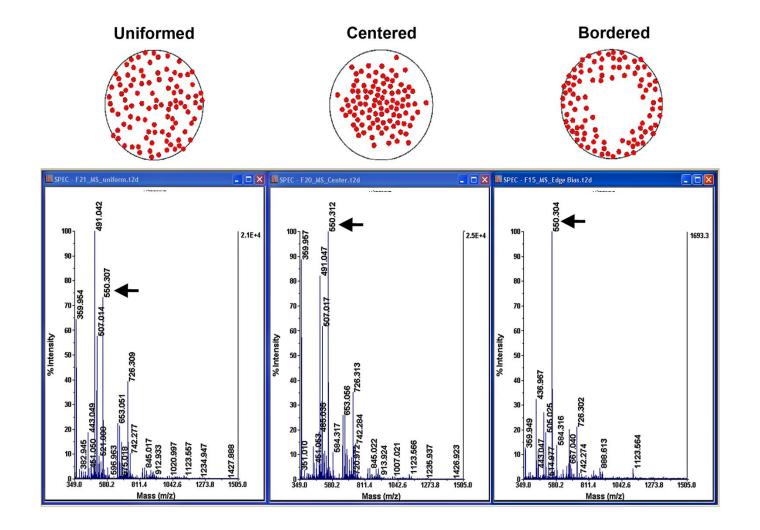
## Supporting information for Mass spectrometry in pharmacokinetic studies of a synthetic compound for spinal cord injury treatment.

María Sánchez-Sierra<sup>1</sup>, Isabel García-Álvarez<sup>1</sup>, Alfonso Fernández-Mayoralas<sup>2</sup>, Sandra Moreno-Lillo<sup>1</sup>, Gemma Barroso García<sup>3</sup>, Verónica Moral Dardé<sup>3</sup>, Ernesto Doncel-Pérez <sup>1\*</sup>

1) Grupo de Química Neuro-regenerativa, Hospital Nacional de Parapléjicos, Servicio de Salud de Castilla La Mancha (SESCAM), Finca La Peraleda s/n, 45071 Toledo, Spain.

2) Instituto de Química Orgánica General, CSIC, Juan de la Cierva 3, 28006 Madrid, Spain.

3) Servicio de Proteómica, Hospital Nacional de Parapléjicos, Servicio de Salud de Castilla La Mancha (SESCAM), Finca La Peraleda s/n, 45071 Toledo, Spain.



**Figure 1 Examples of acquisition of samples in MALDI-TOF MS analysis in this study.** In circles ways of sample acquisition, below examples of mass spectrums in each case. Arrows for IG20 signal at 550,3 m/z.

## **Qualitative Compound Report**

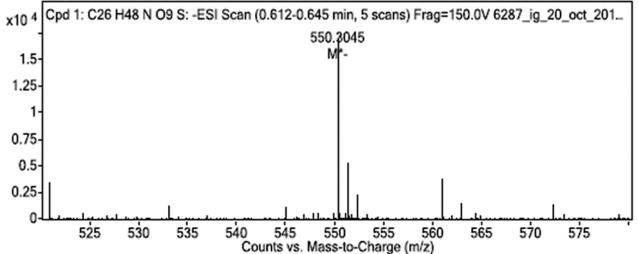
Data File	6287_ig_20_oct_2013_01.d	Sample Name	Unavailable
Sample Type Instrument Name	Unavailable Unavailable	Position User Name	Unavailable Unavailable
Acq Method DA Method	QualDAMethod.m	IRM Calibration Status Comment	Success Sample information is unavailable

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Drff (ppm)
Cpd 1: C26 H48 N O9 S	0.612	550.3039	17028	C26 H48 N O9 S	550.305	-1.92

Compound Label	RT	Algorithm	Mass
Cpd 1: C26 H48 N O9 S	0.612	Find By Formula	550.3039
10.7			

MS Zoomed Spectrum



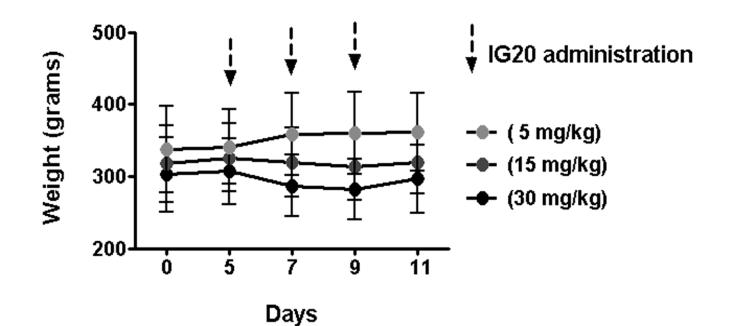
## MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
112.9855				1030501		
113.0529				26526		
113.0819				79022		
113.1143				13098		
113.1392				8905		
113.1597				6448		
113.1835				6726		
113.2082				7051		
113.988				35159		
550.3045	550.3055	-1.88	1	17028	C26 H48 N O9 S	M*-

--- End Of Report ---

**Figure 2. Qualitative compound report for IG20 by ESI-MS analysis.** The final product in the IG20 synthesis was analyzed by Electrospray Ionization Mass Spectrometry, in ion negative mode. The mass/charge at 550.30 and purity of IG20 is shown.

## Weight evolution



**Figure 3. Evolution of weight in rats injected with IG20 compound.** Normal adult rats were injected every two days with different concentrations of IG20 compound. The gaining of weight was used as a health parameter. There was not significant difference in between groups of animals during the period assayed. The higher concentration of IG20 (30mg/kg) was selected for successive experiments.