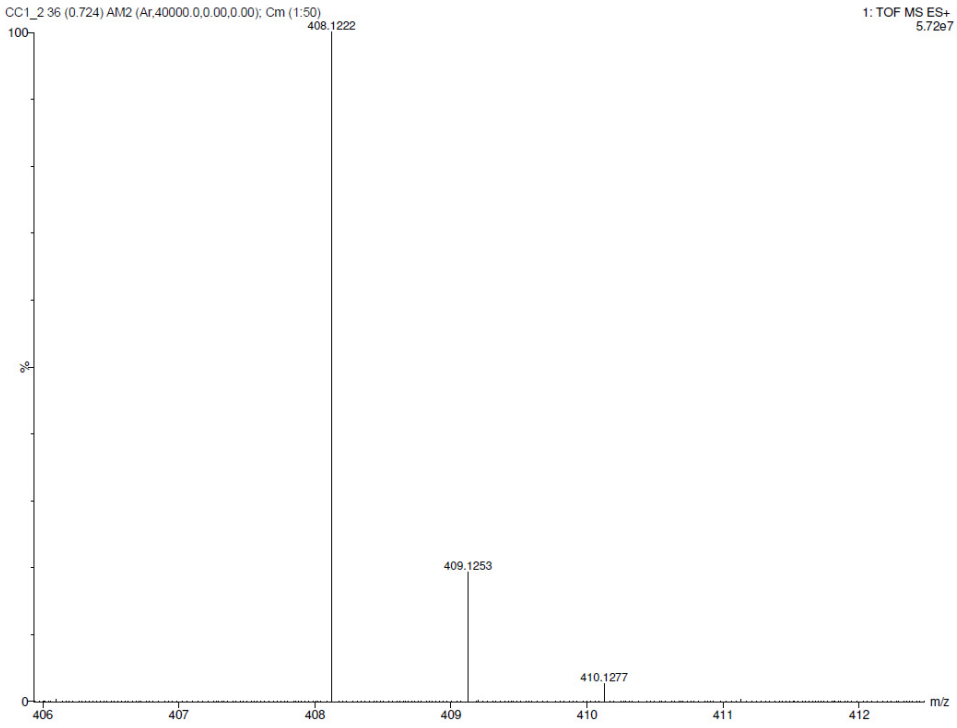
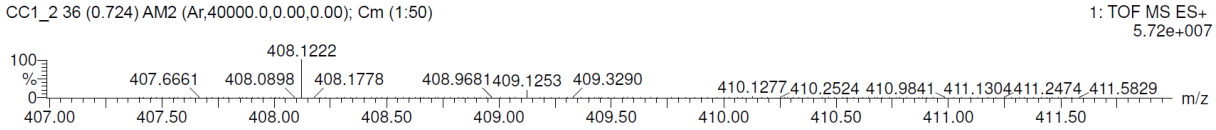


Figure S7. copy of HRMS spectrum of Compound 1b threo in DMSO-d_6

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 21-21 H: 20-21 N: 1-1 O: 5-5 Na: 0-4 F: 1-1



Minimum:				-5.0				
Maximum:		5.0	5.0	300.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.1222	408.1223	-0.1	-0.2	11.5	2001.8	n/a	n/a	C21 H20 N O5 Na F

Figure S8. copy of Elemental Composition Report of Compound 1b threo