ESI

Table S1: Selected bond lengths (Å) and angles (°) of ferrocene-conjugates **1-6.**

3-ferrocenyl-estra-1,3,5 (10)-triene-17β-ol **(1)**

Distance (Å)		**Angle (°)**		**Torsion Angle (°)**	
C(17)-O(2)	1.43(8)	C(17)-C(13)-C(14)	100.1(5)	O(1)-C(19)-C(20)-Fe	88.95(7)
O(1)-C(19)	1.35(9)	C(16)-C(19)-C(20)	111.8(7)	O(1)-C(19)-O(3)-C(21)	3.6(1)

16-ferrocenylidene-3-hydroxyestra-1,3,5 (10)-triene-17-one **(2a)**

Distance (Å)		**Angle (°)**		**Torsion Angle (°)**	
C(17)-O(2)	1.22(3)	C(17)-C(13)-C(14)	128.90(2)	C(16)-C(19)-C(20)-Fe	79.1(3)
C(16)-C(19)	1.35(3)	C(16)-C(19)-C(20)	128.90(2)	C(17)-C(16)-C(19)-C(21)	167.72(2)

16-ferrocenylidene-3-hydroxyestra-1,3,5 (10)-triene-17-one **(2b)**

Distance (Å)		**Angle (°)**		**Torsion Angle (°)**	
C(17)-O(2)	1.22(3)	C(17)-C(13)-C(14)	100.60(2)	C(16)-C(19)-C(20)-Fe	253.34(3)
C(16)-C(19)	1.34(3)	C(16)-C(19)-C(20)	128.90(2)	C(17)-C(16)-C(19)-C(21)	161.44(7)

16-ferrocenylidene-estra-1,3,5-triene-3,17-diol **(3A)**

Distance (Å)		**Angle (°)**		**Torsion Angle (°)**	
C(17)-O(2)	1.42(8)	C(17)-C(13)-C(14)	101.40(6)	C(16)-C(19)-C(20)-Fe	43(1)
C(16)-C(19)	1.34(1)	C(16)-C(19)-C(20)	115.30(6)	C(16)-C(19)-C(20)-C(21)	134.0(1)

16-ferrocenylidene-estra-1,3,5-triene-3,17-diol **(3B)**

Distance (Å)		**Angle (°)**		**Torsion Angle (°)**	
C(17)-O(2)	1.43(8)	C(17)-C(13)-C(14)	99.60(5)	C(16)-C(19)-C(20)-Fe	82.4(9)
C(16)-C(19)	1.32(8)	C(16)-C(19)-C(20)	129.40(7)	C(16)-C(19)-C(20)-C(21)	177.4(8)

16-ferrocenemethyl-3-hydroxyestra-1,3,5(10)-triene-17-one **(4)**

Distance (Å)		**Angle (°)**		**Torsion Angle (°)**	
C(17)-O(2)	1.20(9)	C(17)-C(13)-C(14)	101.40(6)	C(16)-C(19)-C(20)-Fe	172.9(5)
C(16)-C(19)	1.51(1)	C(16)-C(19)-C(20)	115.30(6)		

16-ferrocenemethyl-estra-1,3,5(10)-triene-3,17β-diol **(5)**

	5A	**5B**	**5C**	**5D**	**5E**	**5F**
Bond Distance (Å)						
C(17)-O(2)	1.40(1)	1.442(1)	1.43(1)	1.49(1)	1.43(2)	1.44(1)
C(16)-C(19)	1.44(2)	1.49(1)	1.50(2)	1.47(2)	1.50(2)	1.56(1)
Bond Angle (°)						
C(17)-C(13)-C(14)	99.00(7)	97.54(6)	100.91(7)	97.99(7)	100.48(8)	98.98(7)
C(16)-C(19)-C(20)	119.70(1)	126.75(6)	114.17(1)	97.01(1)	114.54(1)	110.29(8)
Torsion Angle (°)						
C(16)-C(19)-C(20)-Fe	62.95(2)	164.18(7)	202.4(7)	166.33(9)	159.18(9)	206.98(7)

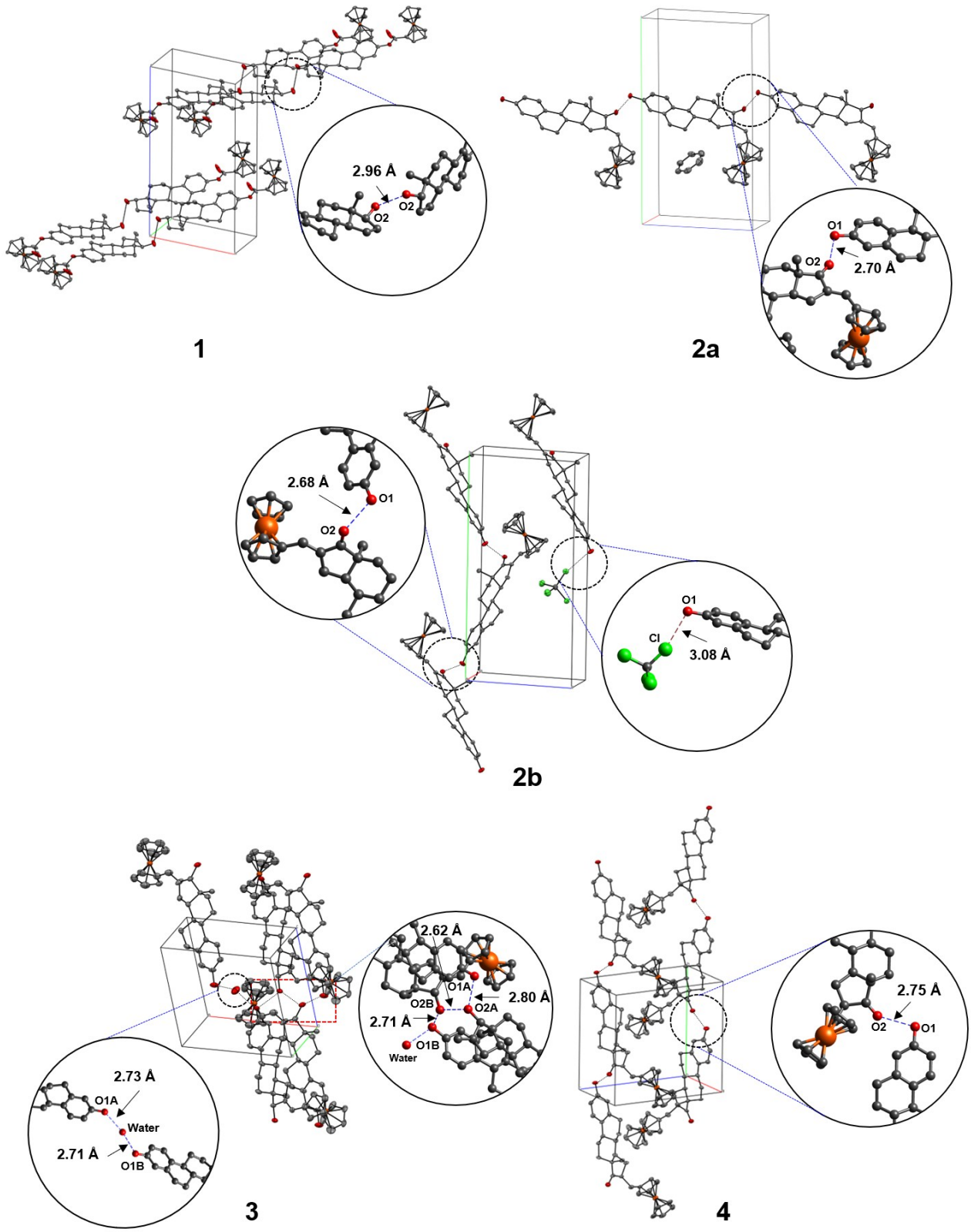


Fig. S1. Illustration of the H-bond assemblies formed in the solid state of the ferrocene-estrogen conjugates **1**, **2a**, **2b**, **3**, and **4**.

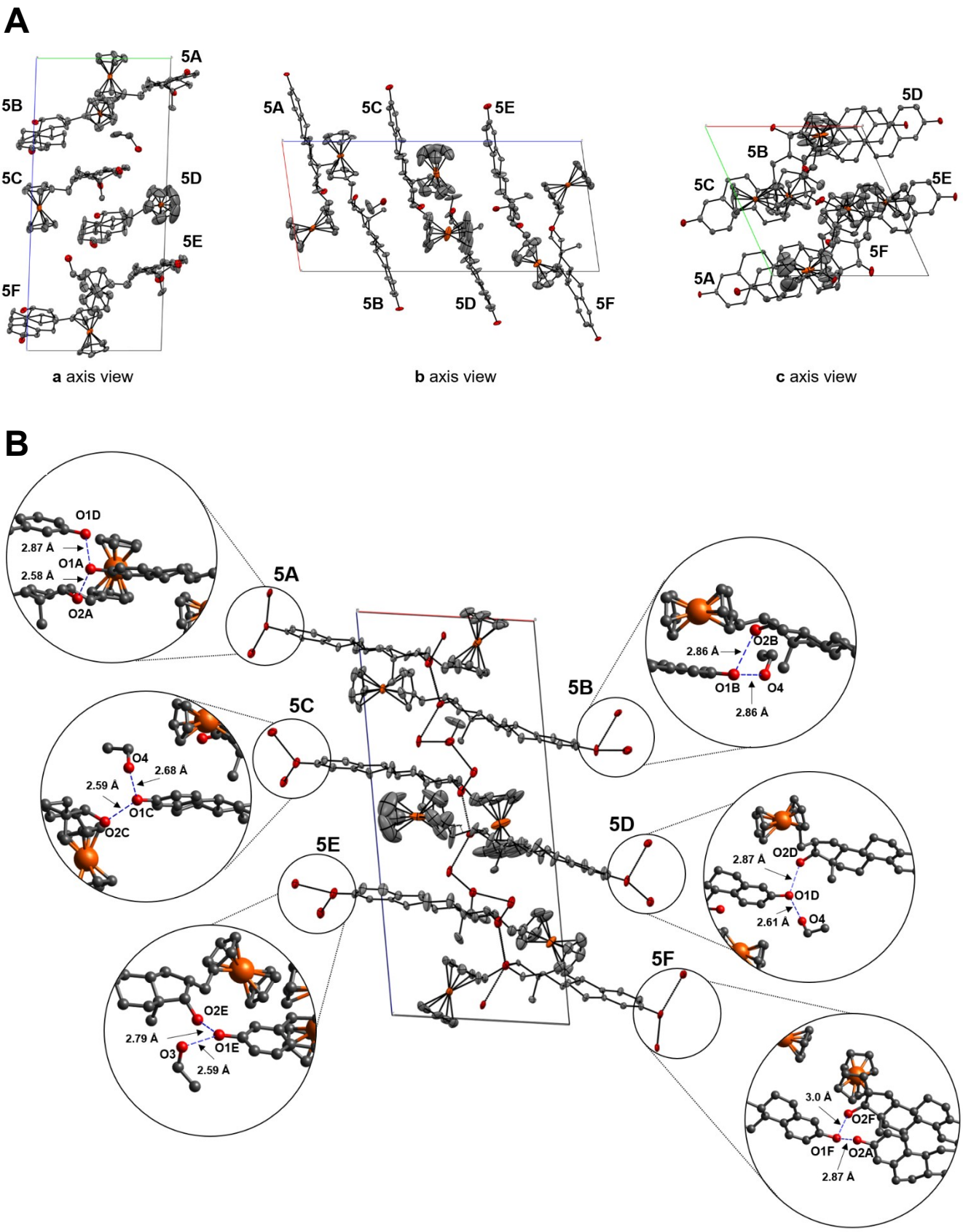


Fig. S2. Illustration of the crystal structure (**A**) along each unit cell axis and the H-bond assemble formed in the solid state of the ferrocene-estrogen conjugates **5** (**B**).

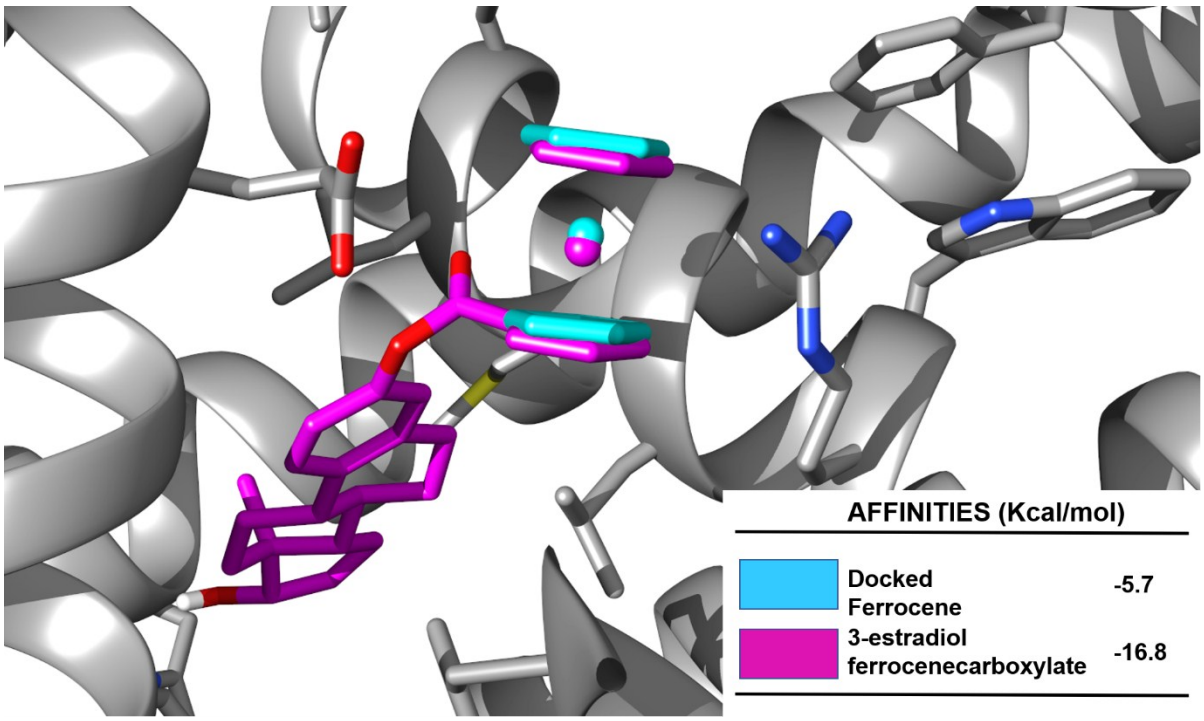


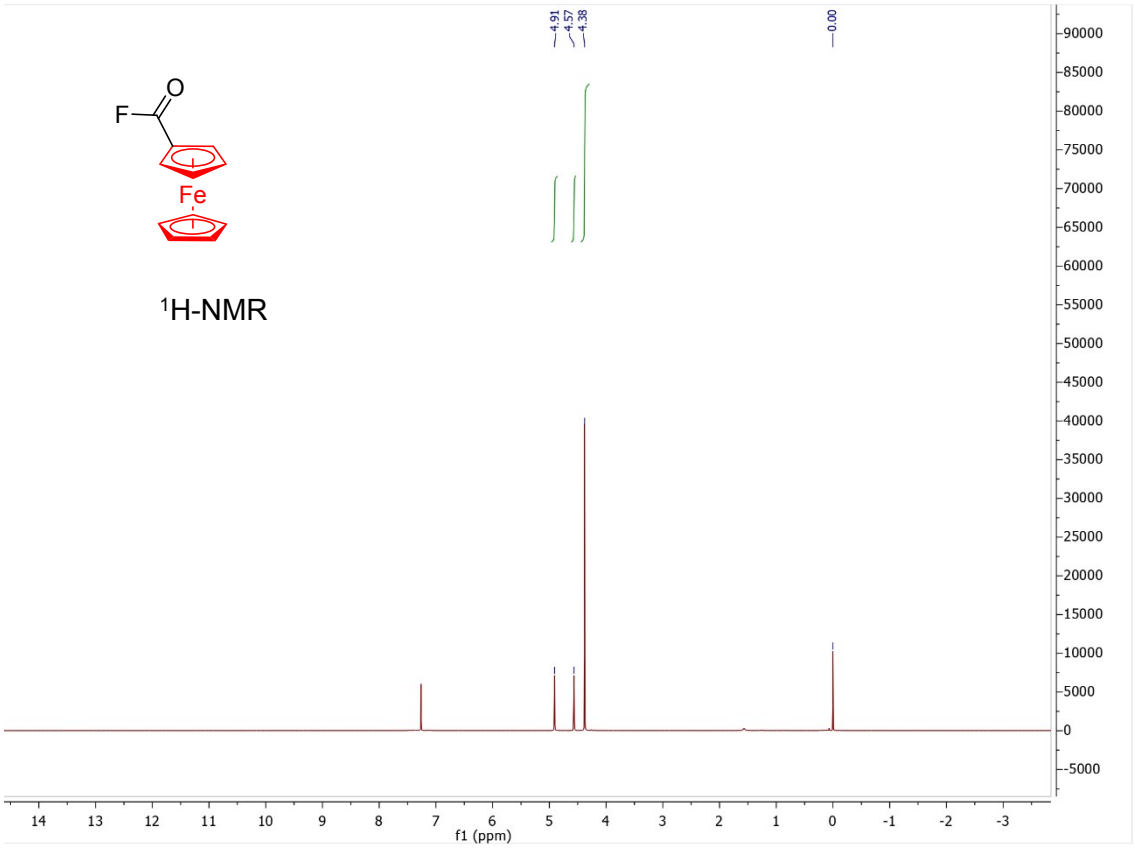
Fig. S3. Ferrocene and 3-estradiol ferrocenecarboxylate (**1**) docking superposition.

Table S2: Tamoxifen Cytotoxic activity on Hormone-Dependent MCF-7 and T-47D and Hormone-Independent MDA-MB-231 Breast Cancer Cell Lines.

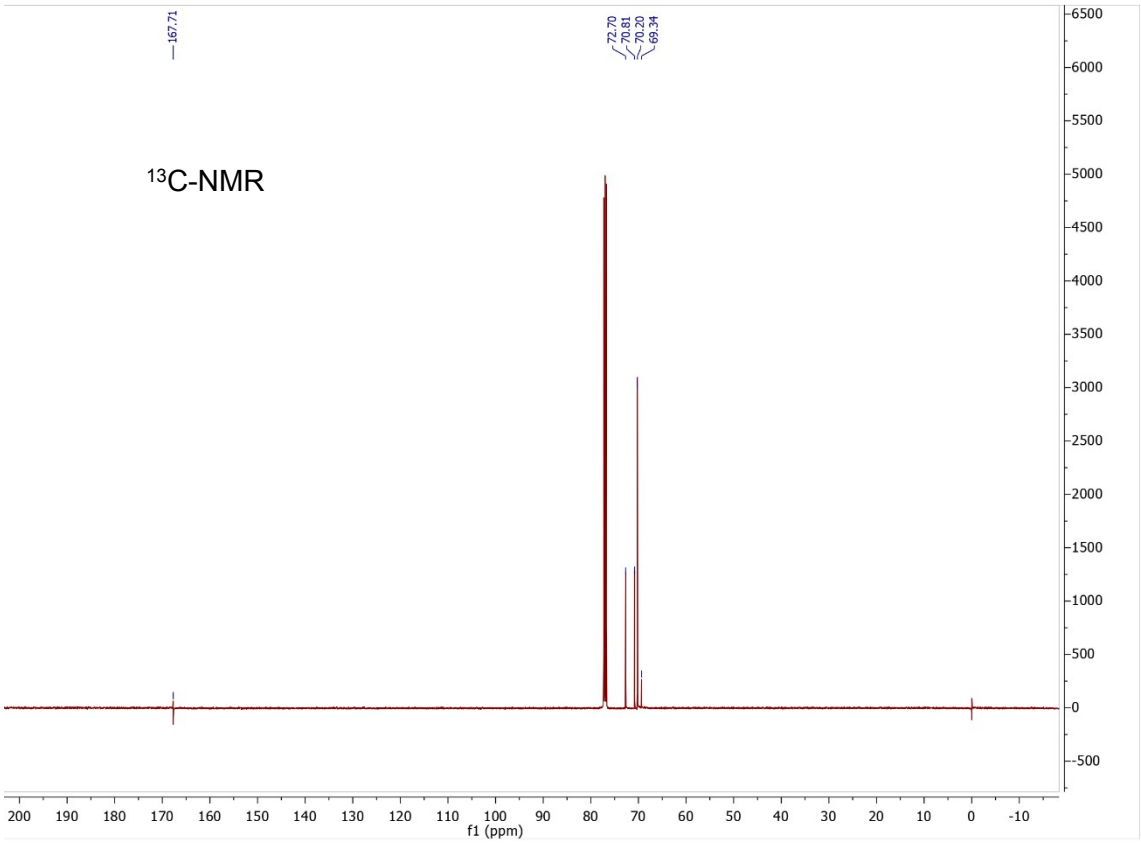
	Tamoxifen IC_{50} on Breast Cancer Cell Lines (μM)		
Method	MCF-7	T-47D	MDA-MB-231
MTT 48Hr	24.76 (0.80)	-	25.84 (1.60)
MTT 72 Hr	17.49 (1.50)	-	25.84 (1.60)
MTT 48 hr	9.06 (0.29)	8.99 (0.55)	13.05 (0.91)

NMR data:

1. Fluorocarbonylferrocene

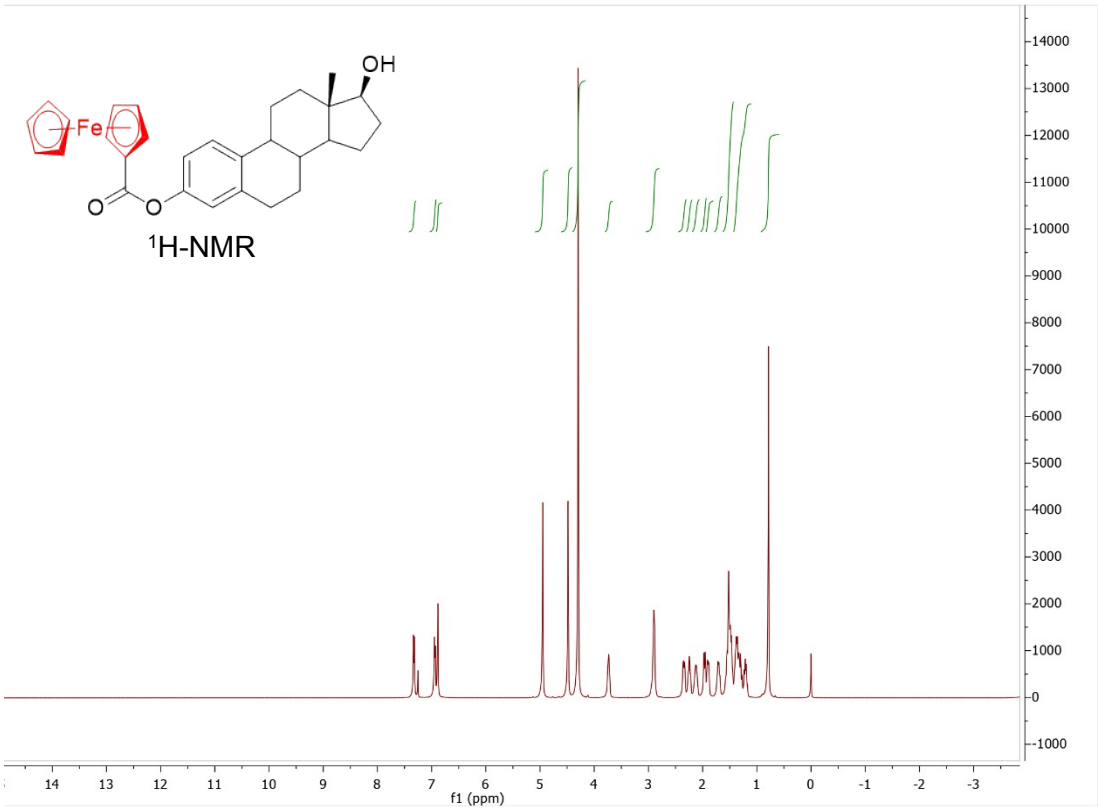


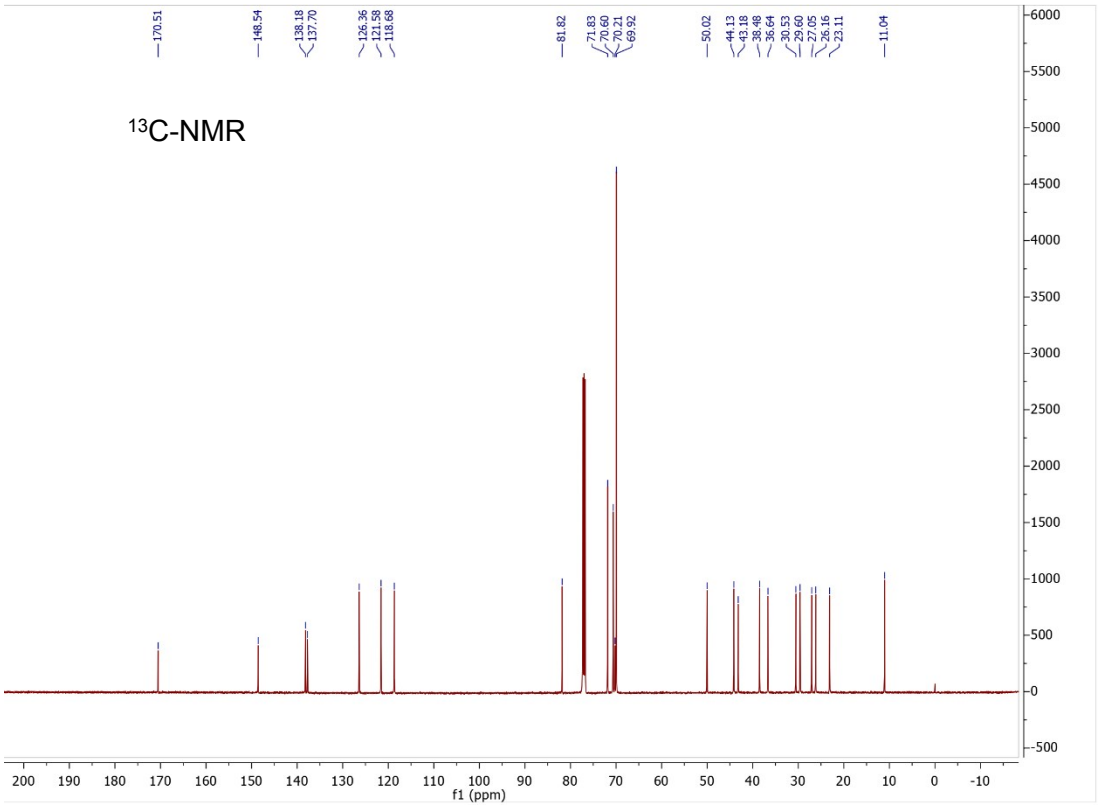
^{1}H-NMR



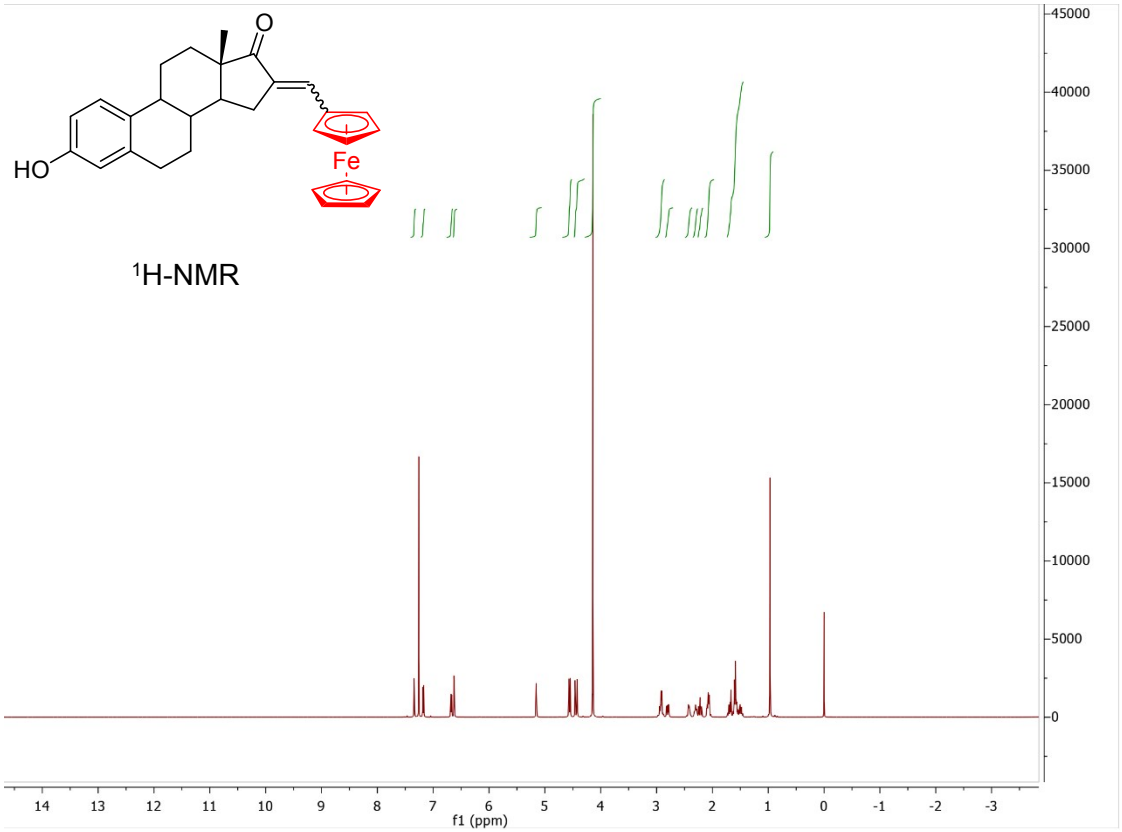
^{13}C-NMR

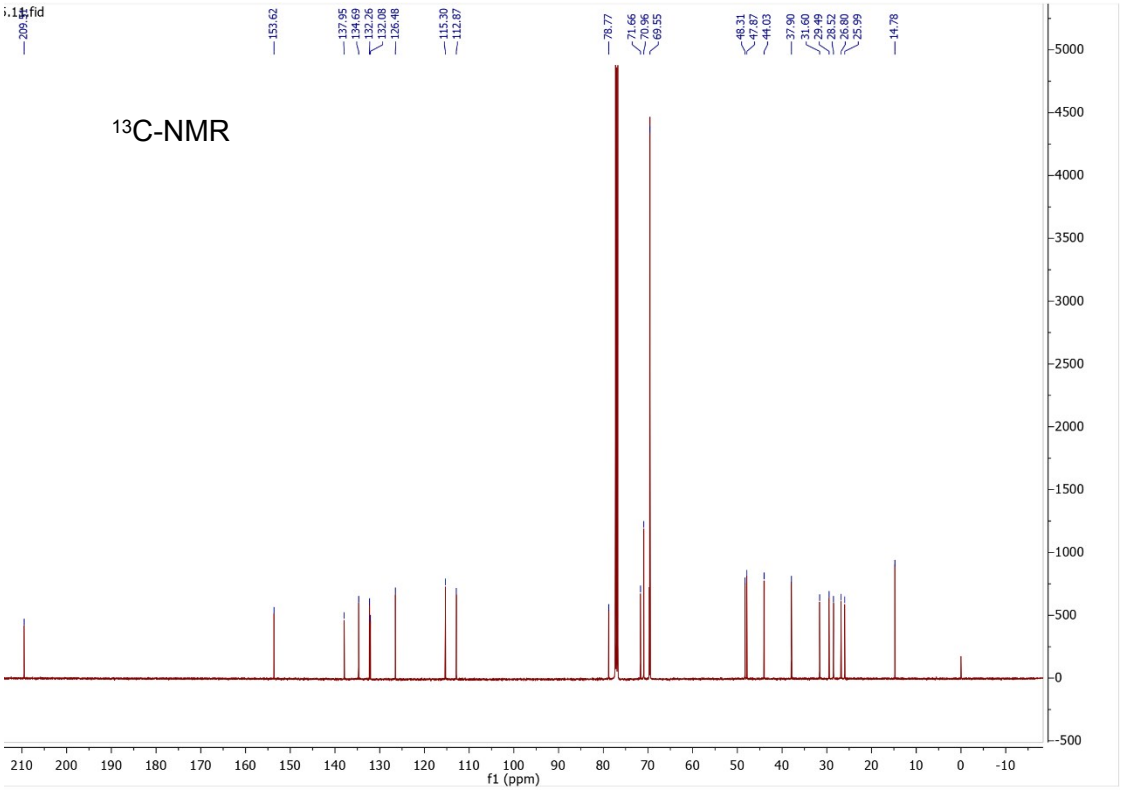
2. 3-estradiol ferrocenecarboxylate (**1**)



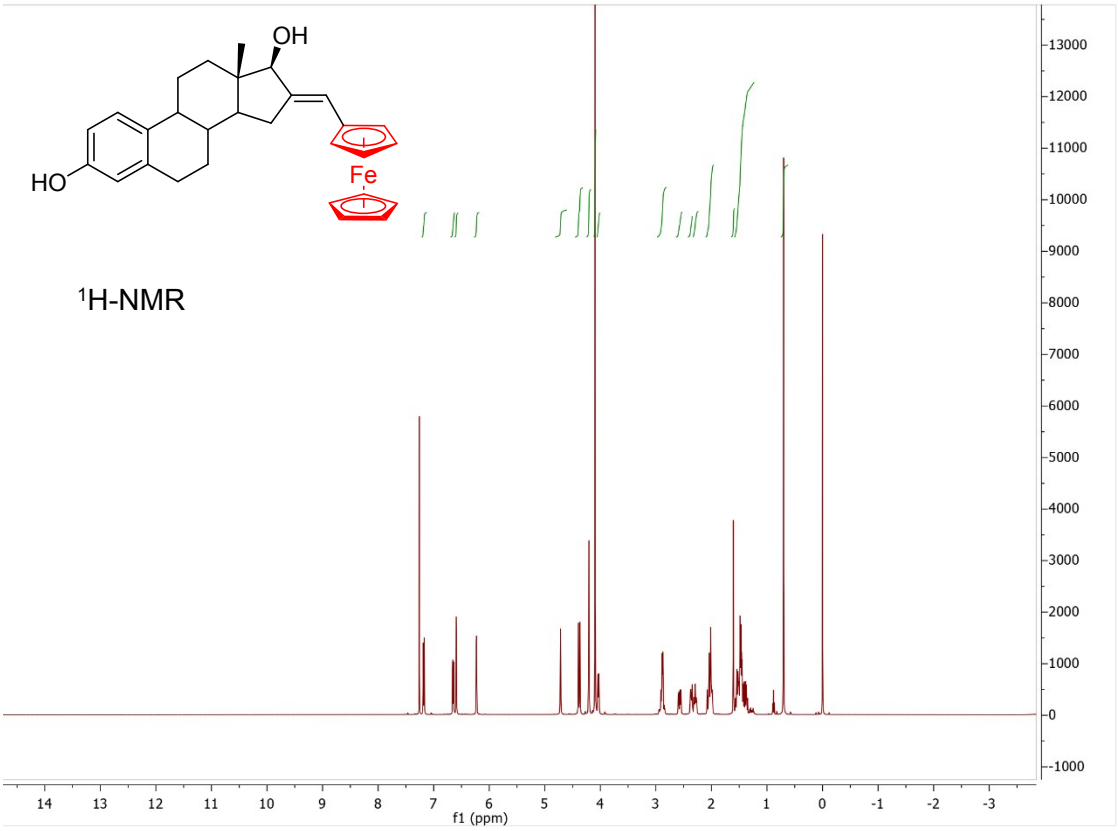


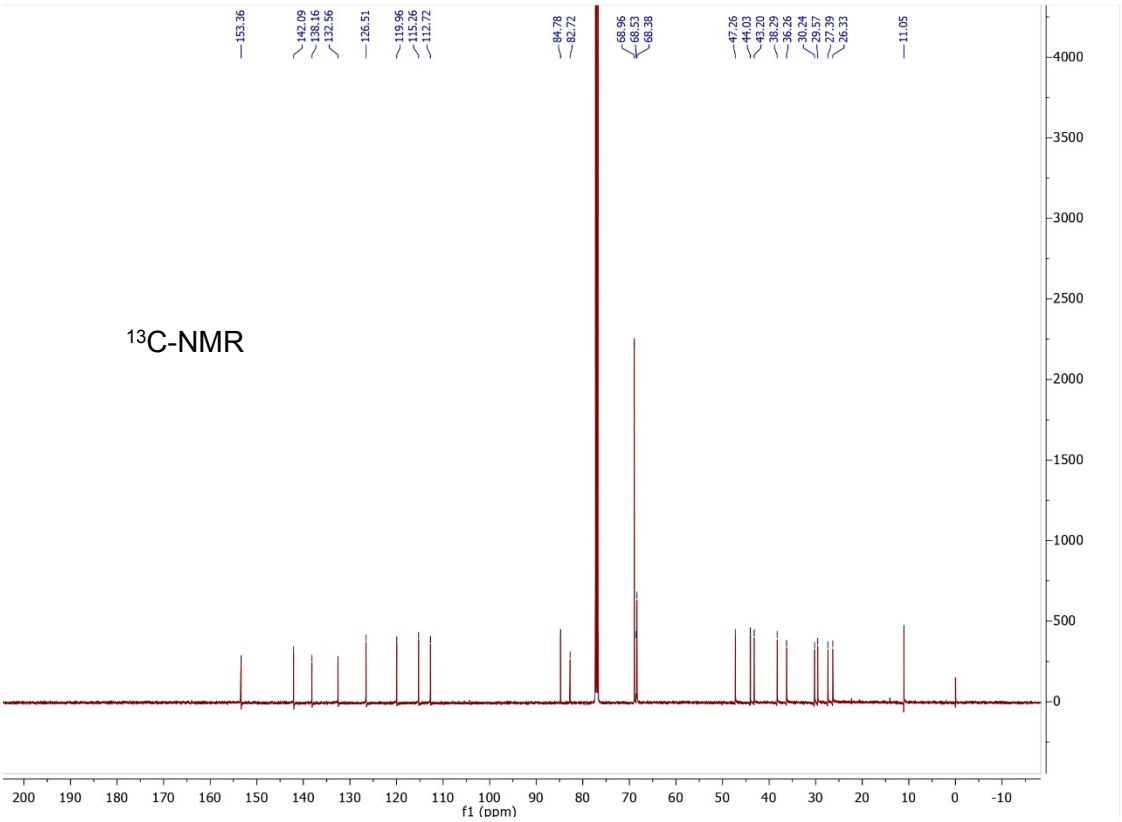
3. 16-ferrocenylidene-3-hydroxyestra-1,3,5 (10)-triene-17-one (**2**)



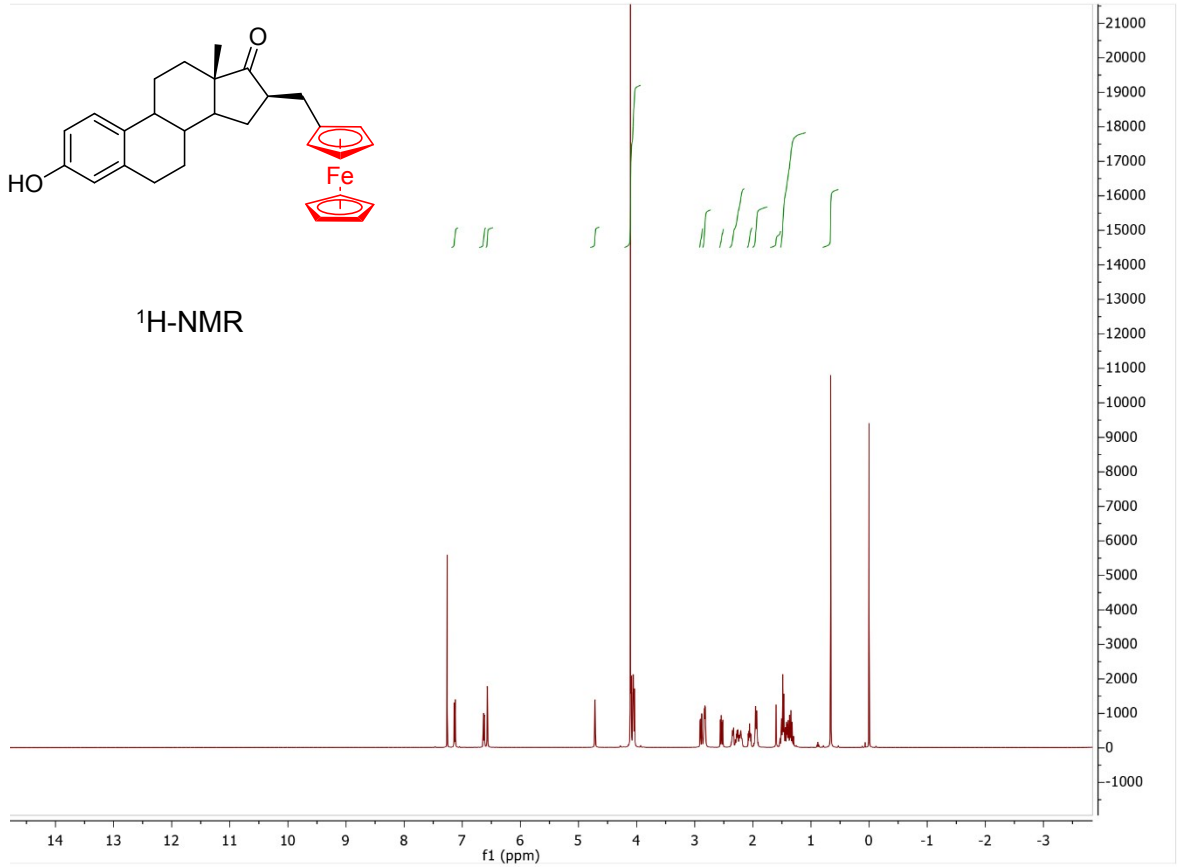


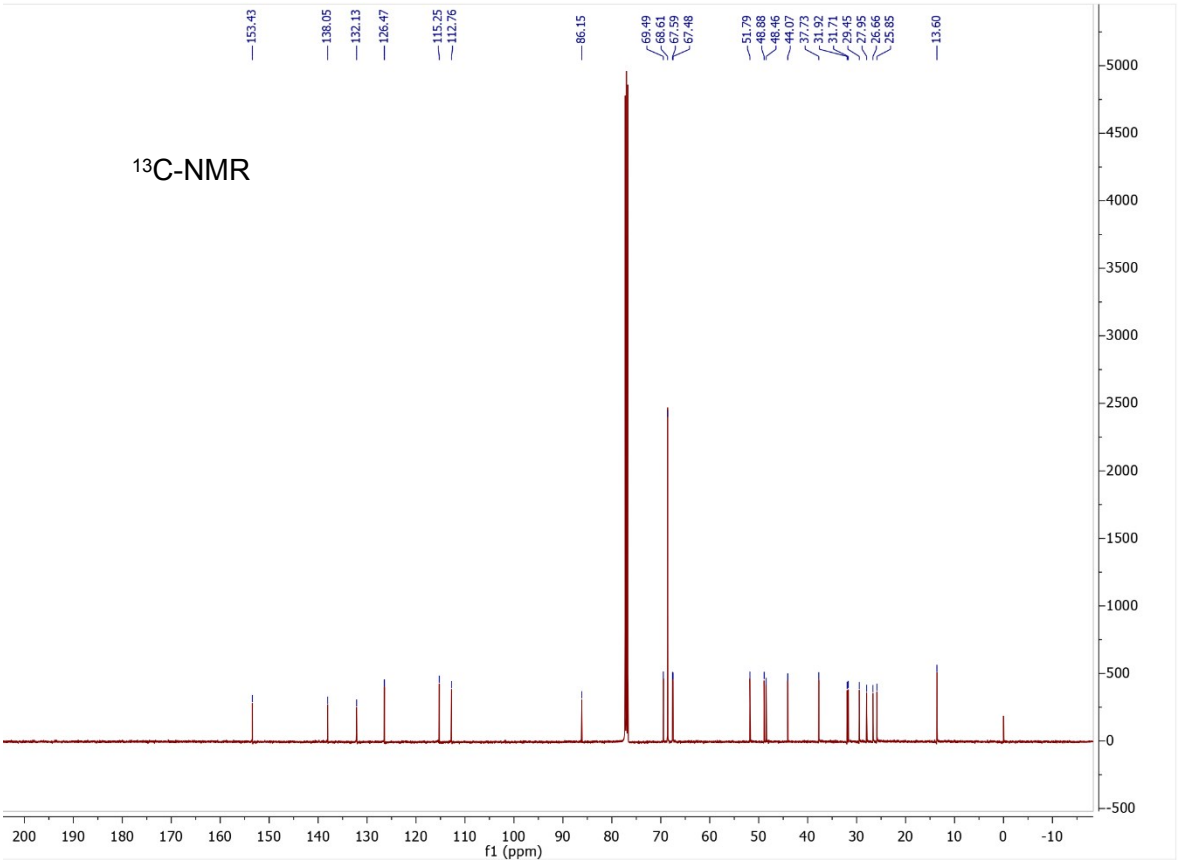
4. 16-ferrocenylidene-estra-1,3,5-triene-3,17-diol (**3**)





5. 16-ferrocenemethyl-3-hydroxyestra-1,3,5(10)-triene-17-one (**4**)





6. 16-ferrocenemethyl-estra-1,3,5(10)-triene-3,17β-diol (**5**)