

Supporting Information

**Synthesis and separation of the enantiomers of the  
Neuropeptide S receptor antagonist (9R/S)-3-Oxo-1,1-diphenyl-  
tetrahydro-oxazolo[3,4-*a*]pyrazine-7-carboxylic acid 4-fluoro-  
benzylamide (SHA 68)**

Claudio Trapella<sup>§‡</sup>, Michela Pela<sup>§‡</sup>, Luisa Del Zoppo<sup>§</sup>, Girolamo Calo<sup>#</sup>, Valeria  
Camarda<sup>#</sup>, Chiara Ruzza<sup>#</sup>, Alberto Cavazzini<sup>¶</sup>, Valerio Bertolasi<sup>¶</sup>, Valentina  
Costa<sup>¶</sup>, Rainer K. Reinscheid<sup>\*</sup>, Severo Salvadori<sup>§</sup>  
and Remo Guerrini<sup>§\*</sup>

<sup>§</sup>*Department of Pharmaceutical Sciences and Biotechnology Center, and  
<sup>#</sup>Department of Experimental and Clinical Medicine, Section of Pharmacology and  
Neuroscience center, and National Institute of Neuroscience, University of Ferrara,  
via Fossato di Mortara 19, 44100 Ferrara, Italy. <sup>¶</sup>Department of Chemistry,  
University of Ferrara,, via L. Borsari 46, 44100 Ferrara, Italy. <sup>\*</sup>Department of  
Pharmaceutical Sciences, University of California Irvine, 360 Med Surge 2, Irvine,  
CA 92697, USA.*

<sup>‡</sup> These authors contributed equally to this work

\*To whom Correspondence should be addressed.  
Remo Guerrini  
Phone: +39-0532-455-988; Fax: +39-0532-455953  
E-mail: [r.guerrini@unife.it](mailto:r.guerrini@unife.it)

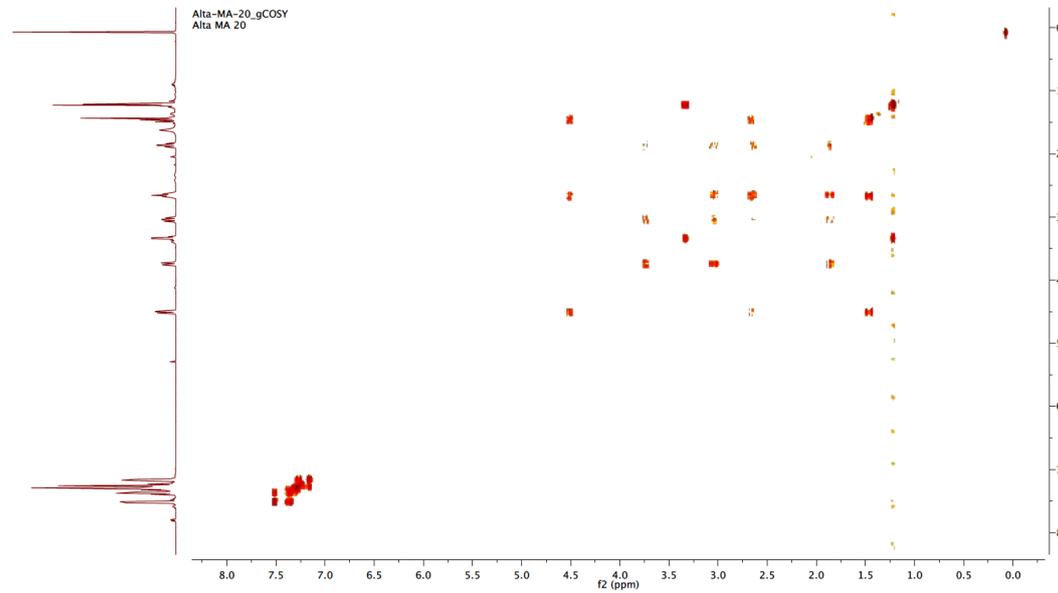
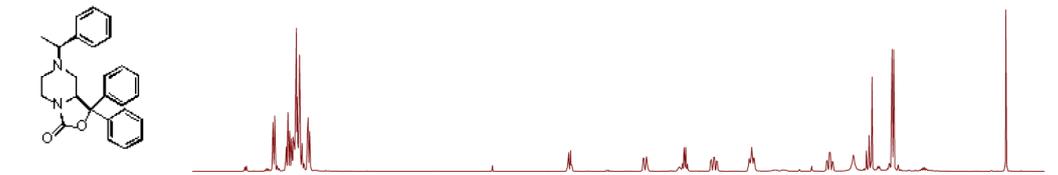
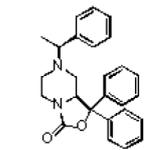
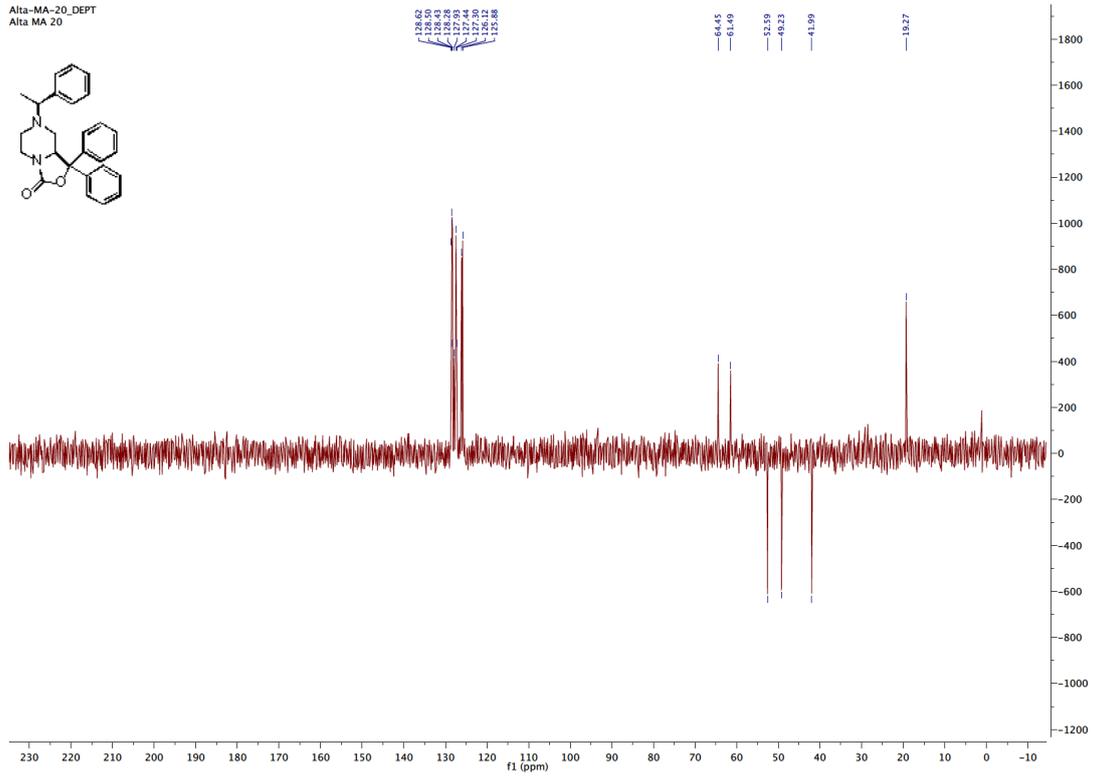
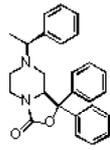
## Contents

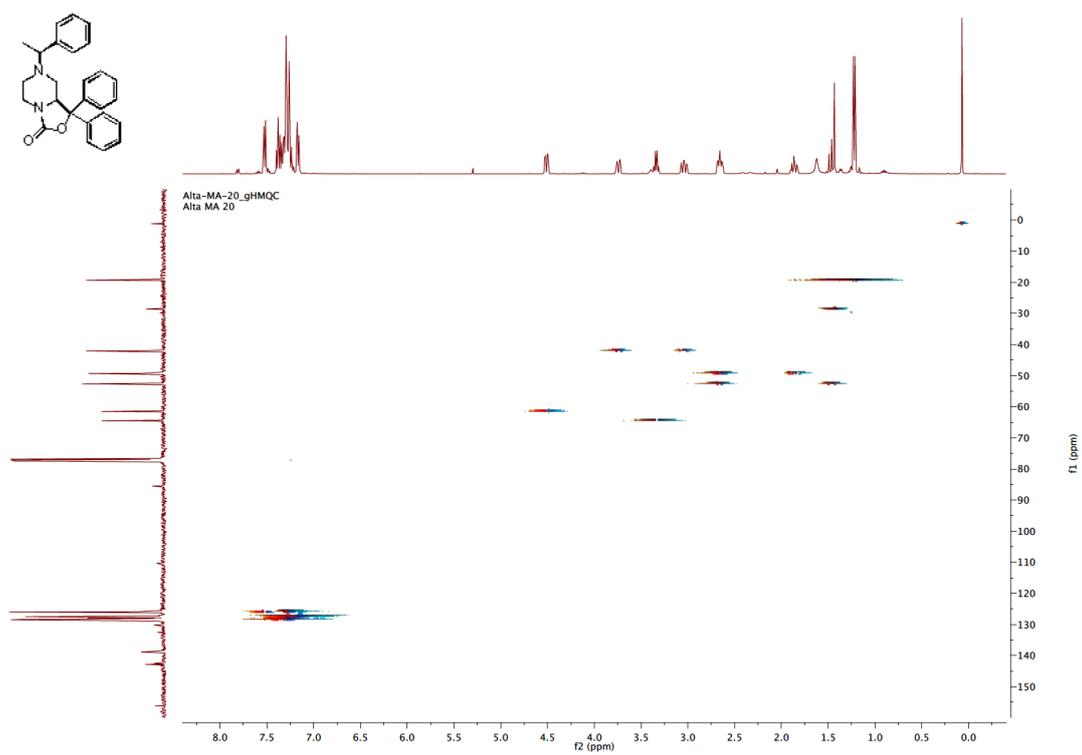
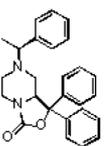
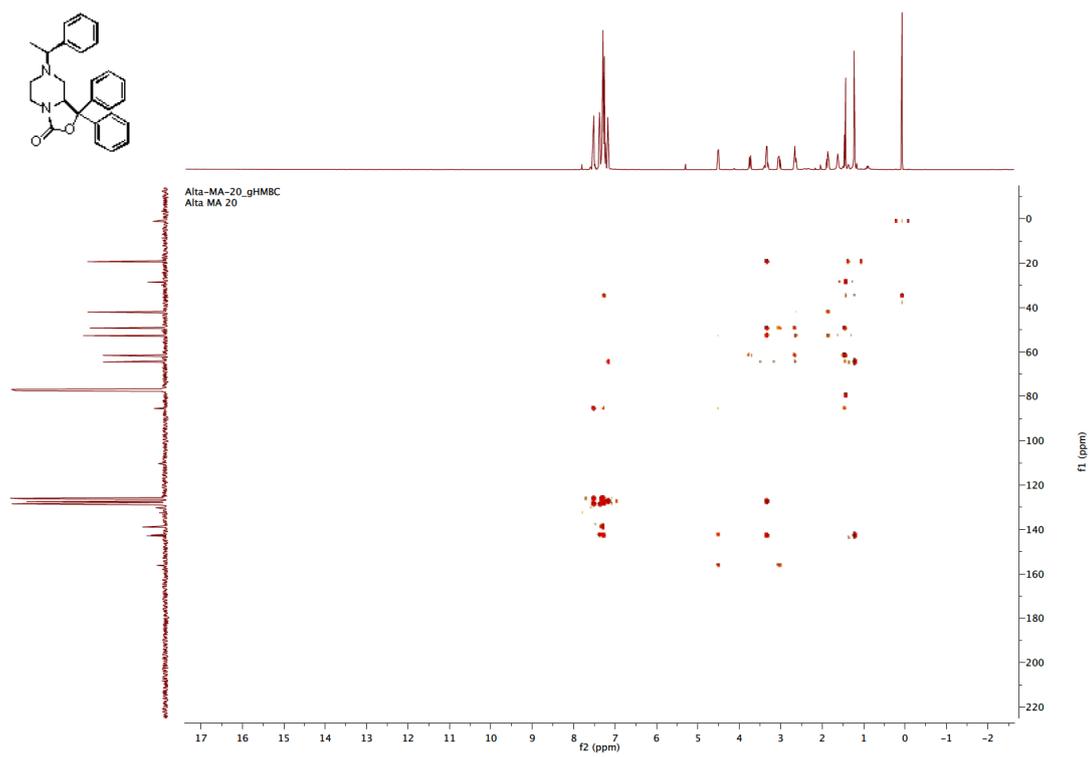
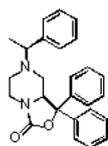
page S3	$^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra of compound 8a
page S4	DEPT-NMR and COSY-NMR spectra of compound 8a
page S5	HMBC-NMR and HMQC-NMR spectra of compound 8a
page S6	$^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra of compound 8
page S7	DEPT-NMR and COSY-NMR spectra of compound 8
page S8	HMBC-NMR and HMQC-NMR spectra of compound 8
page S9	$^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra of compound 10
page S10	DEPT-NMR and COSY-NMR spectra of compound 10
page S11	HMBC-NMR and HMQC-NMR spectra of compound 10
page S12	$^{19}\text{F}$ -NMR spectra of compound 10, $^1\text{H}$ -NMR spectra of compound 10a
page S13	$^{13}\text{C}$ -NMR and DEPT-NMR spectra of compound 10a
page S14	COSY-NMR and HMQC-NMR spectra of compound 10a
page S15	HMBC-NMR and $^{19}\text{F}$ -NMR spectra of compound 10a

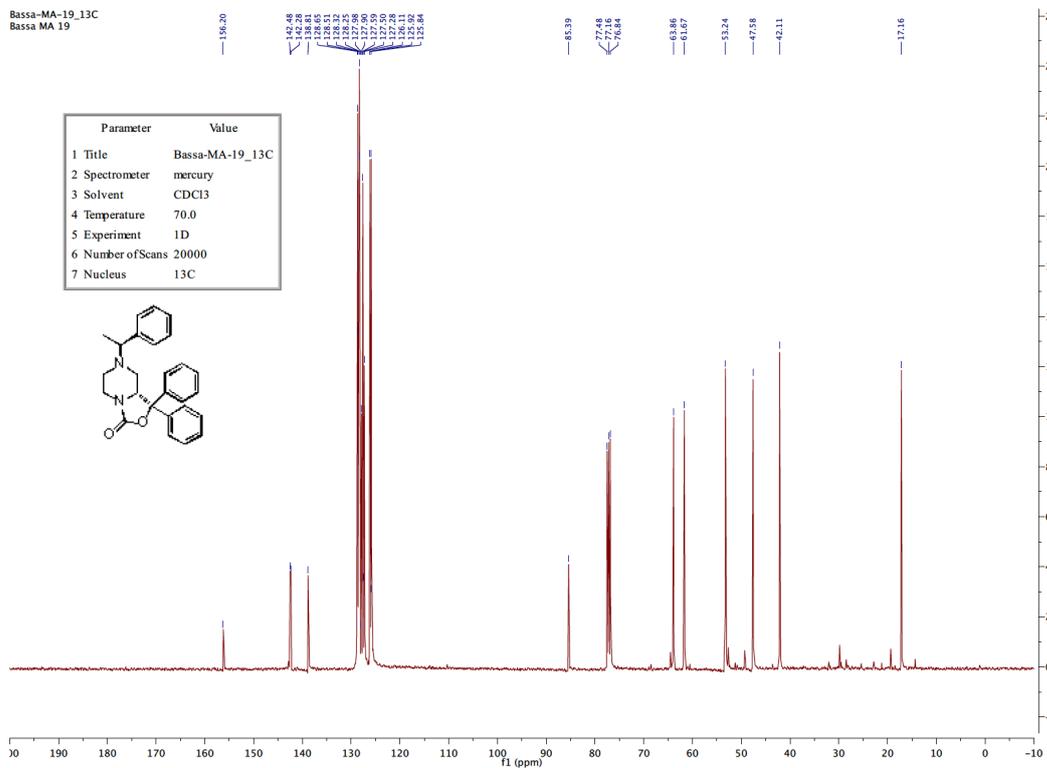
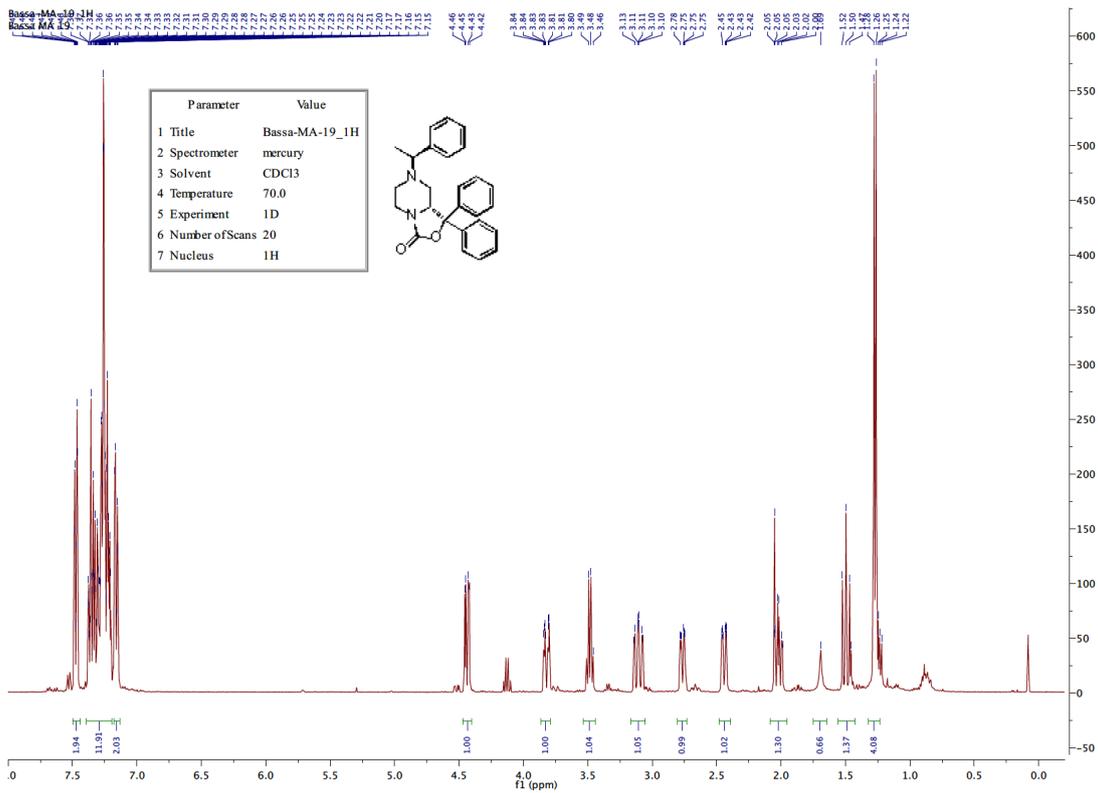
All the spectra were elaborated using MestreNova 6.0.2 software, and FID data are available on request.



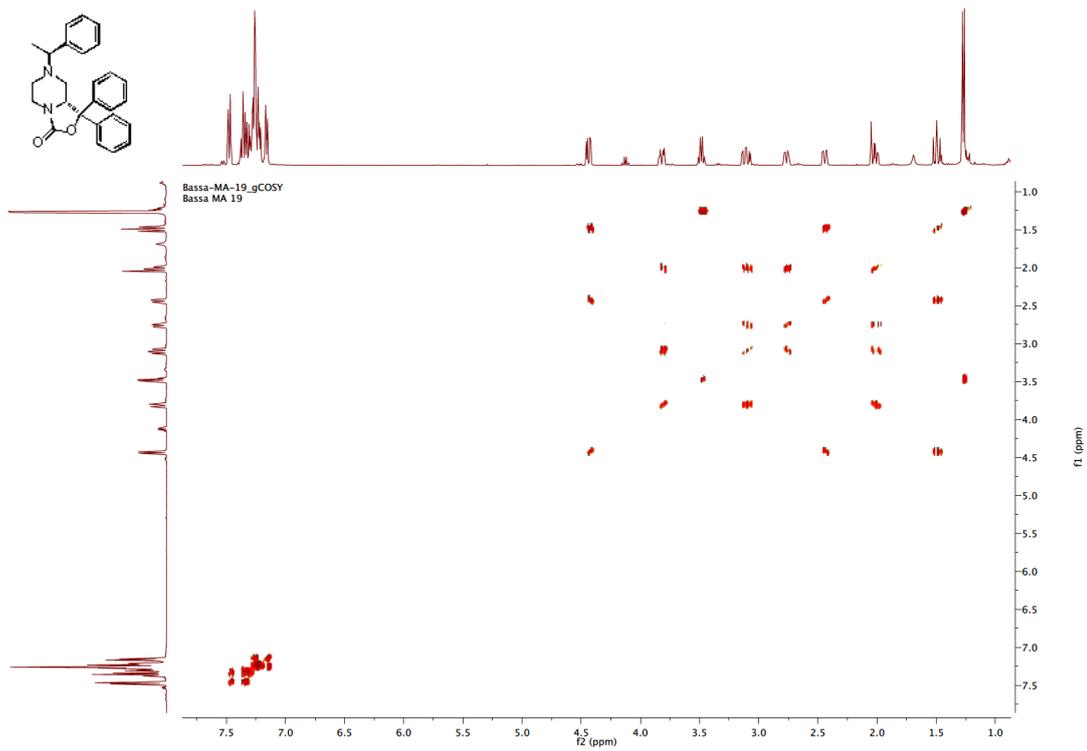
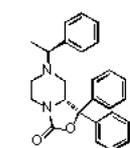
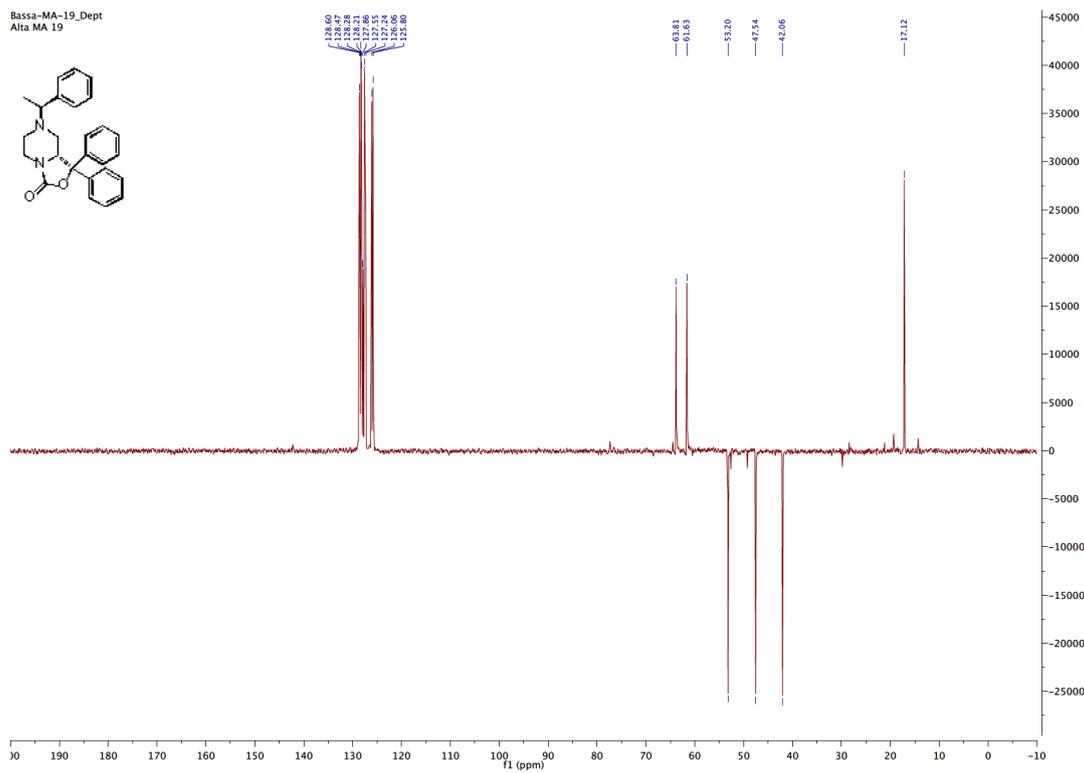
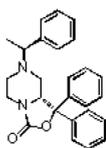
Alta-MA-20\_DEPT  
Alta MA 20

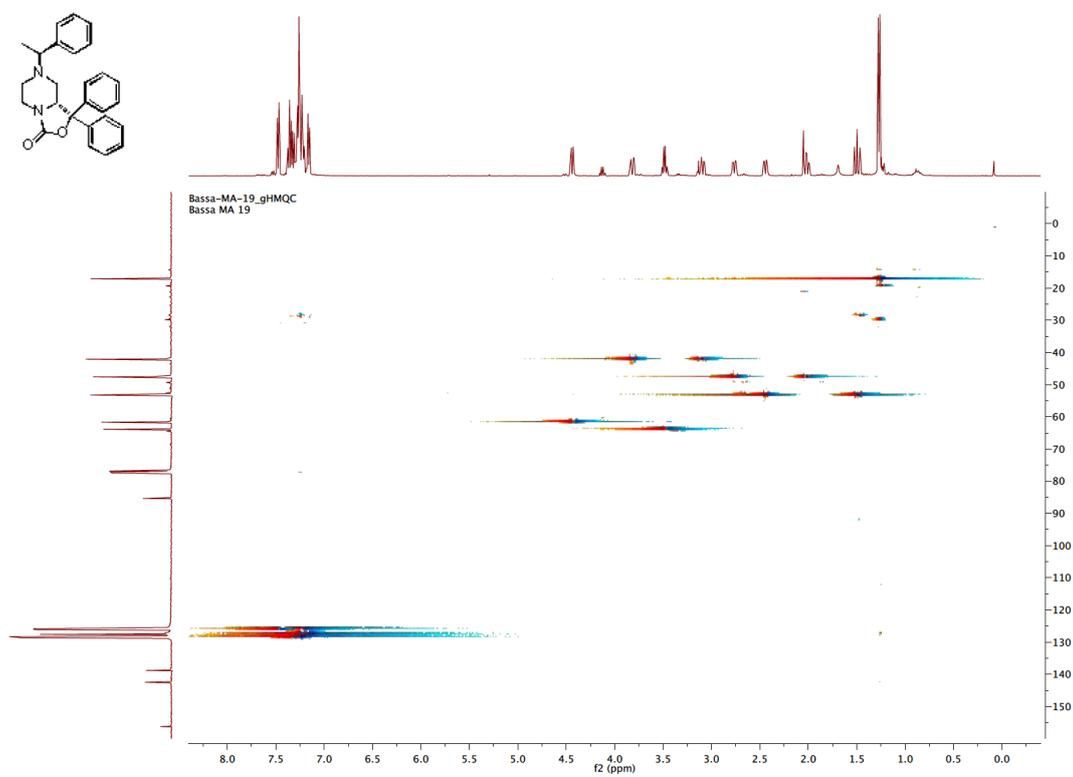
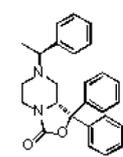
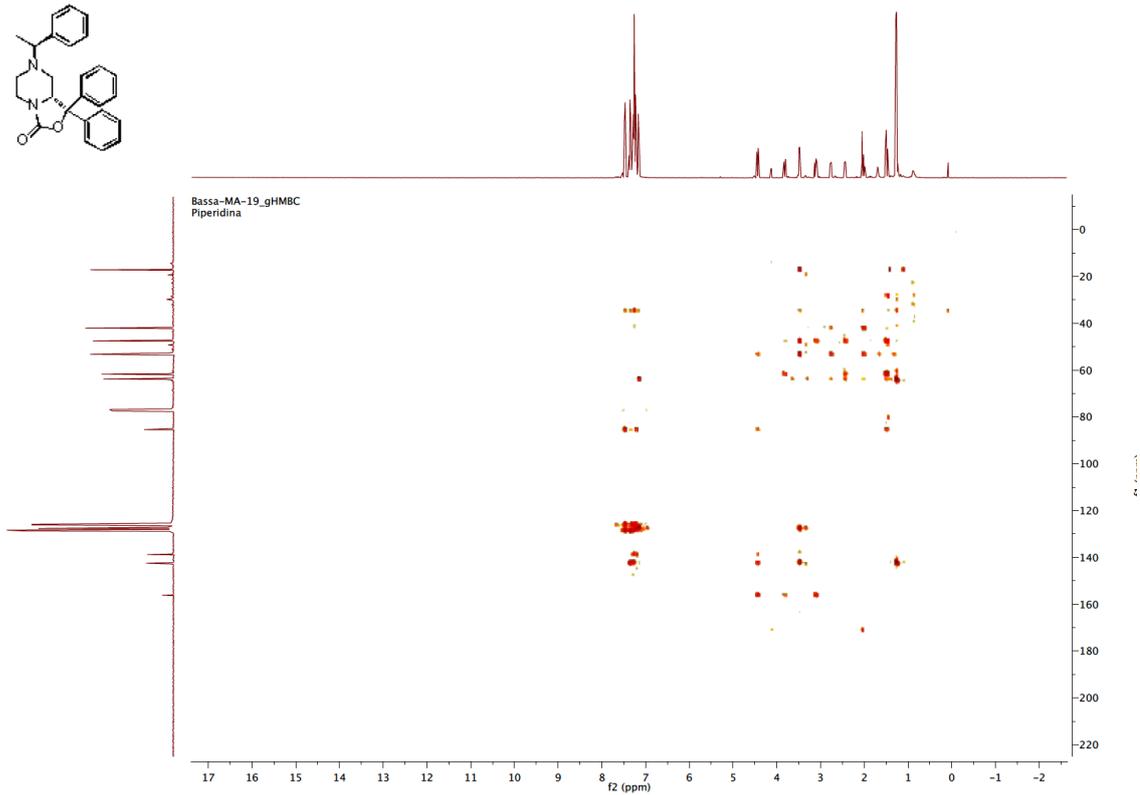
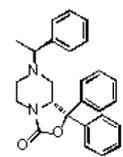


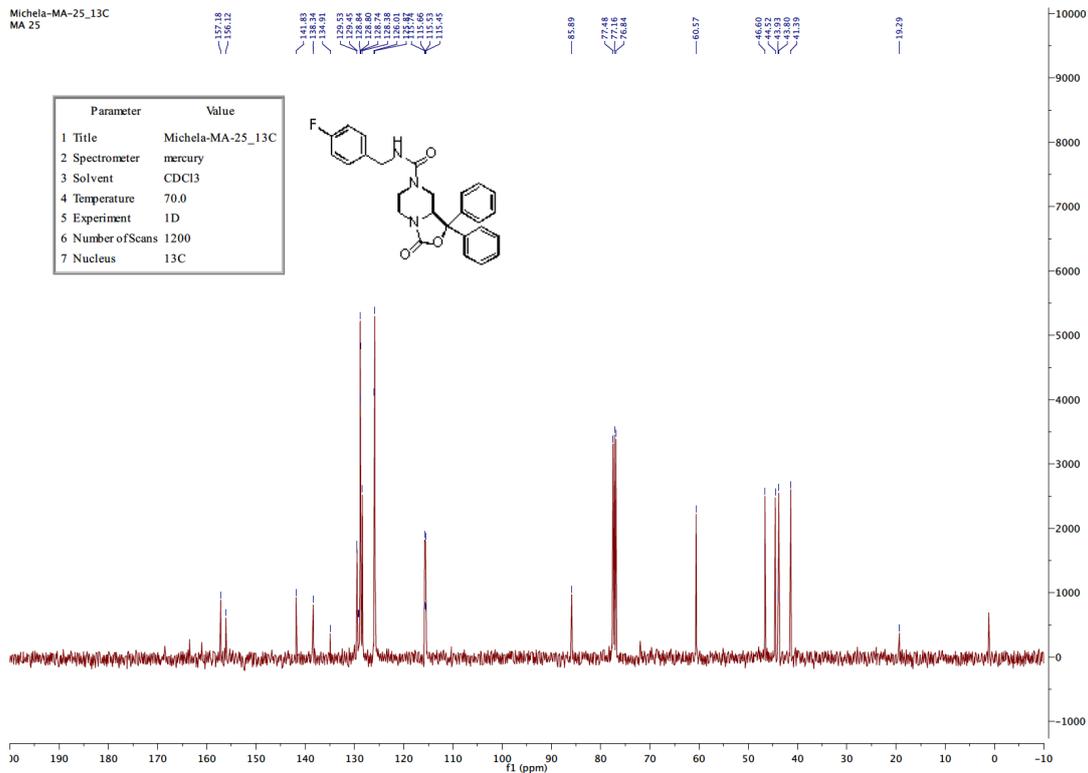
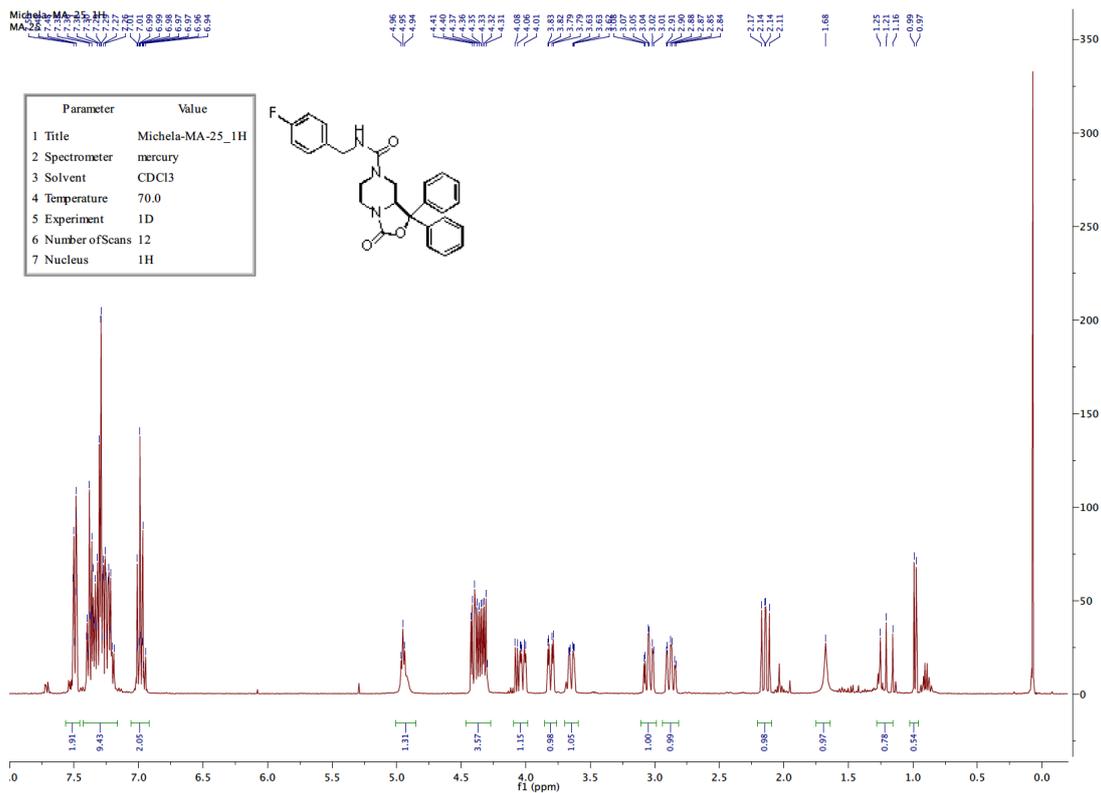


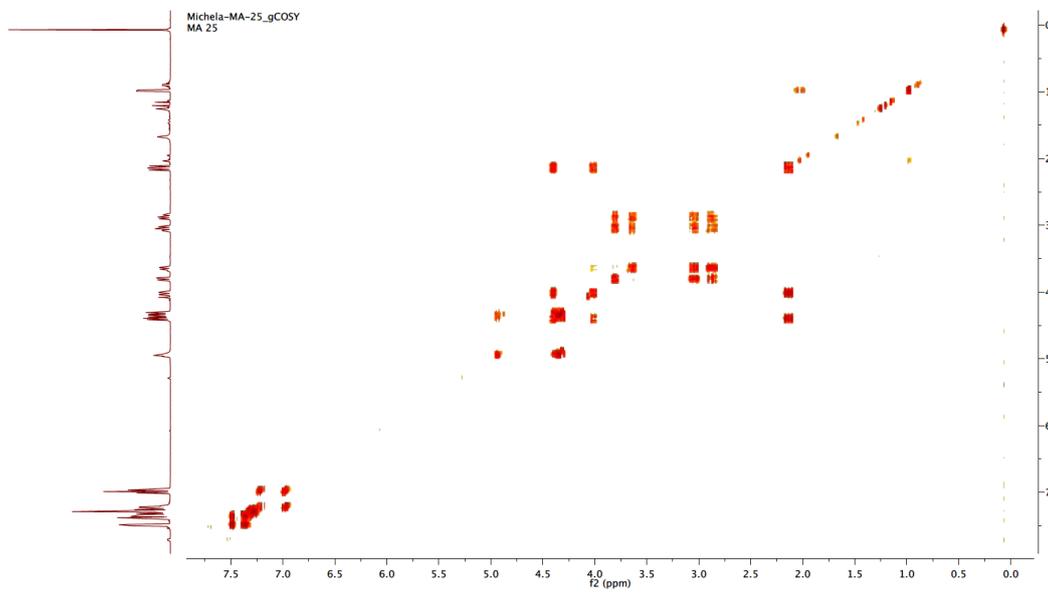
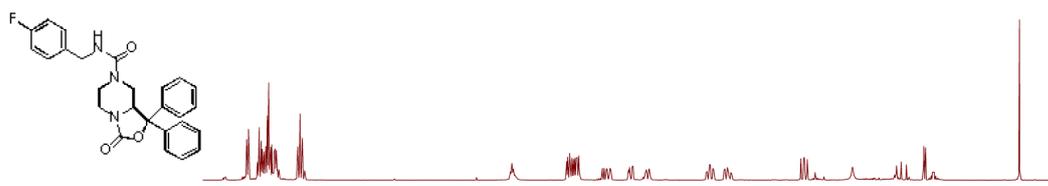
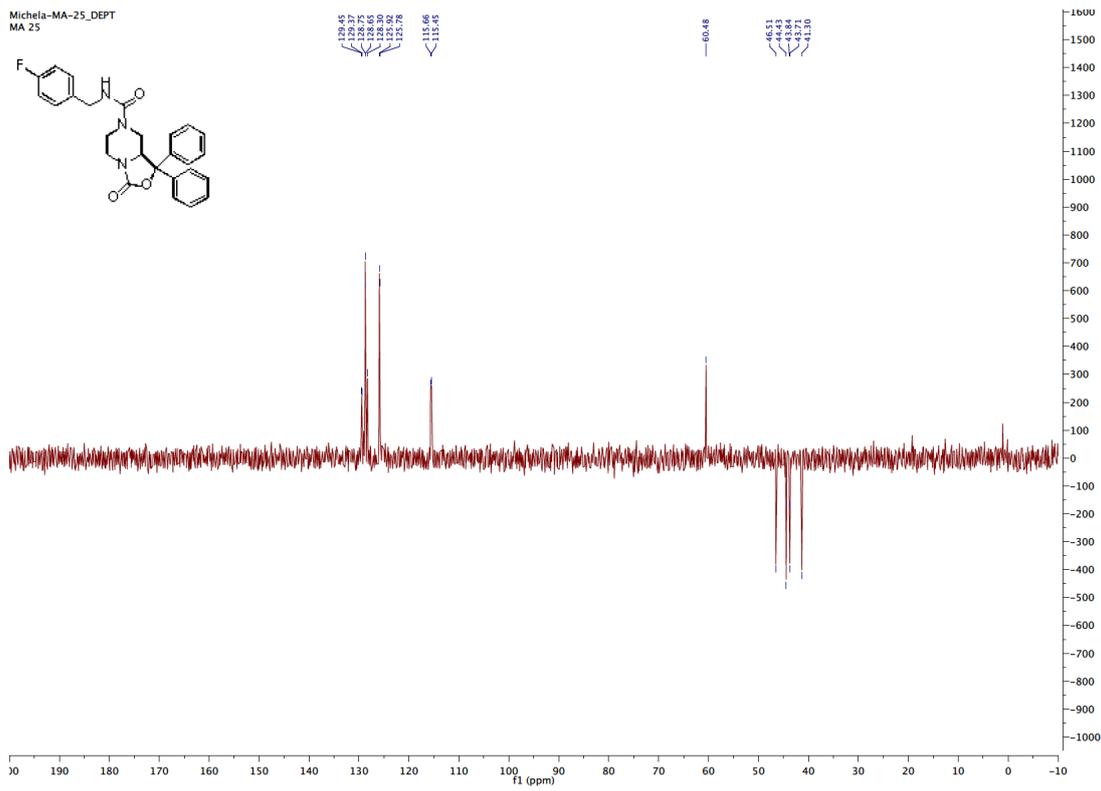


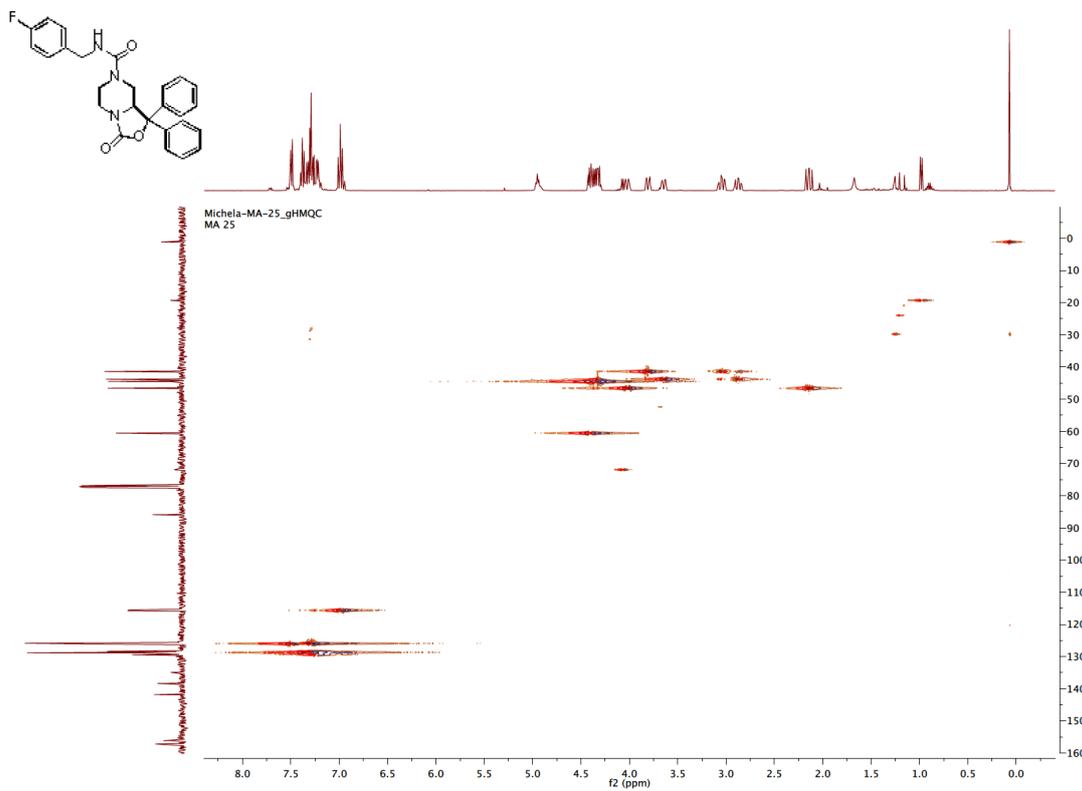
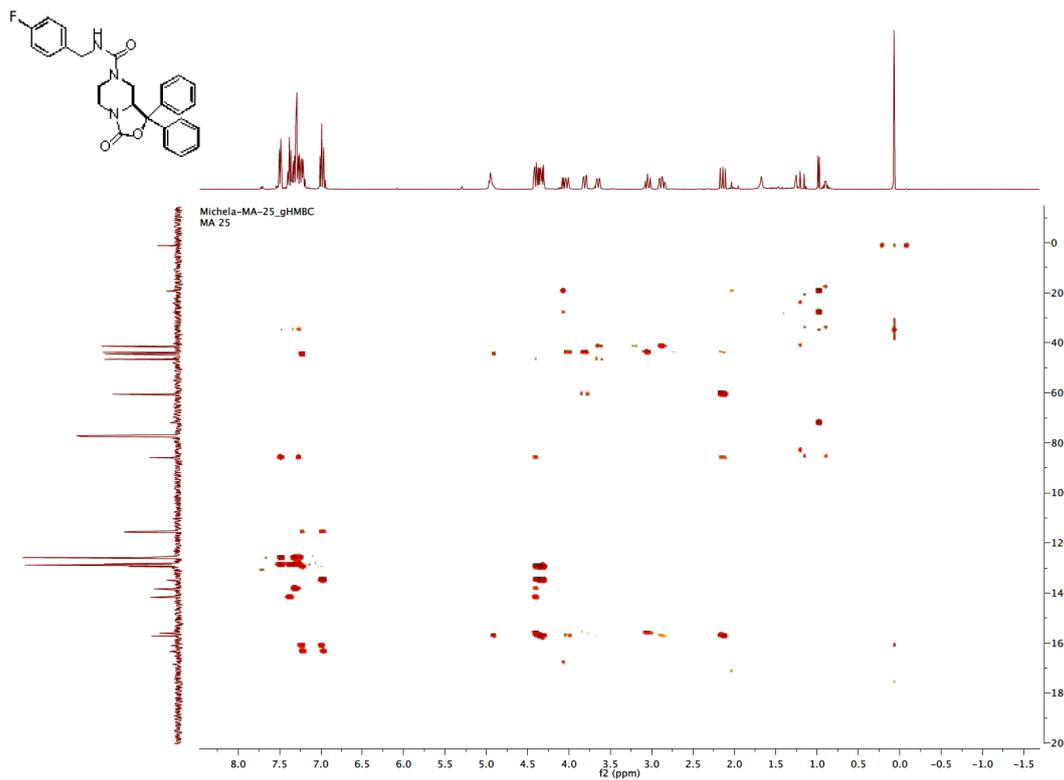
Bassa-MA-19\_Dept  
Alta MA 19



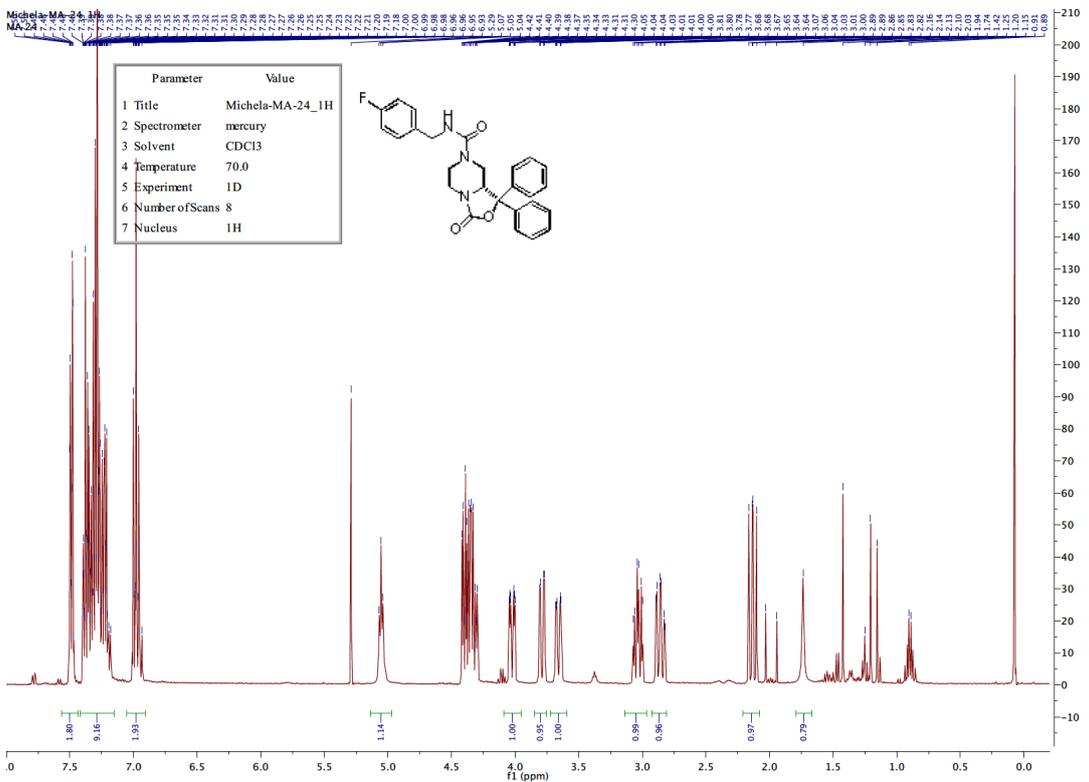
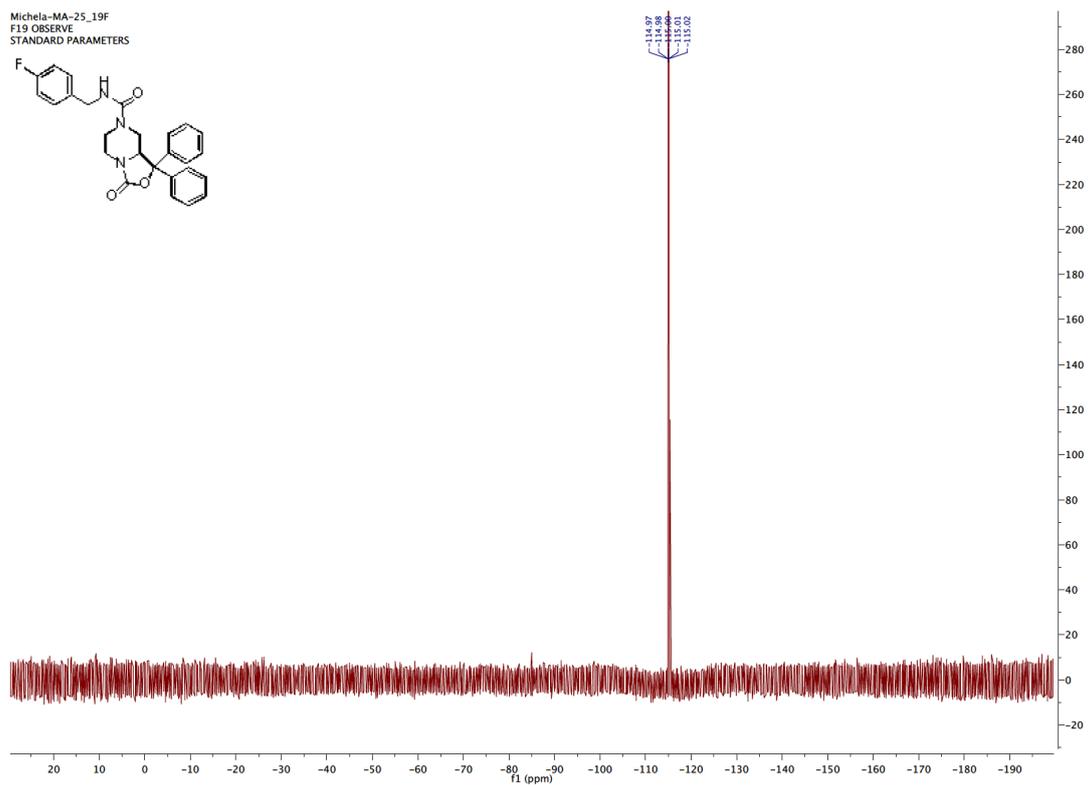
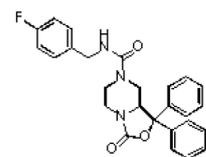








Michela-MA-25\_19F  
 F19 OBSERVE  
 STANDARD PARAMETERS



Michela-MA-24\_13C  
MA 24

163.44  
157.20  
156.11  
141.81  
138.30  
134.91  
129.48  
129.41  
128.82  
128.82  
128.72  
125.99  
115.40  
115.40

85.90

77.16

76.84

60.55

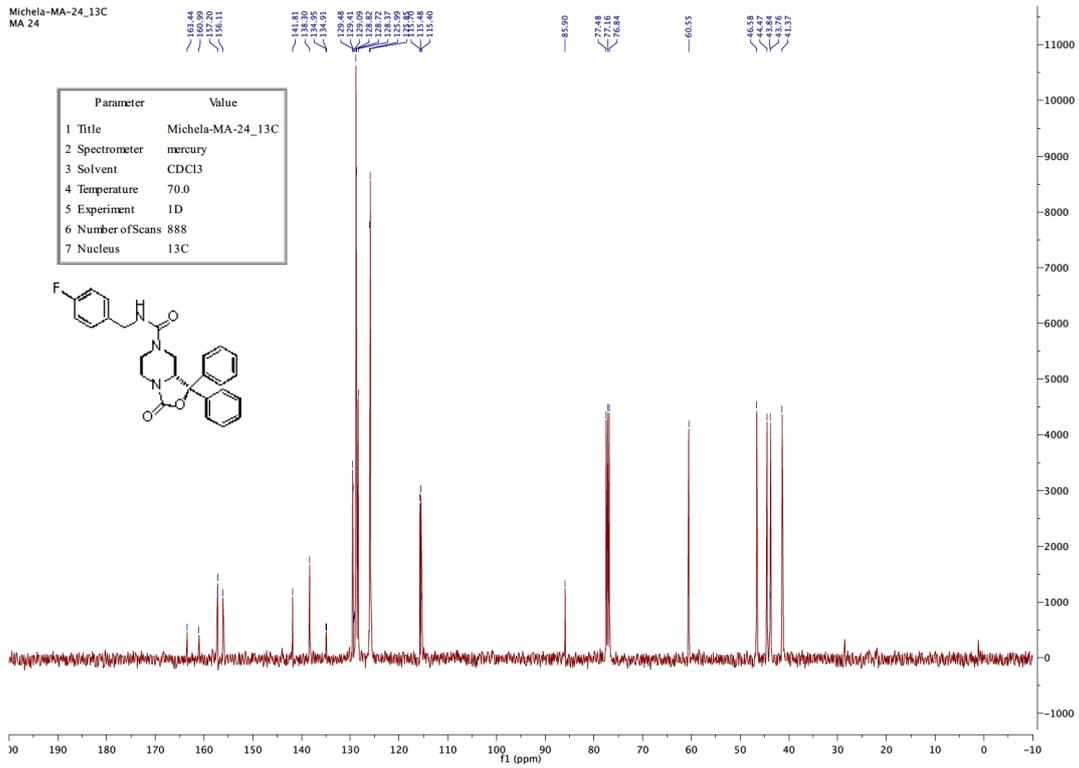
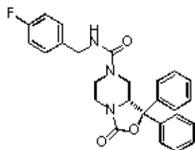
46.58

43.84

41.78

41.29

Parameter	Value
1 Title	Michela-MA-24_13C
2 Spectrometer	mercury
3 Solvent	CDCl3
4 Temperature	70.0
5 Experiment	1D
6 Number of Scans	888
7 Nucleus	13C



Michela-MA-24\_DEPT  
MA 24

129.42  
129.34  
128.82  
128.82  
128.72  
125.99  
115.44  
115.42

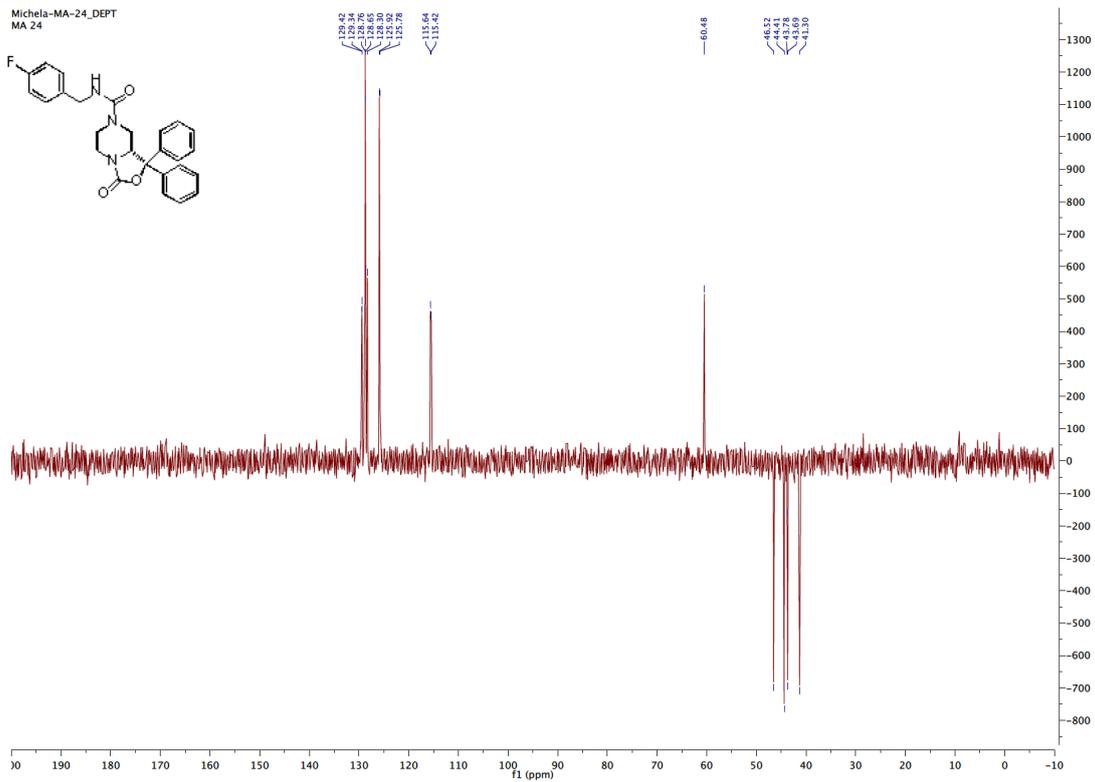
60.48

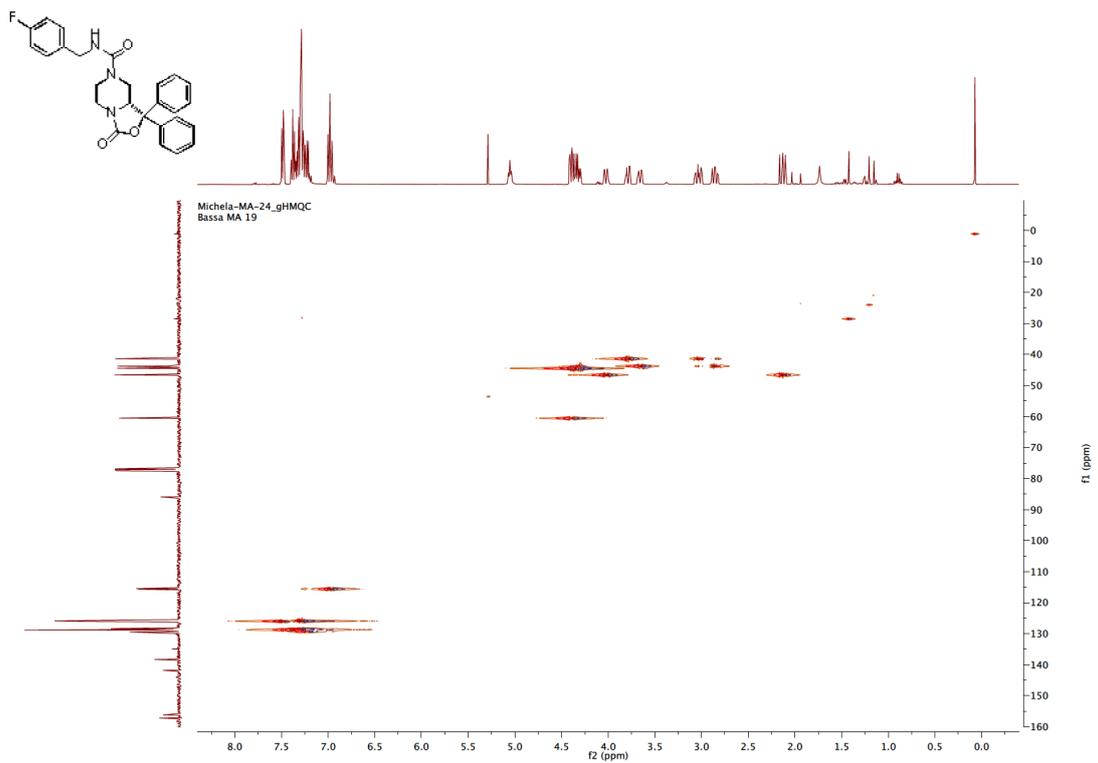
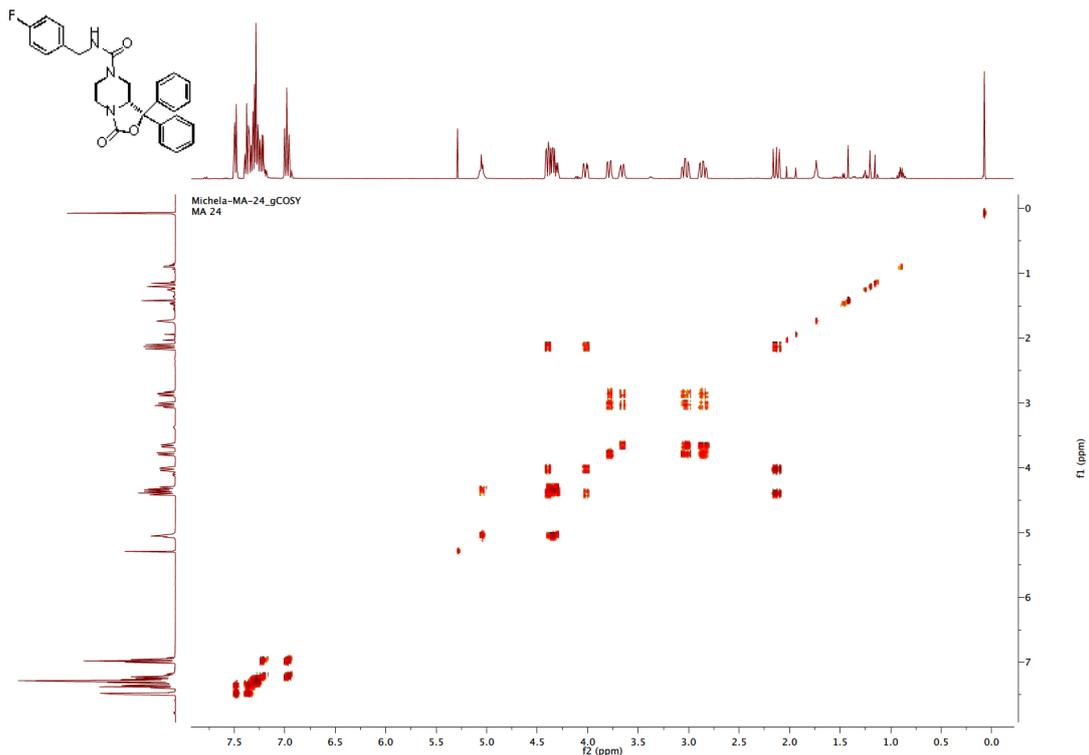
46.52

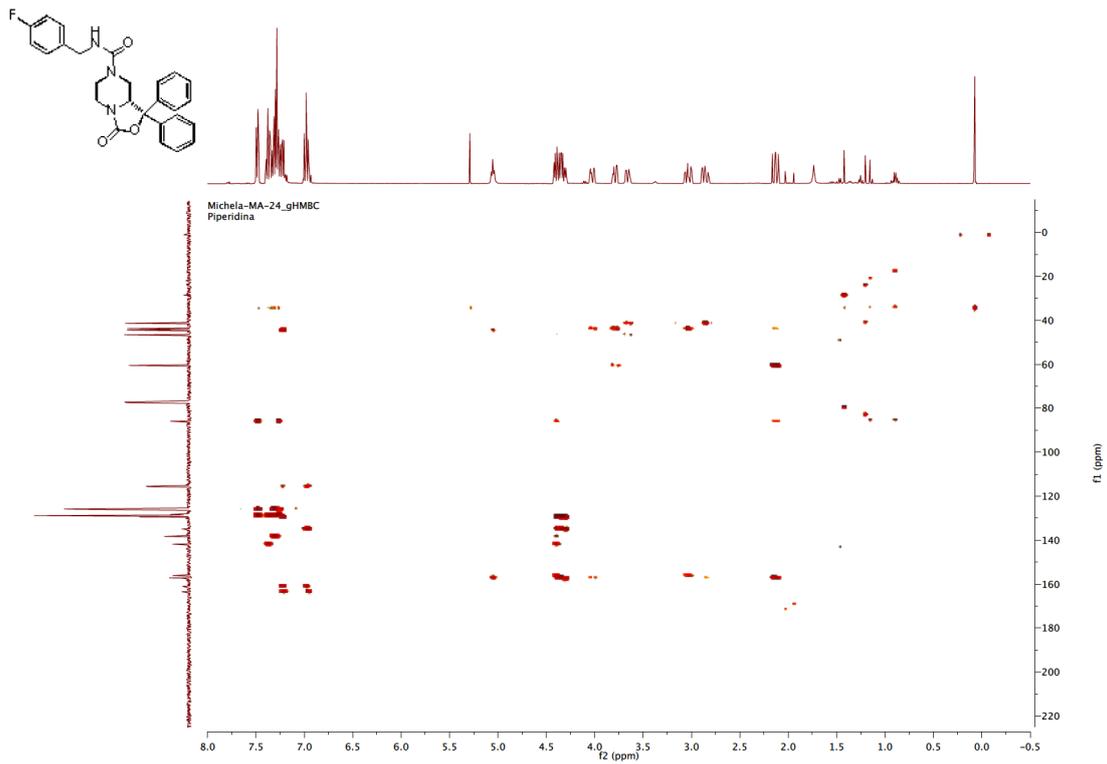
43.78

43.69

41.29







Michela-MA-24\_19F  
MA 24

Parameter	Value
1 Title	Michela-MA-24_19F
2 Spectrometer	mercury
3 Solvent	CDCl3
4 Temperature	70.0
5 Experiment	1D
6 Number of Scans	56
7 Nucleus	19F

