

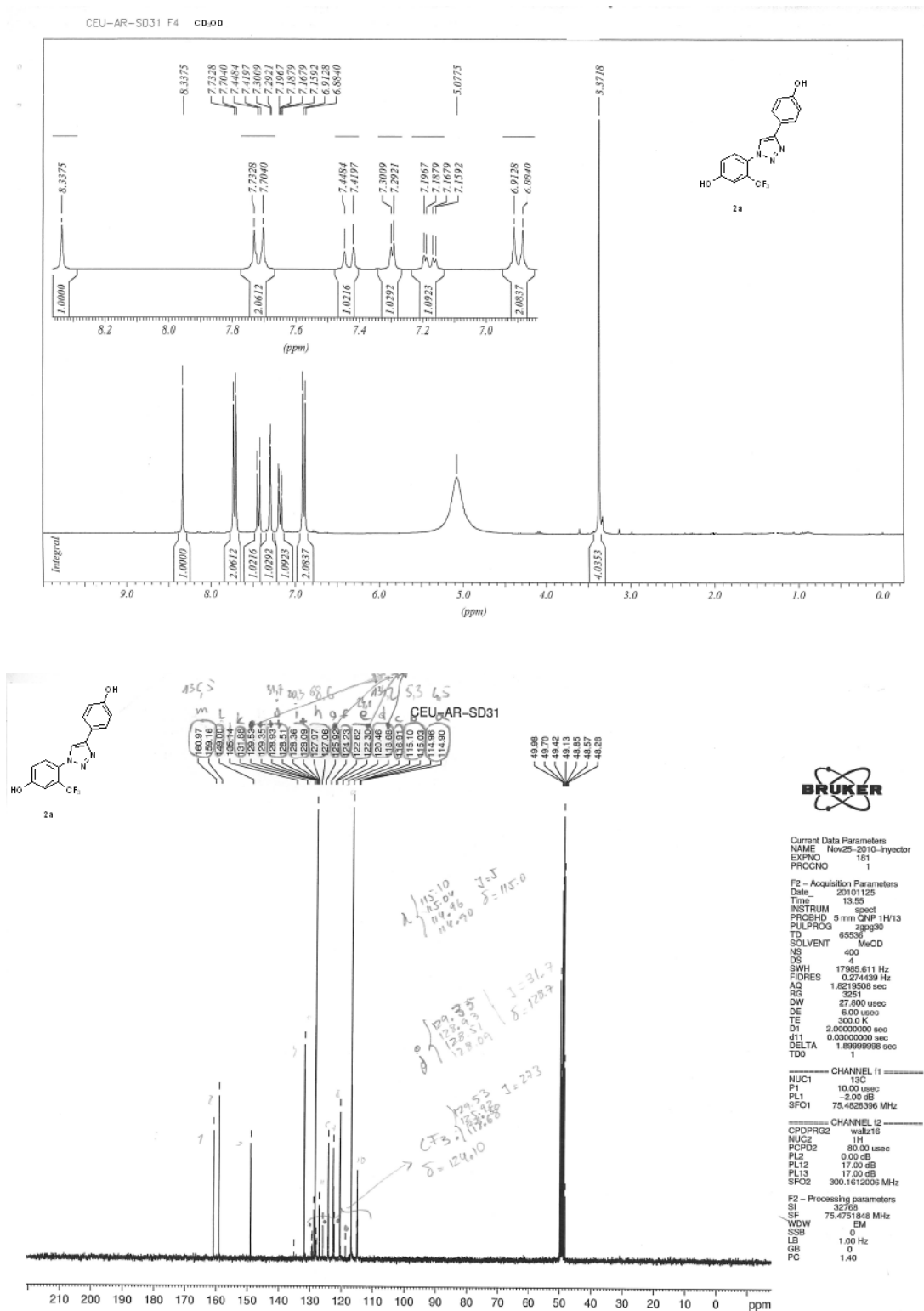
New Clicked Full Agonists of the Estrogen Receptor β

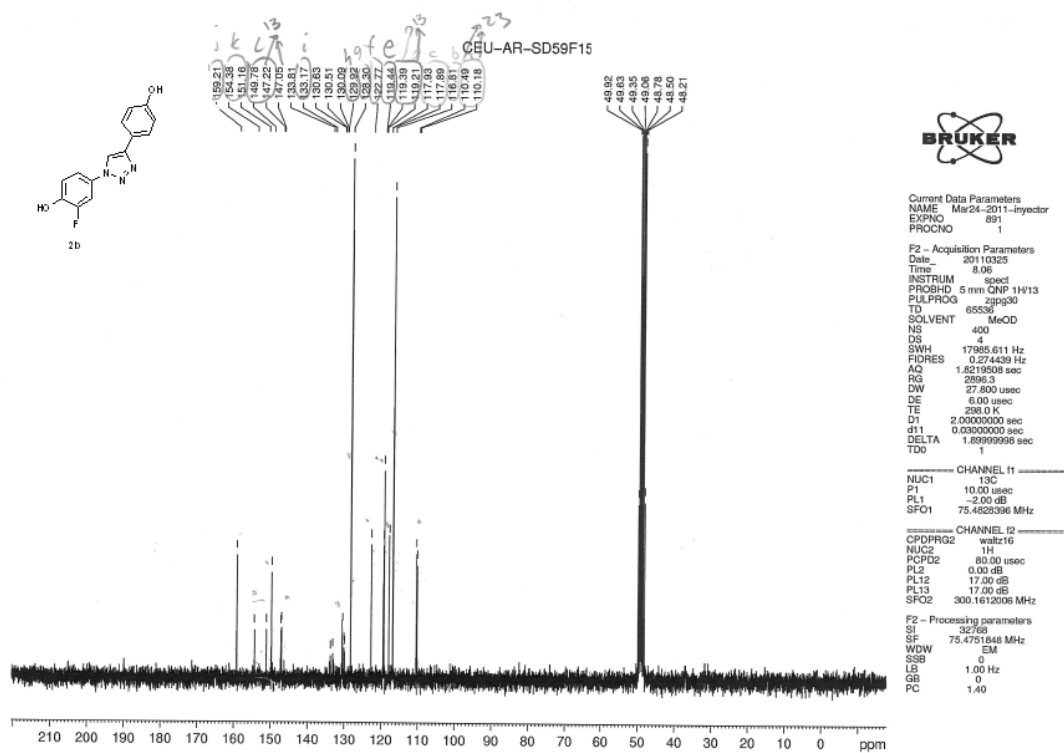
Sebastian Demkowicz,^{a, b} Kamila Filipiak,^{a, c} Maciej Maslyk,^{a, c} Jakub Ciepielski,^{a, d} Sonia de Pascual-Teresa,^e Sonsoles Martín-Santamaría,^a Beatriz de Pascual-Teresa,^{*a} Ana Ramos.^{*a}

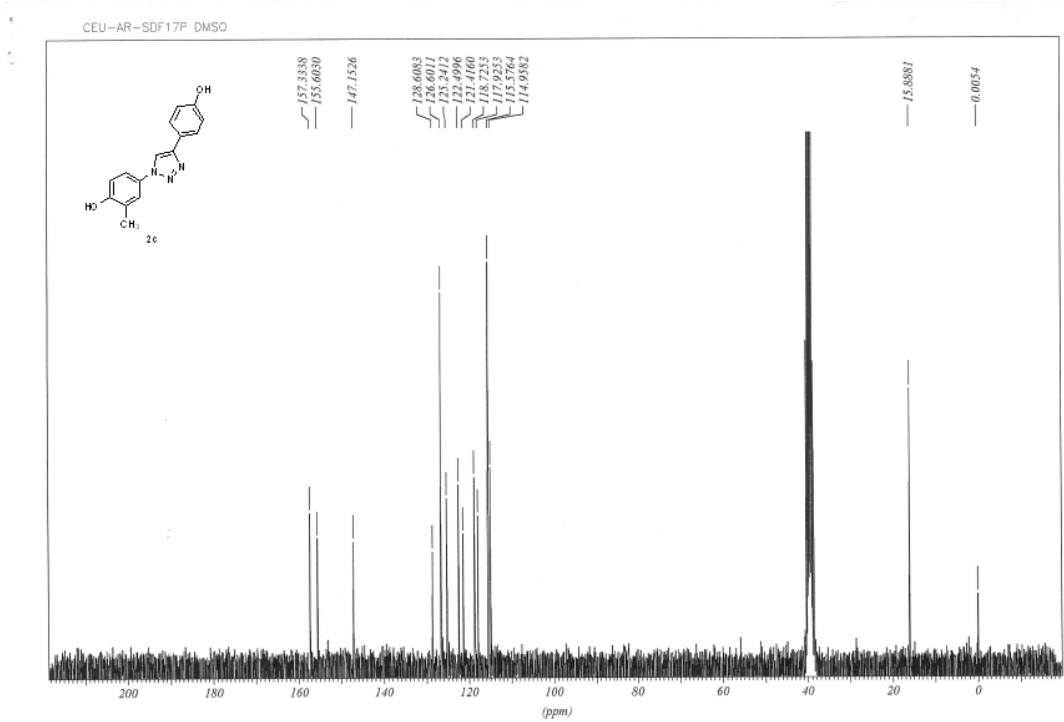
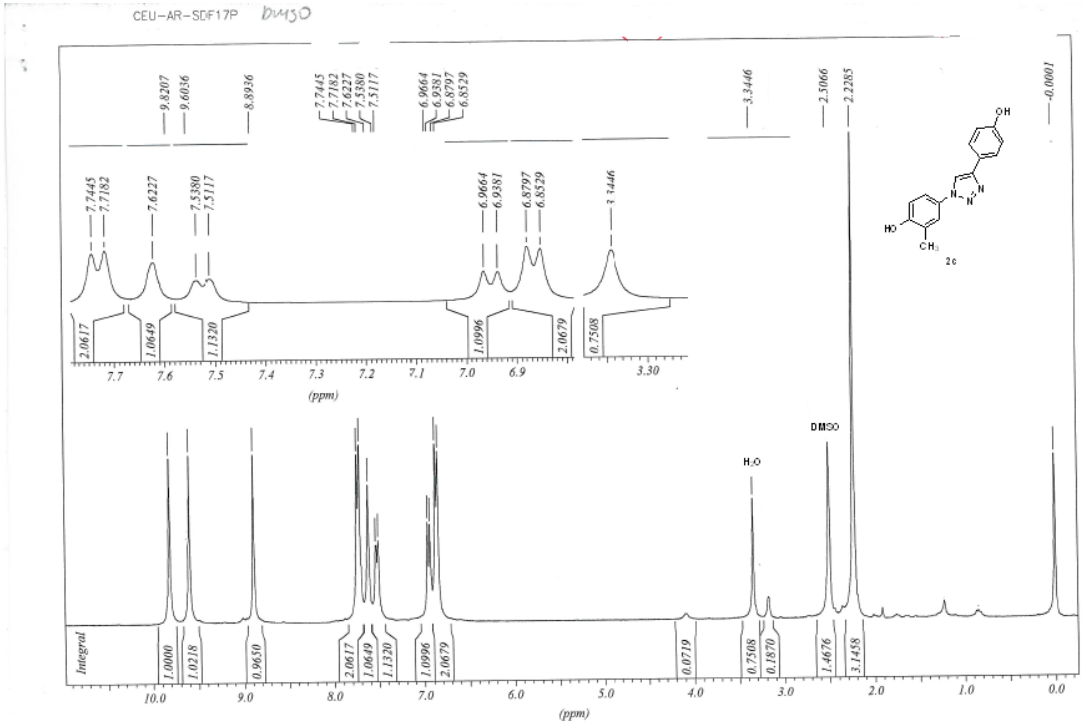
^a Departamento de Química, Facultad de Farmacia, Universidad CEU San Pablo, 28668-Boadilla del Monte, Madrid, Spain.
E-mail: aramgon@ceu.es, bpaster@ceu.es; Fax: (+34)913510496; Tel: (+34)913724796;
^b Department of Organic Chemistry, Gdansk University of Technology, 11/12 G. Narutowicza St., 80-233 Gdańsk, Poland.
^c Department of Molecular Biology, Faculty of Mathematics and Natural Sciences, The John Paul II Catholic University of Lublin, 20-718 Lublin, Poland.
^d Department of Environmental Biochemistry and Chemistry, Faculty of Mathematics and Natural Sciences, The John Paul II Catholic University of Lublin, 20-718 Lublin, Poland.
^e Institute of Food Science, Food Technology and Nutrition (ICTAN), Spanish National Research Council (CSIC), José Antonio Novais 10, 28040-Madrid, Spain.

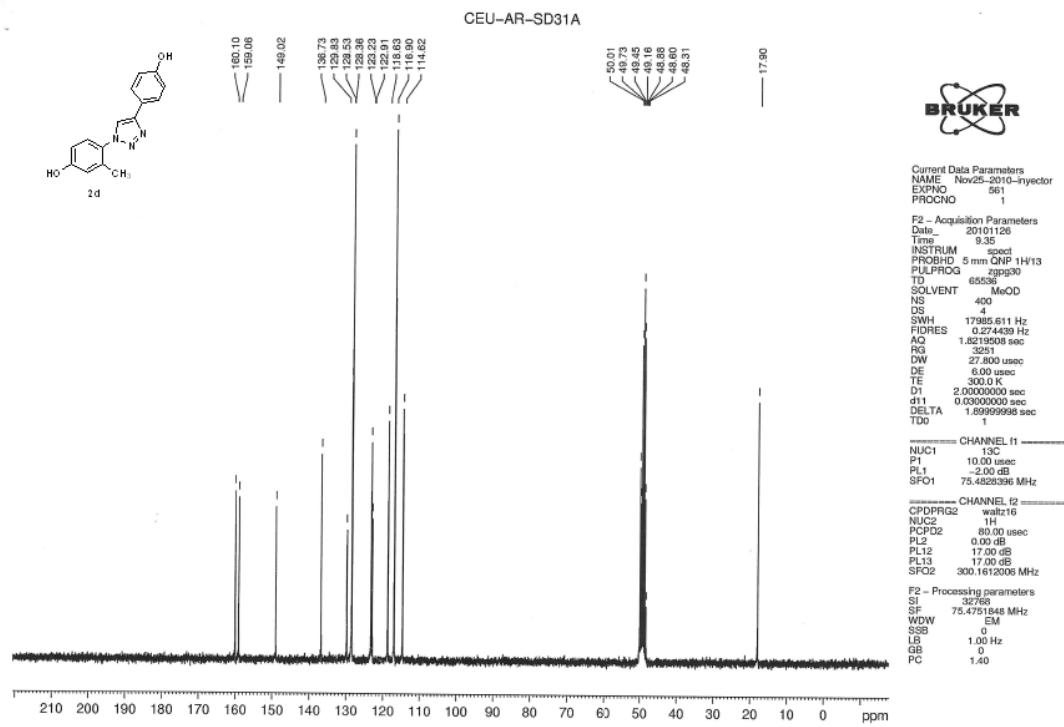
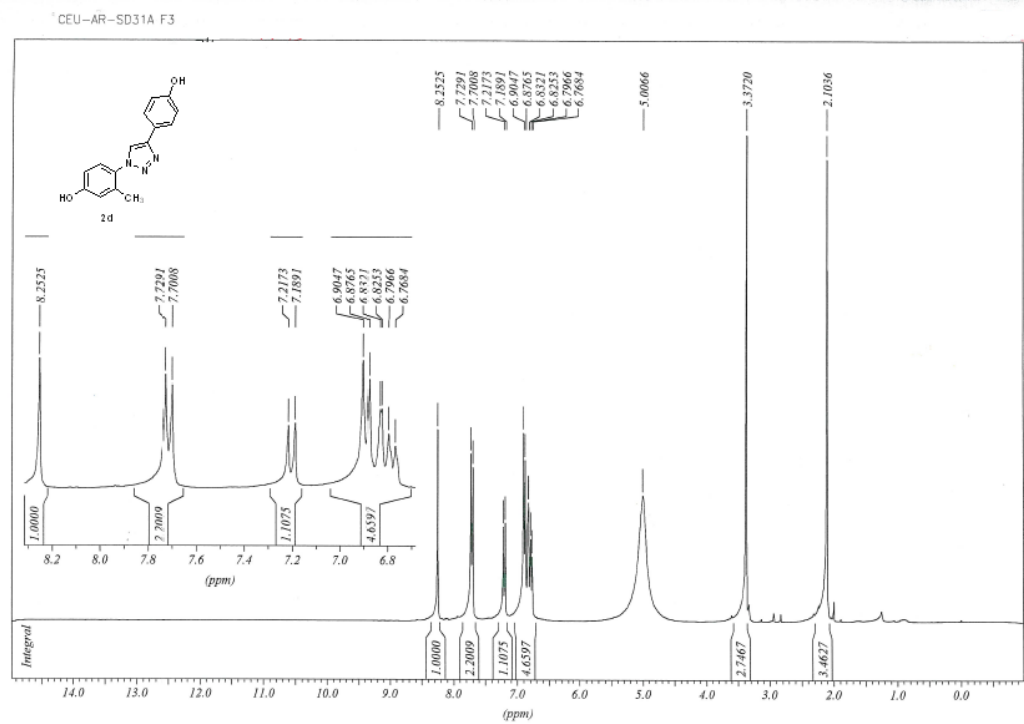
Table of Contents:

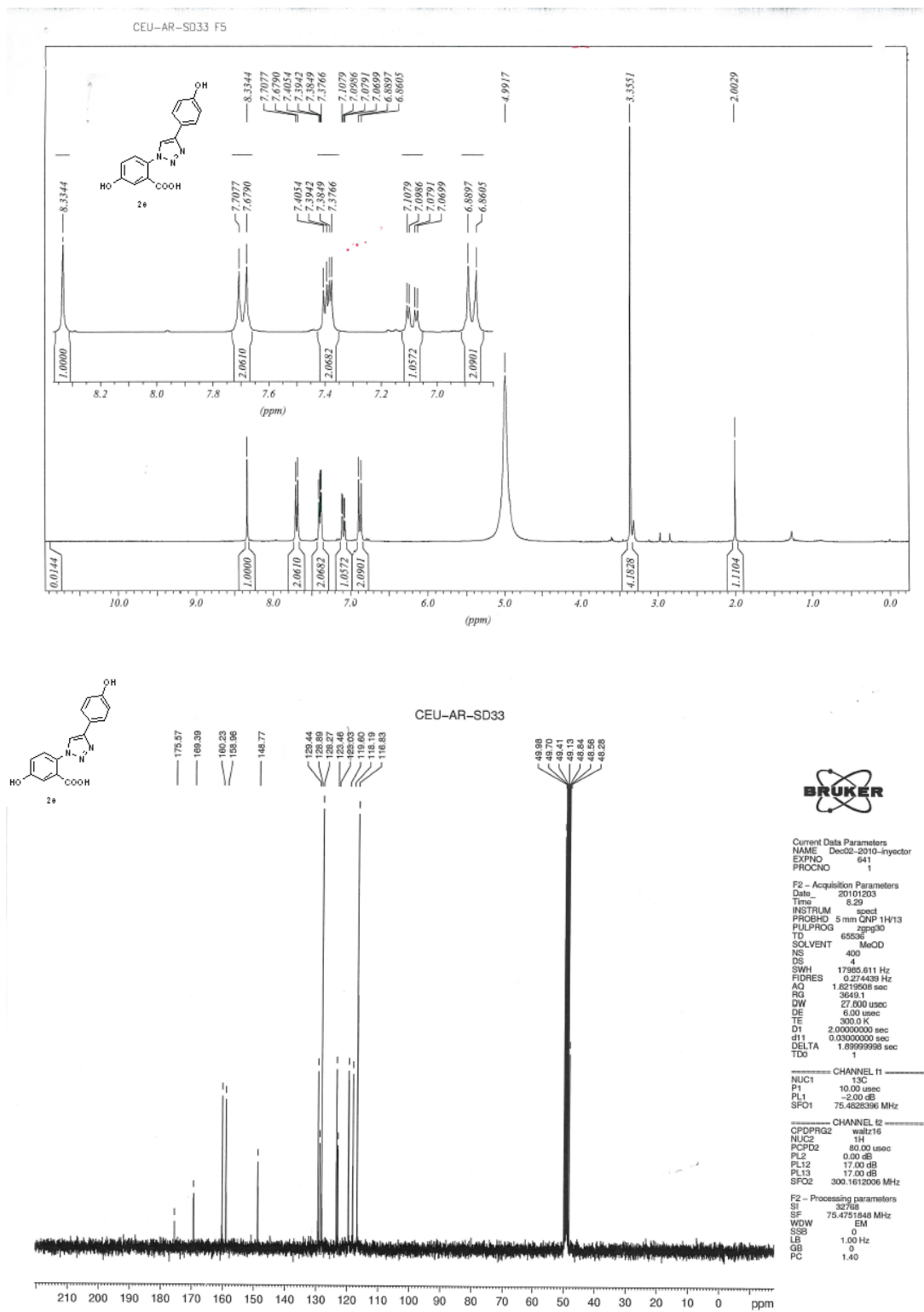
	Pages
1	NMR spectra of compounds 2a-2h , 3a-3f and 3h S2-S16
2	Table S1. Predicted binding energies from the docking studies S17
3	
4	
5	
6	

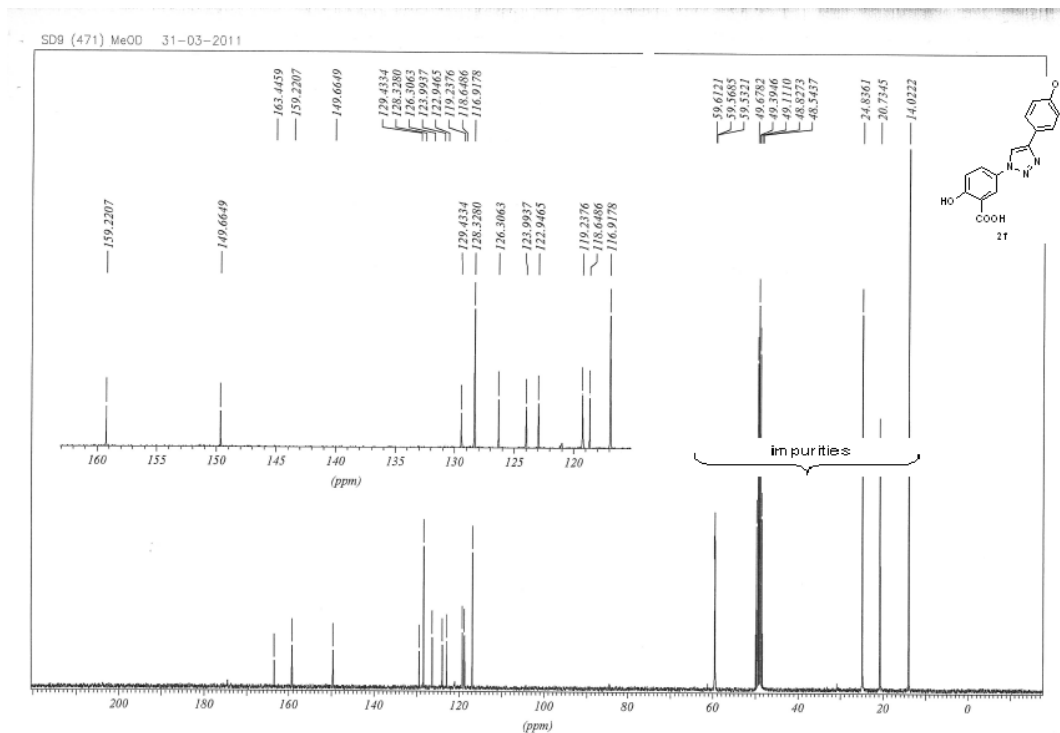
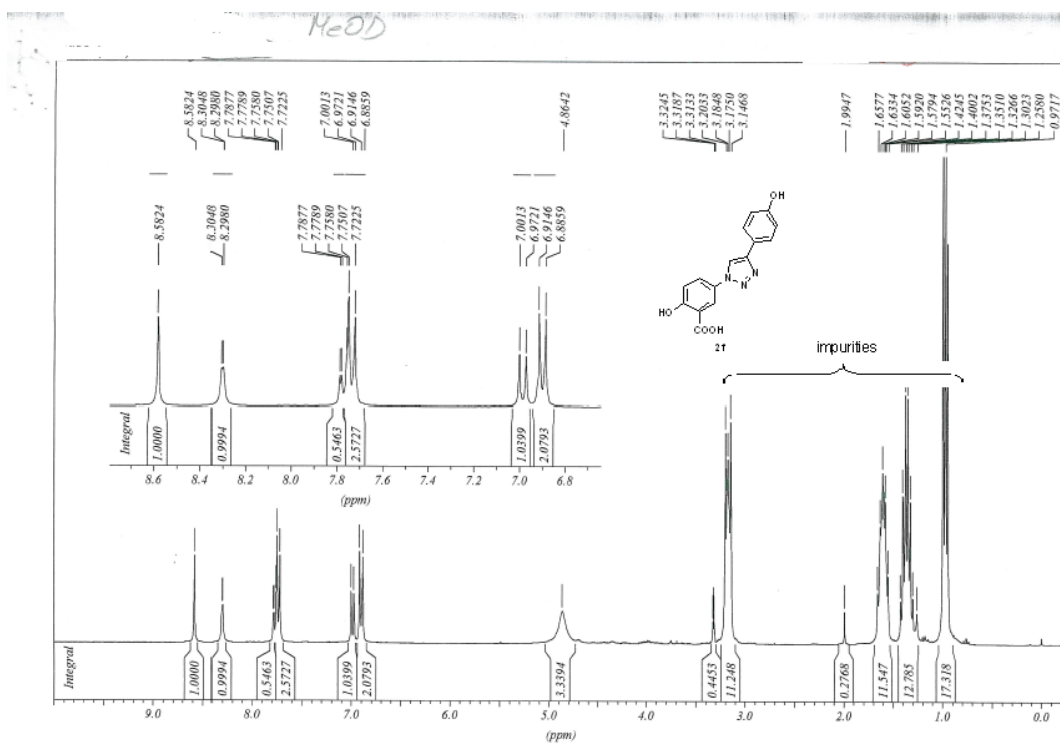




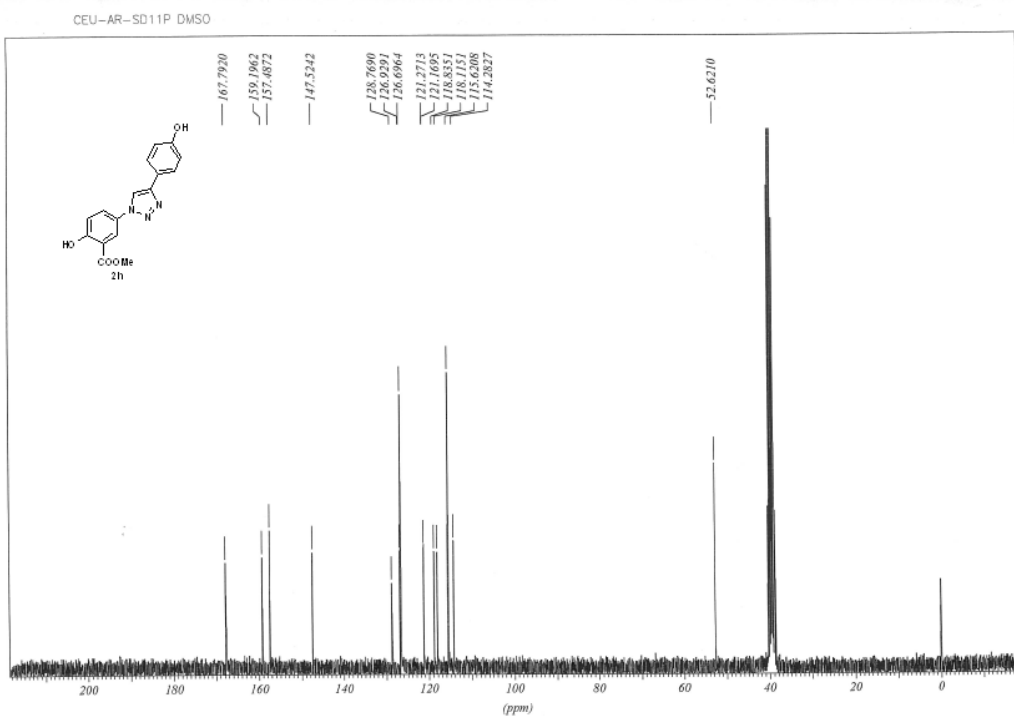
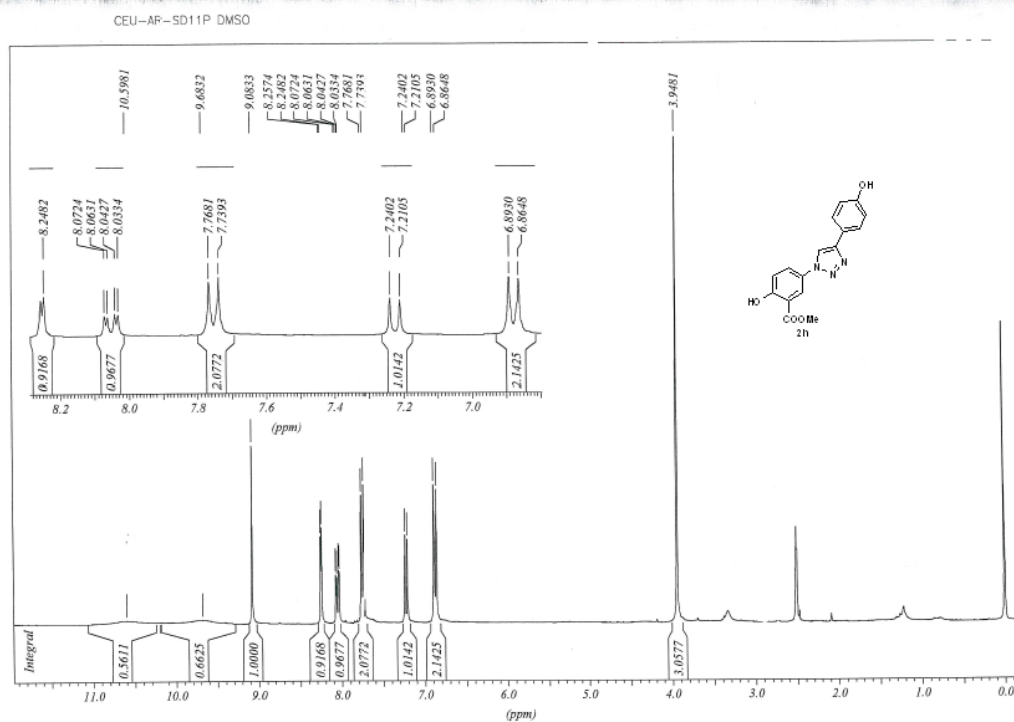


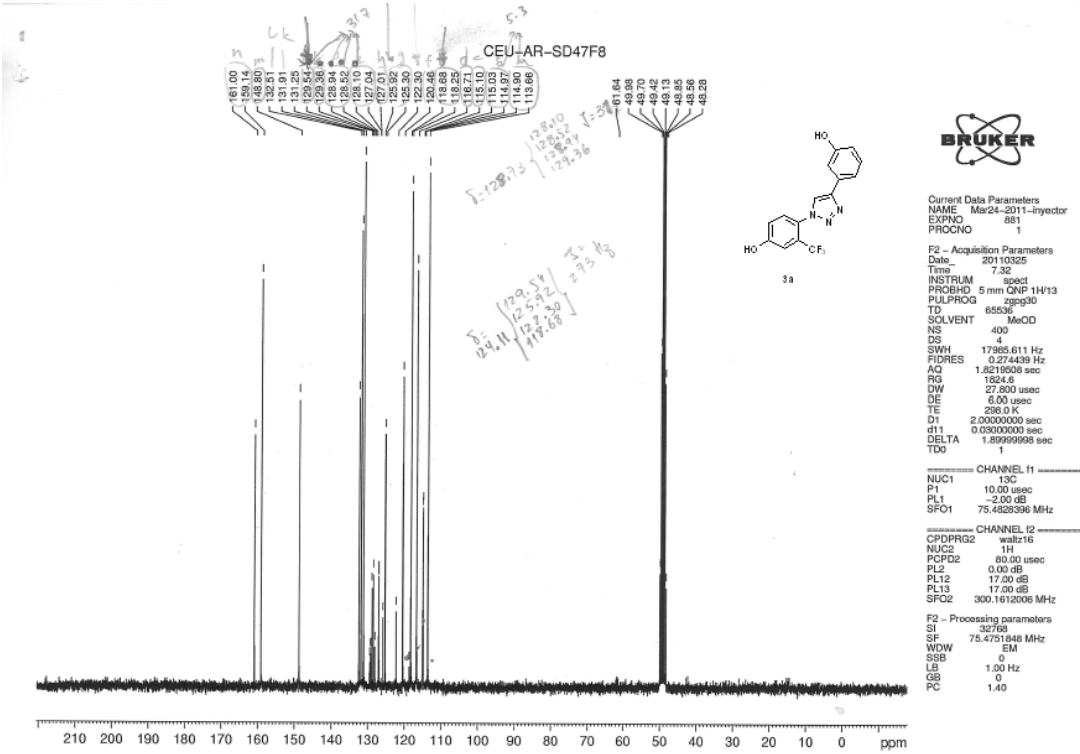
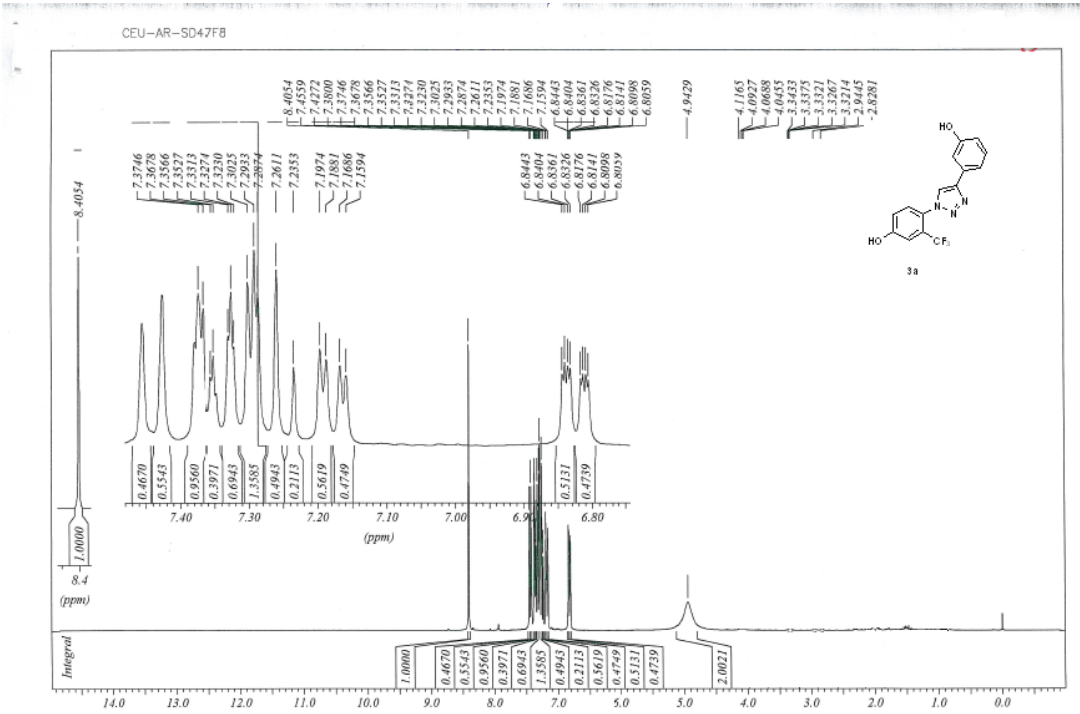


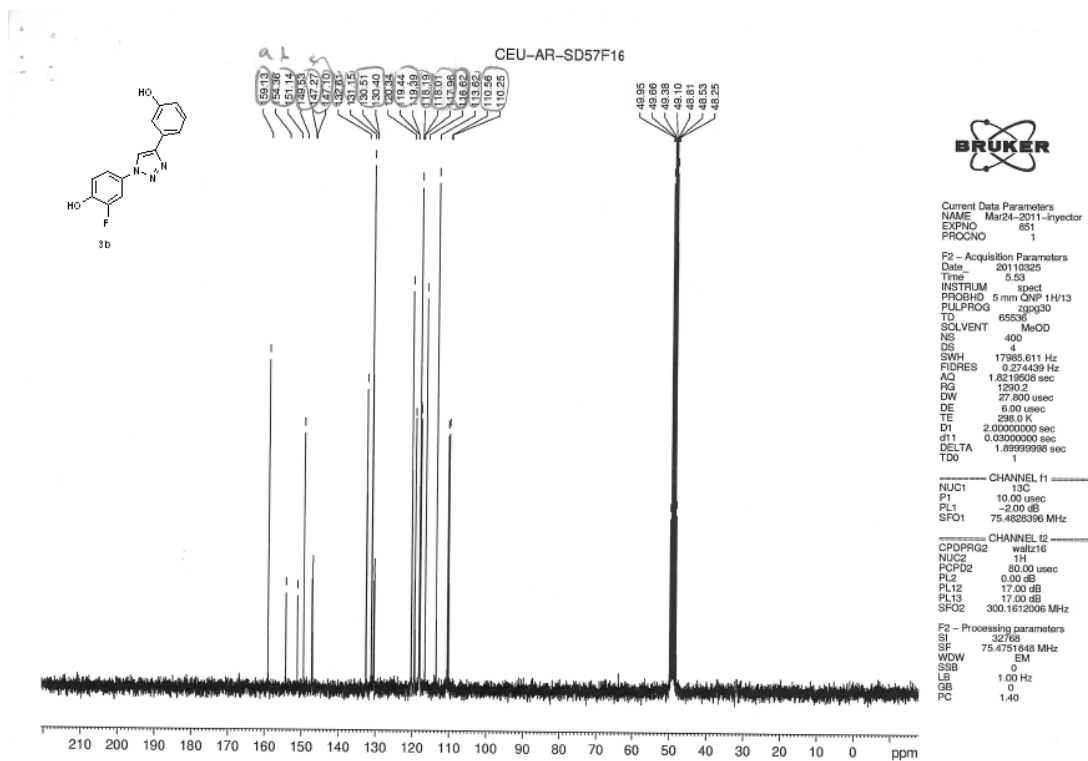


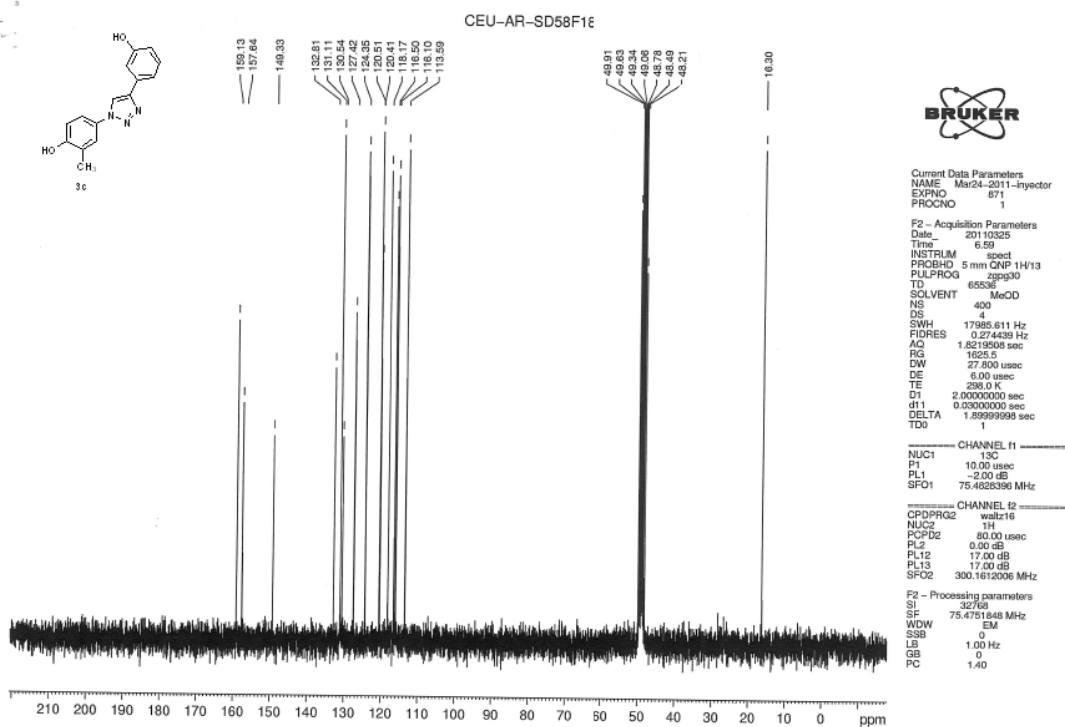


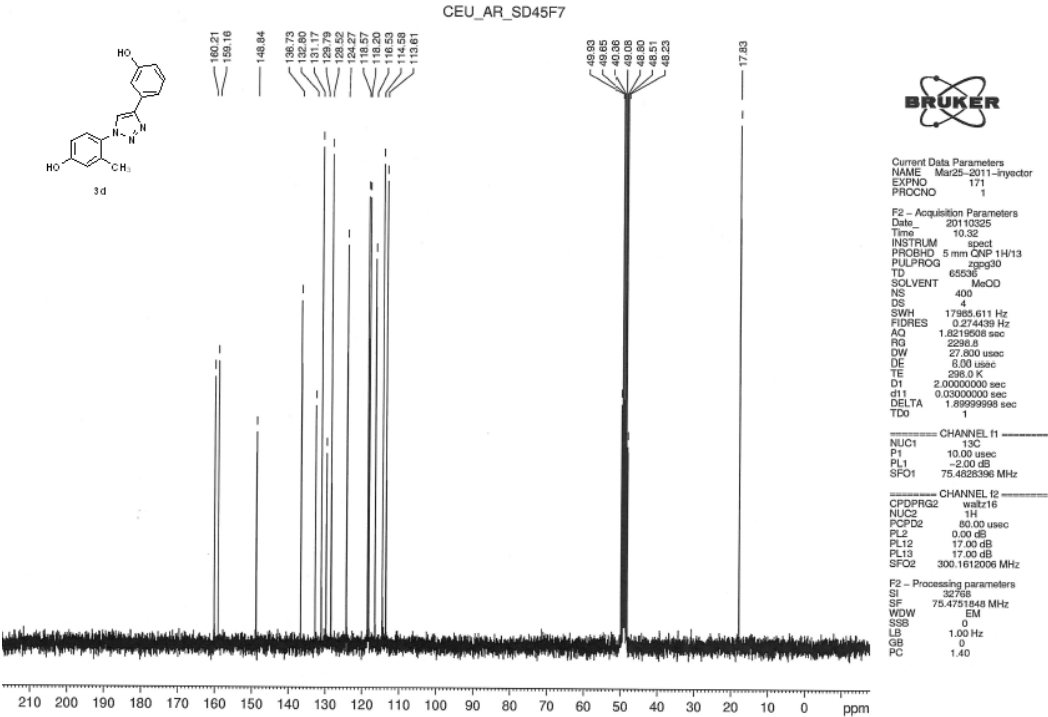
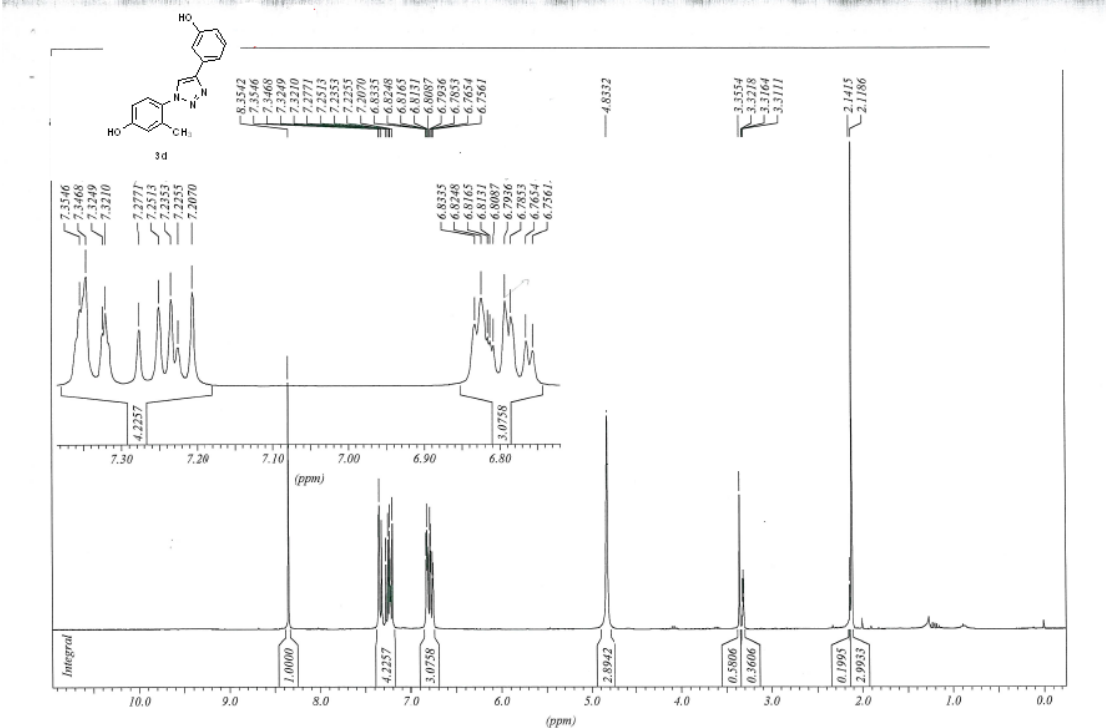


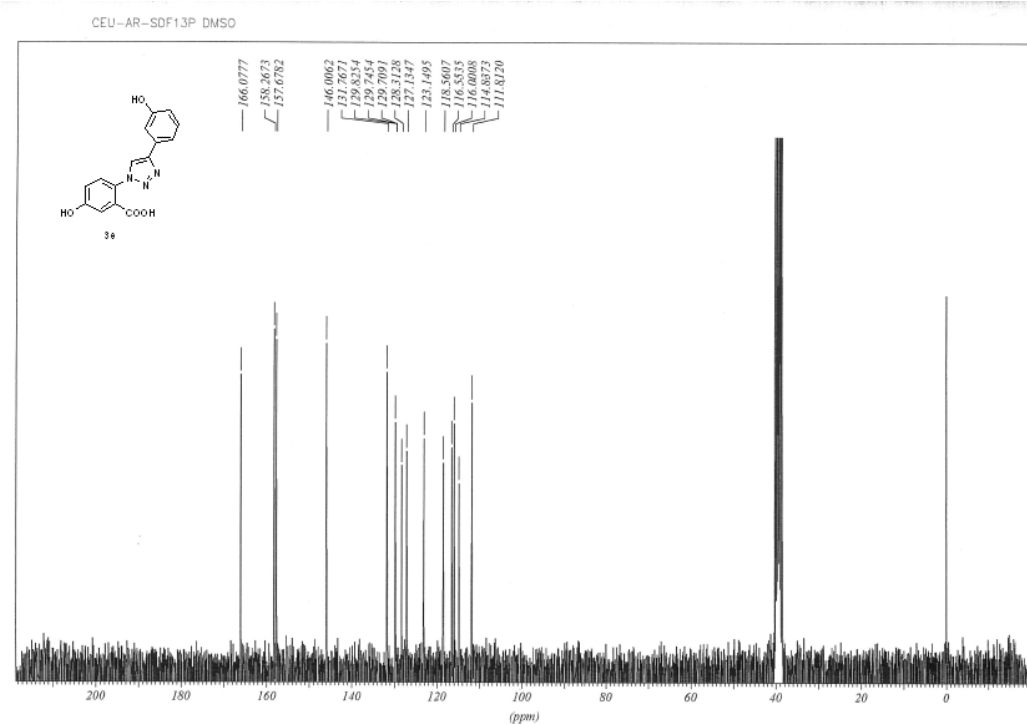
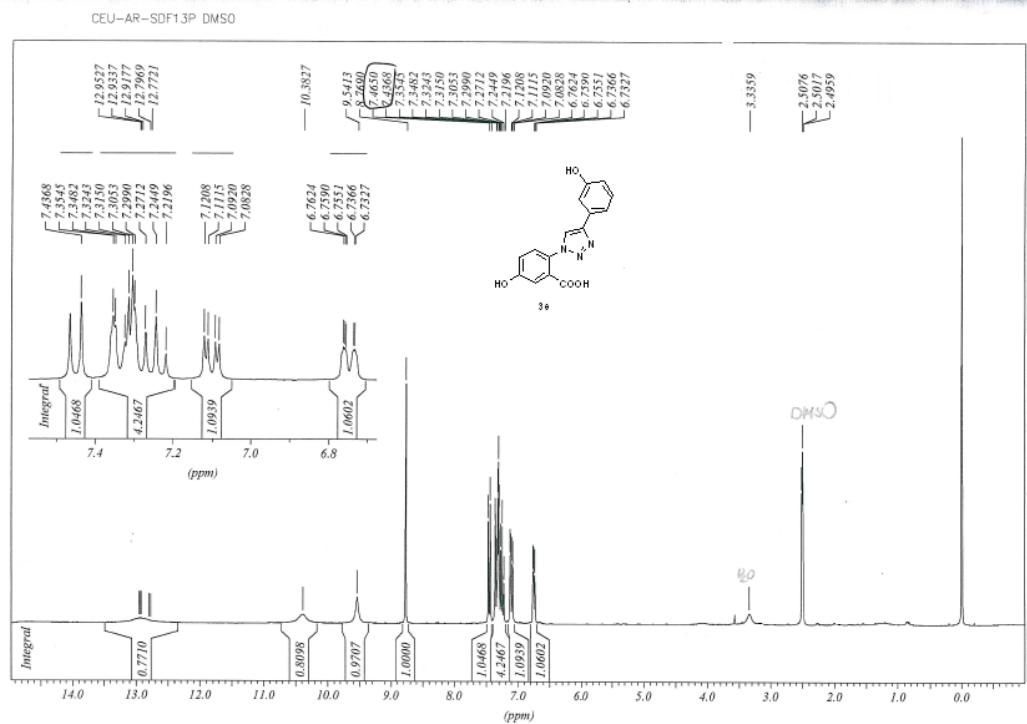


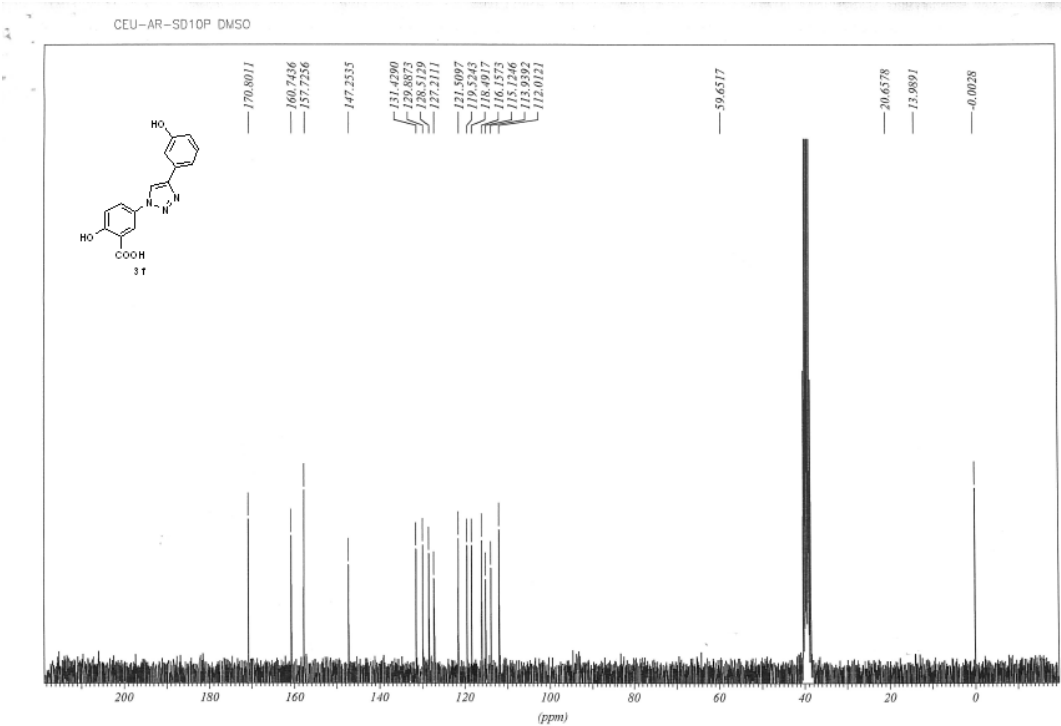
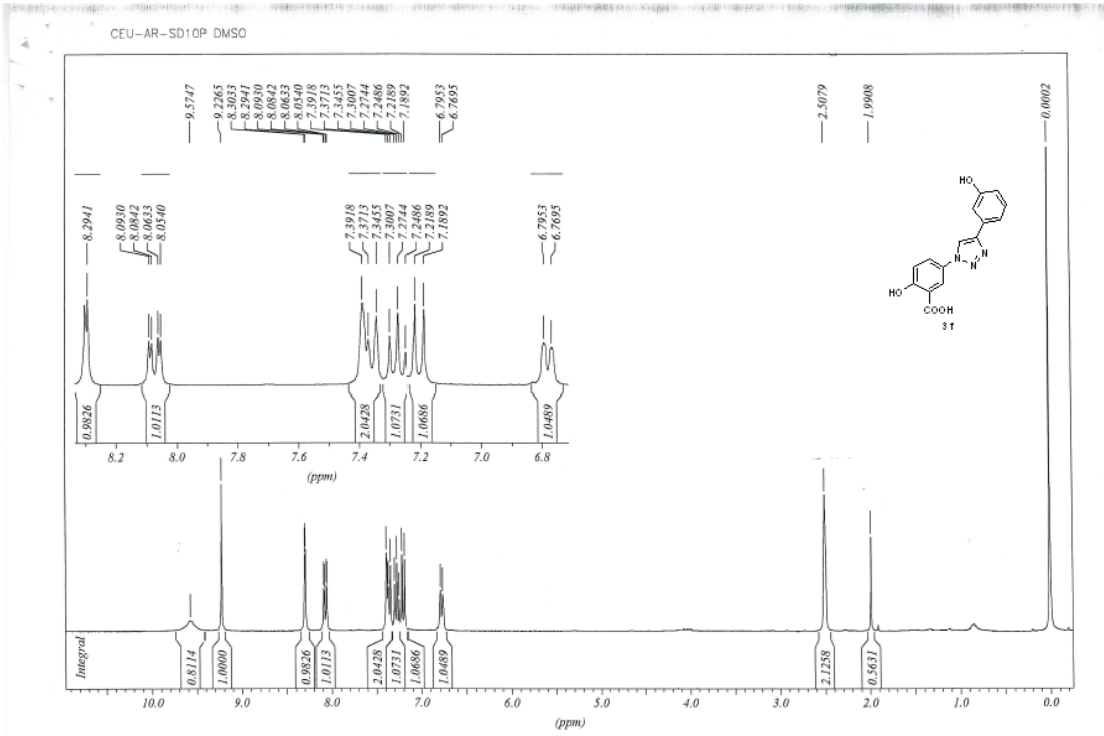












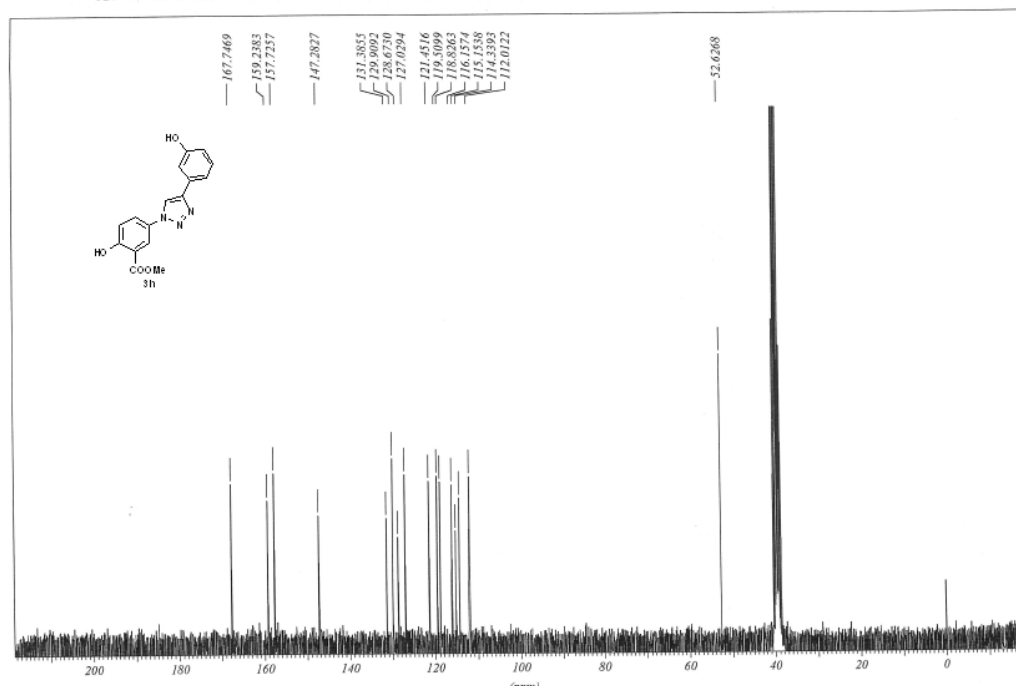
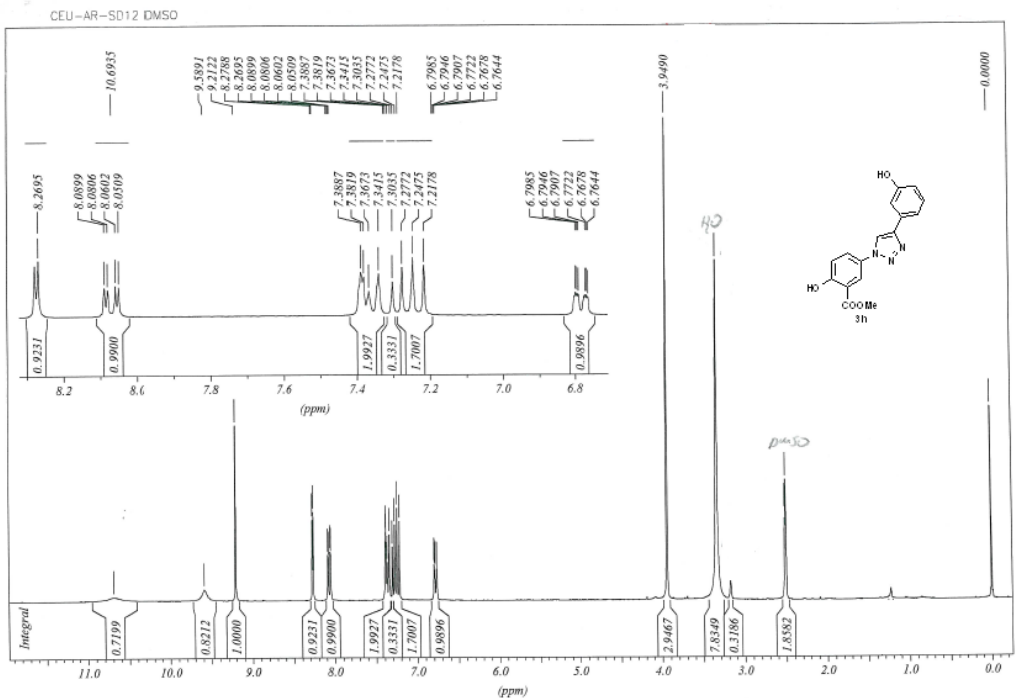


Table S1. Predicted binding energies from the docking studies.

Comp.	Binding energy in ER α^a (kcal/mol)	Binding energy in ER β^b (kcal/mol)
2a	-7.9	-8.1
2b	-4.1	-6.2
2c	-4.9	-9.0
2d	-6.7	-7.8
2e	-6.9	-2.1
2f	-4.8	-9.1
2g	-7.1	-7.3
3a	-7.9 ^c	-8.0
3b	-7.1	-7.4
3c	-5.3	-9.5
3d	-6.8 ^c	-6.8
3e	-2.6 ^d	-2.7
3f	-5.8	-9.7

^aAll binding poses corresponded to non estradiol-like binding modes unless is specified. ^bAll binding poses corresponded to estradiol-like binding modes. ^cEstradiol-like binding pose. ^dOutside the ligand binding domain.