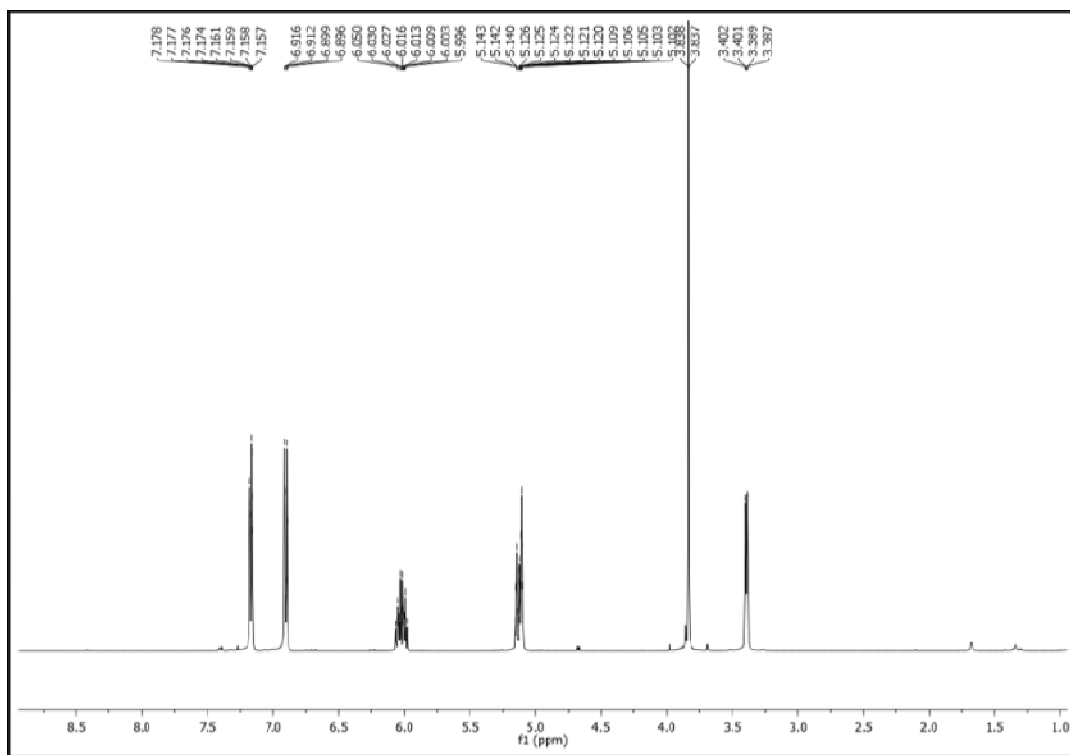
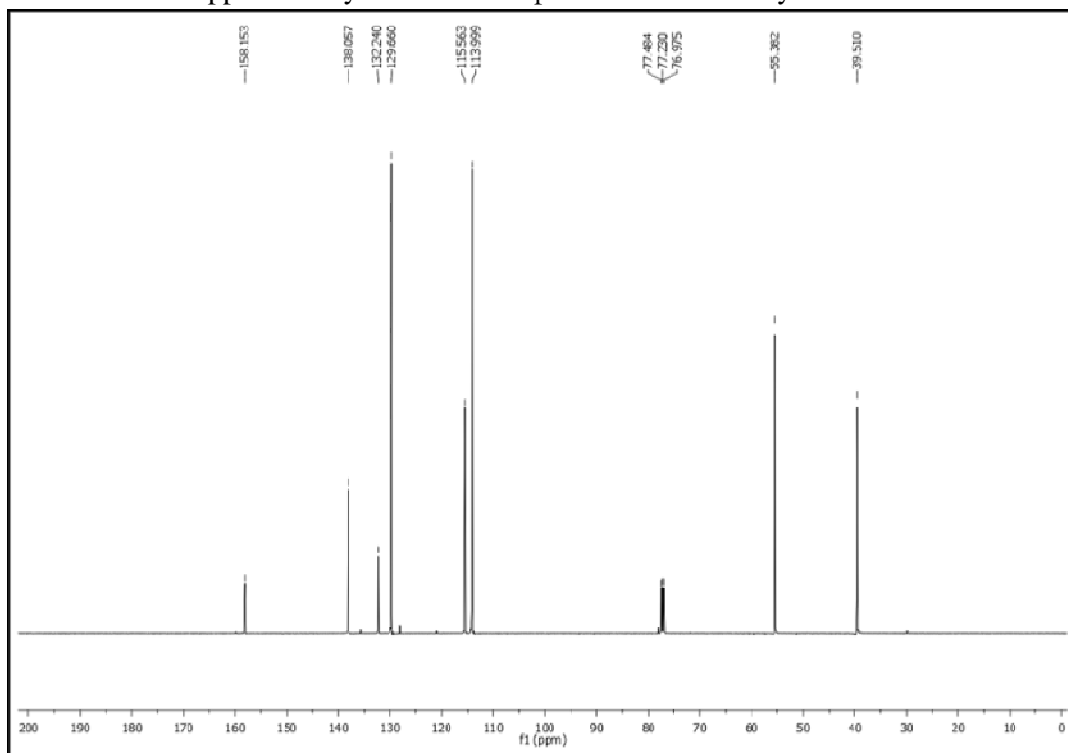


Supplementary 1 -  $^1\text{H}$ NMR spectrum of the methyl chavicol



Supplementary 2 -  $^{13}\text{C}$ NMR spectrum of the methyl chavicol



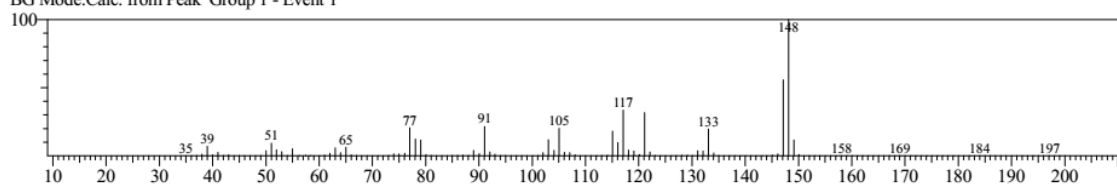
### Supplementary 3 - Mass Spectrum of the methyl chavicol

<< Target >>

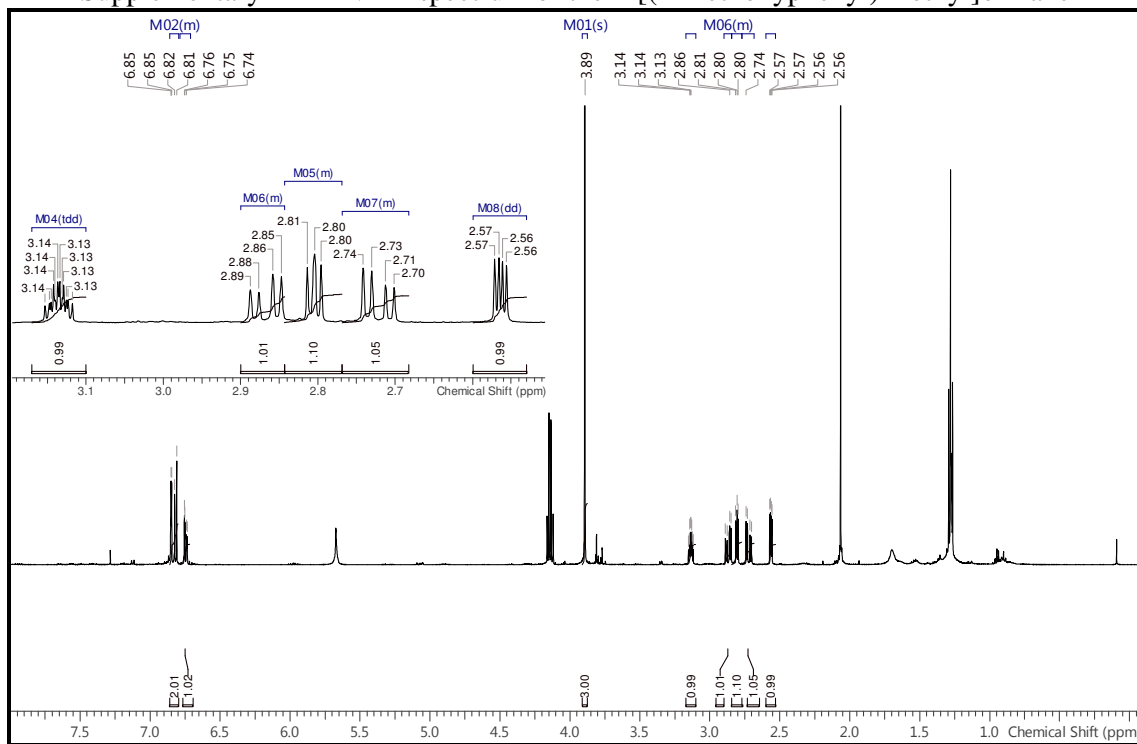
Line#:1 R.Time:9.355(Scan#:872) MassPeaks:166

RawMode:Averaged 9.350-9.360(871-873) BasePeak:148.15(7330228)

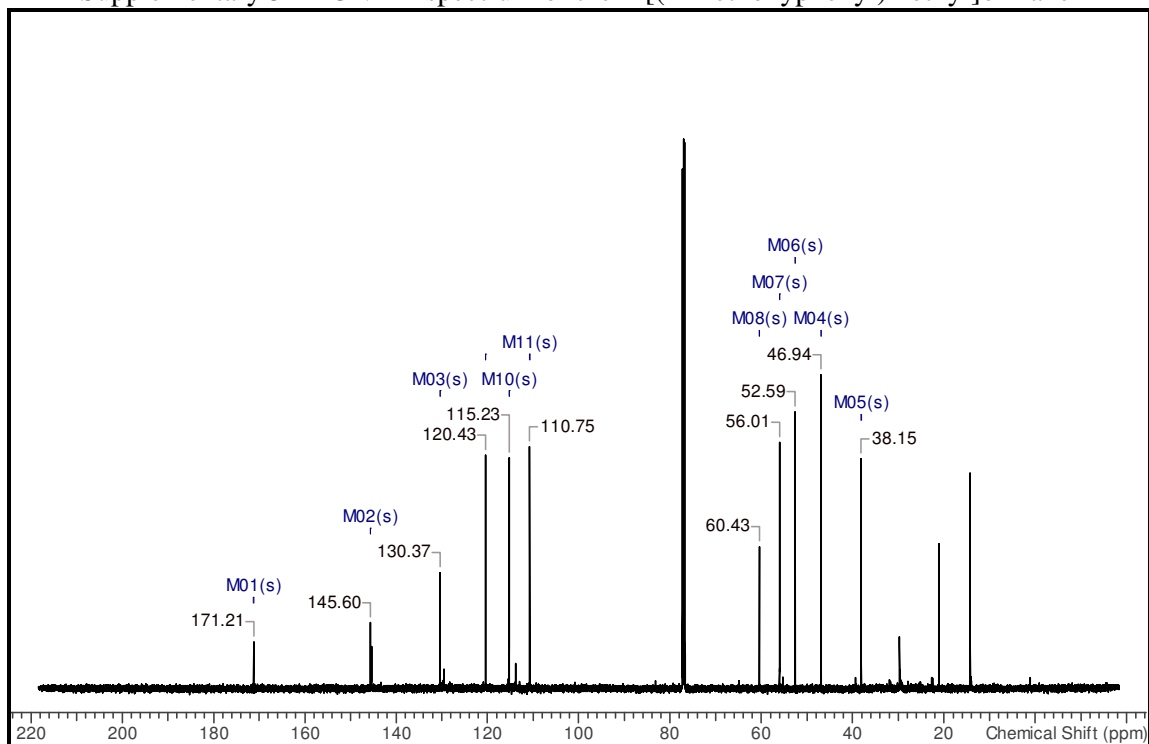
BG Mode:Calc. from Peak Group 1 - Event 1



Supplementary 4 -  $^1\text{H}$ NMR spectrum of the 2-[(4-methoxyphenyl) methyl]oxirane



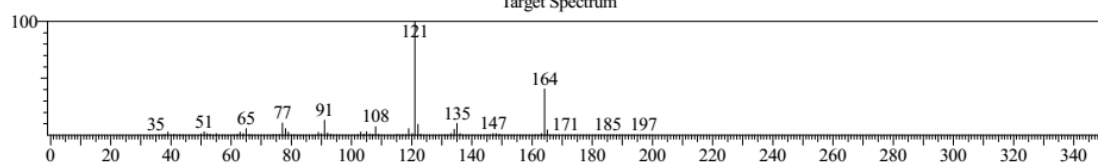
Supplementary 5 -  $^{13}\text{C}$ NMR spectrum of the 2-[(4-methoxyphenyl)methyl]oxirane



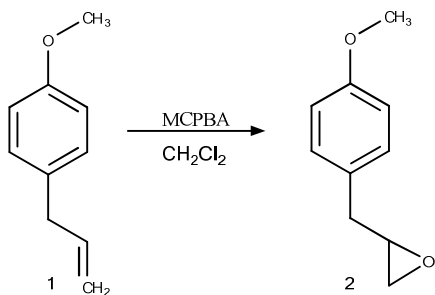
# Supplementary 6 - Mass spectrum of the 2-[(4-methoxyphenyl)methyl]oxirane

Library

<< Target >>  
Line#:1 R.Time:12.890(Scan#:1579) MassPeaks:166  
RawMode:Averaged 12.885-12.895(1578-1580) BasePeak:121.10(6670236)  
BG Mode:Calc. from Peak Group 1 - Event 1  
Target Spectrum



Supplementary 7 - Physico-chemical properties and spectral data of the 2-[(4-methoxyphenyl)methyl]oxirane



**Physical Appearance:** brown oily liquid

**M.F.:** C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>

**M.M.:** 164.204 g.mol<sup>-1</sup>

**Yield:** 75%

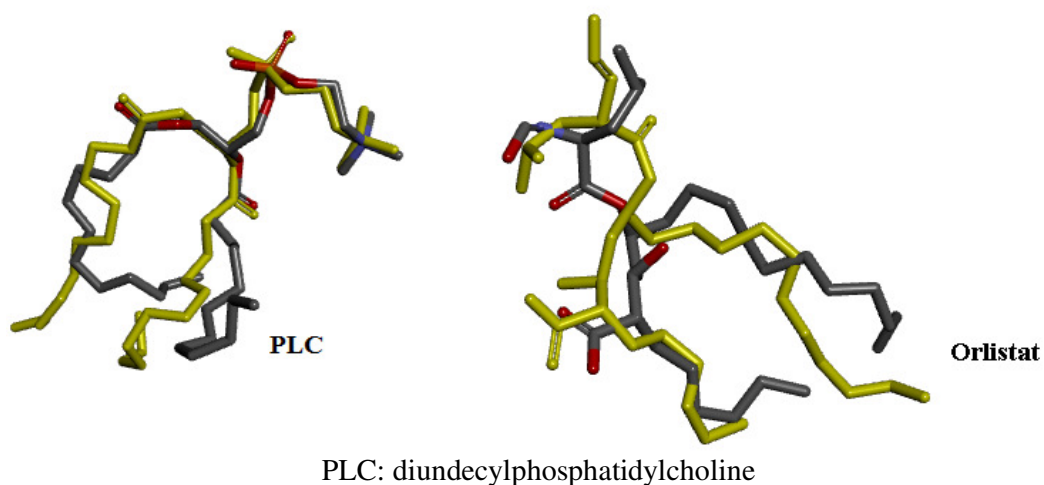
**Purity (GC):** 99%

**<sup>1</sup>HRMN, 500Hz, (CDCl<sub>3</sub>): δ (ppm):** 6.85 (d, 2H, J = 2.14 Hz); 6.74 (d, 2H, J = 2.14 Hz); 3.89 (s, 3H); 3.14 (tdd, 1H, J = 5.53, 5.53, 3.89, 2.75 Hz); 2.70 (m, 3H); 2.56 (dd, 1H, J = 5.04, 2.59 Hz) and 2.11 (m, 3H).

**<sup>13</sup>CRMN, 75Hz, (CDCl<sub>3</sub>): δ (ppm):** 171.395; 145.782; 145.608; 130.553; 120.612; 115.412; 110.935; 60.610; 56.193 and 52.774.

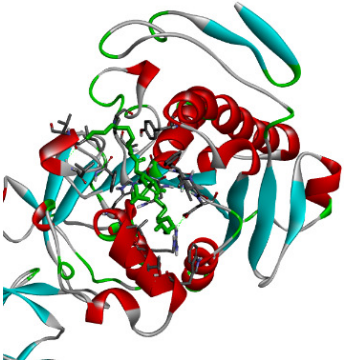
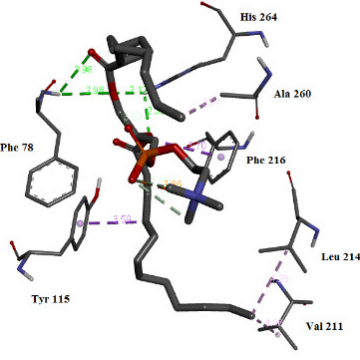
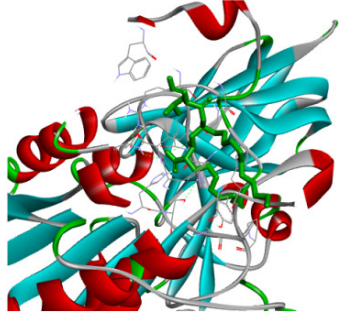
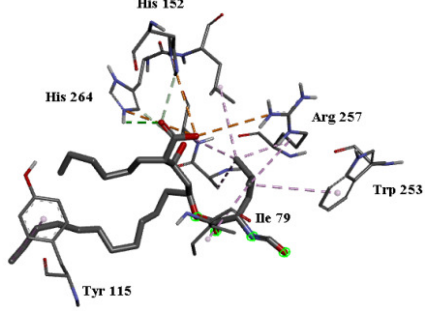
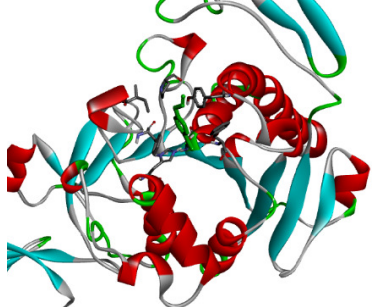
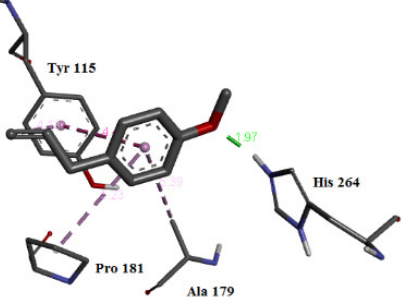
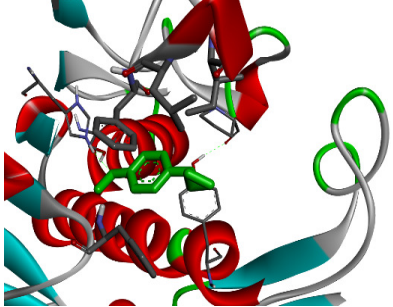
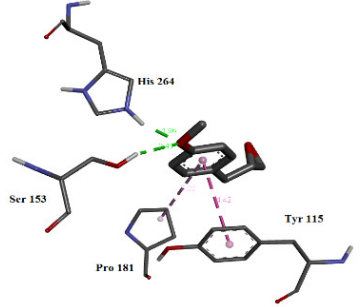
**MS: m/z =** 164 (M<sup>+</sup>); 147; 135; 121; 108; 91; 77 and 65.

Supplementary 8 - Redocking of the crystallographic ligands PLC and orlistat with RMSD  
1.3232 Å and 1.84 Å, respectively.





Supplementary 9 - Molecular orientations of crystallographic ligands at the pancreatic lipase binding site.

Ligands	Molecular interactions between ligands and pancreatic lipase	
	Three-dimensional structure	Aminoacids residues that formed binding site and main interactions
PLC		
Orlistat		
MC		
MPMO		
PLC: diundecylphosphatidylcholine; MC: methyl chavicol; MPMO: 2-[(4-methoxyphenyl)methyl]oxirane.		