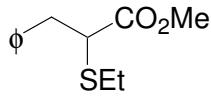


7. APÊNDICES

7.1 Dados espectroscópicos dos produtos

2-etiltio-3-fenil-propanoato de metila **IVF**



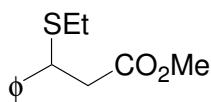
¹H - RMN: 1,26 (t, 3H, J = 11,2 Hz); 2,65 (q, 2H, J = 11,2 Hz); 2,96

(dd, 1H, J = 20,7 e J = 9,5 Hz); 3,21 (dd, 1H J = 20 e J = 13,8 Hz); 3,54 (dd, 1H, J = 13,5 e J = 9,5 Hz); 3,67 (s, 3H); 7,18 – 7,40 (m, 5H)

¹³C – RMN: 14,1; 25,6; 37,8; 47,8; 52,0; 126,7; 128,4; 128,9; 130,8; 138,0; 172,6

E.M.(70 eV) m/z: 224; 164 (-SEt)

3-fenil-3-etiltio-propanoato de metila **IIIA**

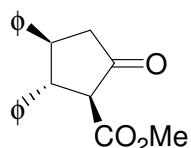


¹H - RMN: 1,57 (t, 3H, J = 7,5 Hz); 2,34 (dq, 2H, J = 7,35 Hz, J = 2,4 Hz); 2,87 (dd, 2H, J = 7,6 Hz, J = 2,4 Hz); 3,61 (s, 3H); 4,30 (t, 1H, J = 7,6 Hz); 7,20 – 7,51 (m, 5H)

¹³C – RMN: 14,2; 25,1; 41,3; 44,9; 51,6; 127,3; 127,5; 128,4; 141,4; 171,1

E.M.(70 eV) m/z: 224; 195 (-Et)

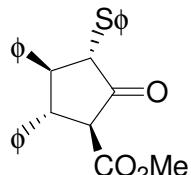
2-metoxi-carbonil-3,4-difenil-ciclopentanona **33**



¹H - RMN: 2,72 (dd, 1H, J = 18,9 e J = 12,3 Hz); 2,98 (dd, 1H, J = 18,6 e J = 7,5 Hz); 3,50 (dt, 1H, J = 12,6 e J = 7,5 Hz); 3,61 (d, 1H, J = 12 Hz); 3,71 (s, 3H); 3,92 (t, 1H, J = 12 Hz); 7,12 – 7,26 (m, 5H)
¹³C – RMN: 47,1; 47,7; 52,8; 53,6; 63,9; 127,4; 127, 6; 128,8; 128,9; 138,5; 139,4; 168,4; 207,8

E.M.(70 eV) m/z: 237 (ión molecular - CO₂Me);

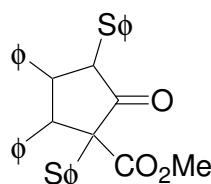
2-metoxicarbonil-3,4-difenil-5-feniltio-ciclopantanona **IIC**



¹H - RMN: 3,22 (t, 2H, J = 11,4Hz); 3,44 (d, 2H, J = 12,6 Hz); 3,72 (s, 6H); 3,79 (2H, d, J = 11,7Hz); 3,86 (t, 2H, J = 12 Hz); 6,94 – 7,44 (m, 15H)
¹³C – RMN: 50,8; 52,6; 53,2; 60,8; 62,2; 127,5; 127,7; 129,1; 131,8; 134,4; 138,0; 138,1; 168,2; 205,2

E.M.(70 eV) m/z: 344 (ión molecular - CO₂Me); 235 (-S phi)

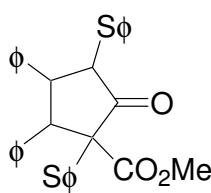
2-metoxicarbonil-2,5-difeniltio-3,4-difenil-ciclopantanona **IIB**



¹H - RMN: 3,41 (s, 6H); 3,56 (dd, 2H, J = 13,2 Hz, J = 6,6 Hz); 4,08 (2d, 2H, J = 13, 2 Hz); 4,21 (d, 2H, J = 6,6 Hz); 6,67 – 7,44 (m, 20H)
¹³C – RMN: 51,2; 53,3; 54,0; 55,6; 127,1; 127,3; 127,8; 127,9; 128,0; 128,4; 128,8; 129,3; 130,1; 134,6; 136,4; 167,2; 207,03

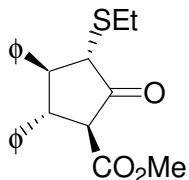
E.M.(70 eV) m/z: 510 ; 401 (-Sphi); 369 (-MeOH)

2-metoxicarbonil-2,5-difeniltio-3,4-difenil-ciclopantanona **IIA**



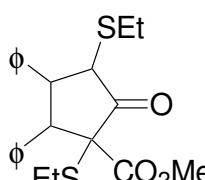
¹H - RMN: 3,79 (d, 2H, J = 10,5 Hz); 3,83 (s, 6H); 4,28 (dd, 2H, J = 12,3 Hz, J = 10,2 Hz); 4,44 (d, 2H, J = 12,3 Hz); 7,64 – 7,68 (m, 20H)
¹³C – RMN: 49,8; 53,5; 55,5; 61,0; 70,9; 127,8; 128,3; 128,4; 128,6; 129,0; 129,2; 130,0; 132,5; 134,9; 137,9; 138,5; 150,1; 169,7; 199,2
E.M.(70 eV) m/z: 510; 401 (-S_{Ph}); 369 (-MeOH)

2-metoxicarbonil-5-ethylthio-3,4-difenil-ciclopentanona **IVC**



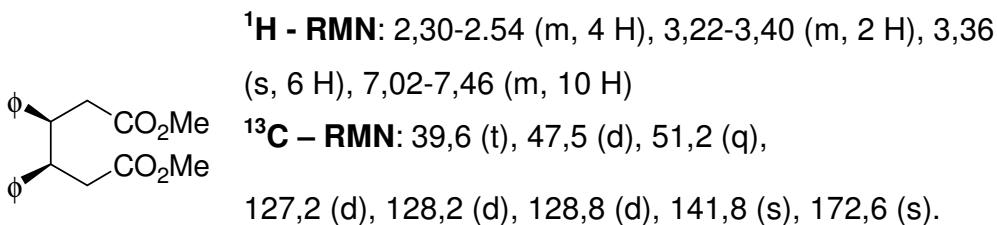
¹H - RMN: 2,63 (q, 4H, J = 7,5 Hz); 3,19 (t, 2H, J = 10,8 Hz); 3,51 (d, 2H, J = 11,1 Hz); 3,73 (s, 6H); 3,79 – 3,95 (m, 4H) 7,09 – 7,37 (m, 10H)
¹³C – RMN: 14,2; 25,8; 51,1; 52,6; 54,6; 56,1; 61,6; 127,2; 127,4; 127,6; 127,8; 128,6; 138,1; 168,4; 205,9
E.M.(70 eV) m/z: 396 (ión molecular – CO₂Me); 236 (-SEt)

2-metoxicarbonil-2,5-diethylthio-3,4-difenil-ciclopentanona **IVD**

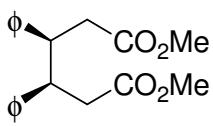


¹H - RMN: 1,16 (q, 6H); 2,48-2,74 (m, 4H); 3,43 (d, 2H, J = 10,2Hz); 3,87 (s, 6H); 4,02 (dd, 2H, J = 10 Hz e J = 12 Hz); 4,42 (d, 2H, J = 12,4 Hz); 7,15-7,37 (m, 10H),
¹³C – RMN: 13,2; 14,5; 24,2; 26,5; 49,2; 53,3; 54,8; 56,9; 67,1; 127,4; 127,8; 128,2; 128,7; 128,8; 133,0; 138,7; 169,3; 200,6
E.M.(70 eV) m/z: 414; 383 (-OMe)

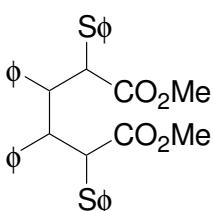
3,4-difenil – hexanoato de dimetila **IIID**



E.M.(70 eV) m/z: 326



2,5-difeniltio-3,4-difenil-hexanoato de dimetila **IID**

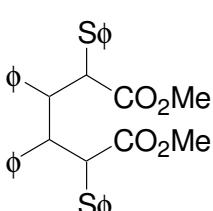


1H - RMN: 3,59 (s, 6H); 3,84 (s, 2H); 4,38 (s, 2H); 6,9 – 7,46 (m, 20H)

13C - RMN: 48,7; 51,5; 52,3; 54,6; 57,1; 88,2; 92,8; 127,5; 127,4;
128,3; 129,4; 135,1; 169,5

E.M.(70 eV) m/z: 433 (íon molecular – Sphi); 361(-CHCO2Me)

2,5-difeniltio-3,4-difenil-hexanoato de dimetila **IIIE**

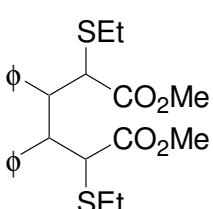


1H - RMN: 3,85 (d, 2H, J = 12 Hz); 4,31 (d, 2H, J = 11,7 Hz); 3,21 (s, 6H); 7,08 – 7,61 (2m, 20H)

13C - RMN: 45,8; 51,6; 53,4; 127,4; 128,1; 129,0; 132,8; 136,5; 171,2

E.M.(70 eV) m/z: 433 (íon molecular – Sphi); 361(-CHCO2OH)

2,5-dietyltilio-3,4-difenil-hexanoato de dimetila **IVE**

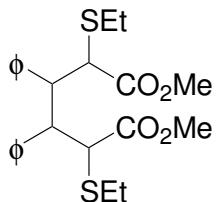


1H - RMN: 1,35 (t, 6H, J = 7,5 Hz); 2,79 (q, 4H, J = 10,5 Hz); 3,33 (s, 6H); 3,48 (d, 2H, J = 11,7 Hz); 4,11 (d, 2H, J = 11,4 Hz); 6,98 – 7,28 (m 10H)

13C - RMN: 14,0; 24,6; 42,9; 49,0; 51,7; 127,3; 128,0; 129,1; 137,1;
171,4

E.M.(70 eV) m/z: 384 (íon molecular – SEt)

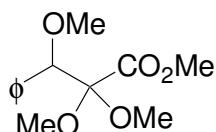
2,5-dietiltio-3,4-difenil-hexanoato de dimetila **IVF**



¹H - RMN: 1,32 (t, 6H, J = 7,2 Hz); 2,72 (q, 4H, J = 7,2 Hz); 3,35 (s, 6H); 3,78 (d, 2H, J = 10,8 Hz); 4,11 (d, 2H, J = 10,8 Hz); 6,98 – 7,28 (m 10H)
¹³C – RMN: 14; 25,9; 44,3; 48,4; 50,1; 127,1; 128,0; 129,1; 139,6; 171,5

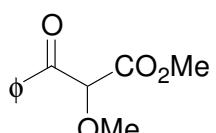
E.M.(70 eV) m/z: 384 (íon molecular – SEt)

2,2,3-trimetoxi-3-fenil-propanoato de metila **IIa**



¹H - RMN: 3,25 (s, 3H); 3,29 (s, 3H); 3,45 (s, 3H); 3,67 (s, 3H); 4,53 (s, 1H); 7,29 – 7,37 (m, 5H),
¹³C – RMN: 50,9; 51,4; 52,0; 84,5 102, 6; 127,7; 128,0; 135,6; 167,7
E.M.(70 eV) m/z:

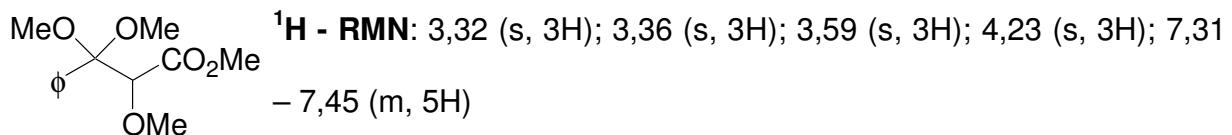
2,-metoxi-3-oxo-3-fenil-propanoato de metila **IIIg**



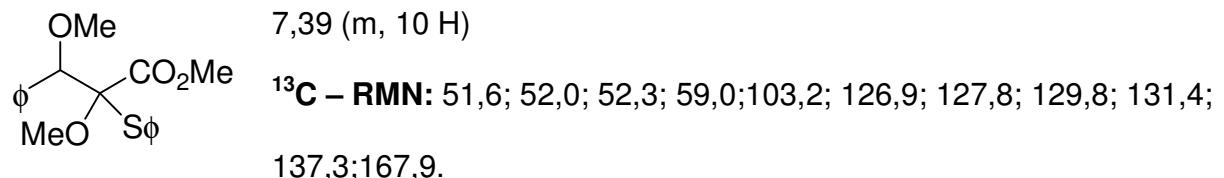
¹H - RMN: 3,53 (s,3H); 3,77 (s, 3H); 4,96 9s,1H); 7,42 – 8,08 (m, 5H)
¹³C – RMN: 52,7; 58,6; 84,9; 128,6; 129,3; 167,9; 192, 3

E.M.(70 eV) m/z: 208

2,3,3-trimetoxi-3-fenil-propanoato de metila **Ia**

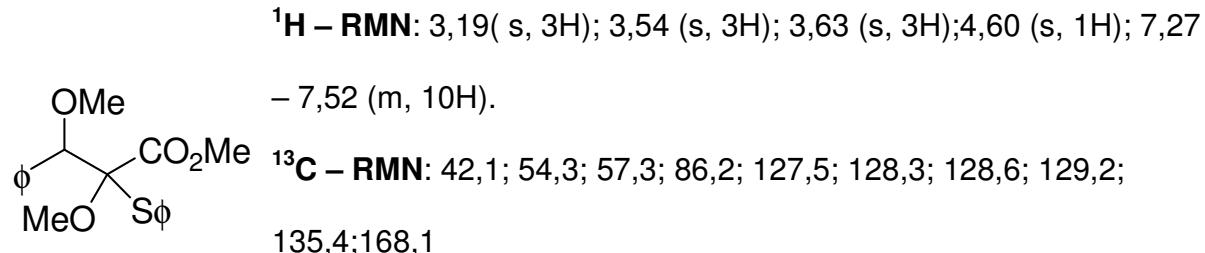


2,3-dimetoxi-2-feniltio-3-fenil-propanoato de metila **IIb**



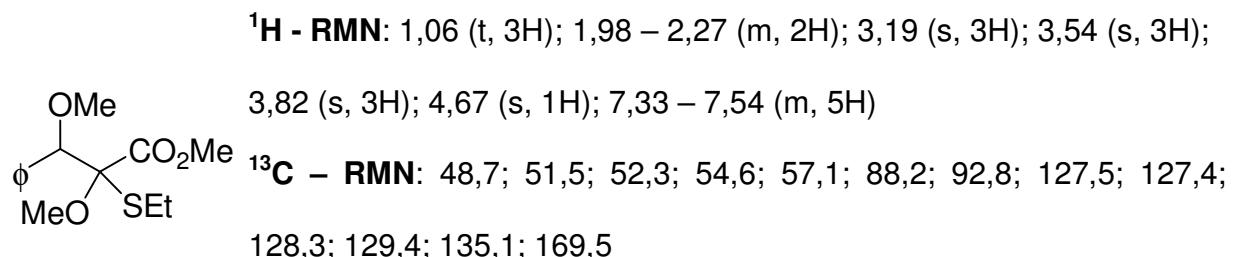
E.M.(70 eV) m/z:: 273 (íon molecular – CO₂Me)

2,3-dimetoxi-2-feniltio-3-fenil-propanoato de metila **IIc**



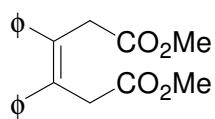
E.M.(70 eV) m/z:: 273 (íon molecular – CO₂Me)

2,3-dimetoxi-2-etiltio-3-fenil-propanoato de metila **IVa**



E.M.(70 eV) m/z: 284; 163 (-SEt, CO₂Me)

3,4-difenil-hexanoato de dietila **III E**

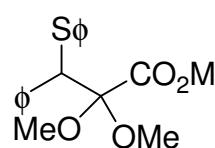


¹H - RMN: 3,29 (6H, s); 3,53 (s, 4H); 7,27 – 7,40 (m, 10 H)

¹³C – RMN: 41,7; 51,7; 128,4; 140,8; 171,6,

E.M.(70 eV) m/z: 324; 292 (-MeOH)

2,2-dimetoxi-3-feniltio-3-fenil-propenoato de metila **II d**



¹H - RMN: 3,29 (s, 3H); 3,38 (s, 3H); 3,90 (s, 3H); 5,07 (s, 1H);

¹³C – RMN:

E.M.(70 eV) m/z:: 223 (ión molecular – phi)