The Mistake in Carl Bosch´s PhD Thesis - a Contribution to “Retro-Chemistry”

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S 15-16 \(^1\)H, \(^{13}\)C and HRMS of Compound 5a/b
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$^1$H and $^{13}$C assignment for Diethyl 2-oxo-1-(2-oxo-2-phenylethyl)-4-phenyl-cyclopent-3-ene-1,3-dicarboxylate (4)

$^1$H of compound 4
$^{13}$C of compound 4

APT of compound 4
H,H-COSY of compound 4

Edited HSQC of compound 4
HMBC of compound 4

HRMS of compound 4 (C_{23}H_{24}O_{6}Na, m/z = 443.15)
$^{1}H$ and $^{13}C$ assignment for Diethyl 4-(4-bromophenyl)-1-(2-(4-bromophenyl)-2-oxoethyl)-2-oxocyclopent-3-ene-1,3-dicarboxylate (4a)

$^{1}H$ of compound 4a
$^{13}$C of compound 4a

HRMS of compound 4a ($C_{25}H_{13}O_6Br_2$, m/z = 576.99)
$^1$H and $^{13}$C assignment for Diethyl 4-(4-nitrophenyl)-1-(2-(4-nitrophenyl)-2-oxoethyl)-2-oxocyclopent-3-ene-1,3-dicarboxylate (4b)

$^1$H of compound 4b
$^{13}$C of compound 4b

HRMS of compound 4b ($C_{25}H_{32}O_{19}N_2Na$, m/z = 533.12)
$^1$H and $^{13}$C assignment for Diethyl 4-(4-cyanophenyl)-1-(2-(4-cyanophenyl)-2-oxoethyl)-2-oxocyclopent-3-ene-1,3-dicarboxylate (4c)

$^1$H of compound 4c
$^{13}$C of compound 4c

HRMS of compound 4c ($C_{27}$H$_{22}$O$_6$N$_2$Na, m/z = 493.14)
$^{1}H$ and $^{13}C$ assignment for Diethyl 4-(3-methoxyphenyl)-1-(2-(3-methoxyphenyl)-2-oxoethyl)-2-oxocyclopent-3-ene-1,3-dicarboxylate (4d)

$^{1}H$ of compound 4d
$^{13}$C of compound 4d

HRMS of compound 4d (C$_{27}$H$_{28}$O$_{2}$Na, m/z = 503.17)
Diethyl 3-oxo-2,4-bis(2-oxo-2-phenylethyl)pentane-dioate (5a/b)

$^1$H-NMR of diastereomeric byproduct 5a/b

$^{13}$C of diastereomeric byproduct 5a/b
HRMS of diastereomeric byproduct 5a/b (C_{25}H_{26}O_2Na, m/z = 461.16)

ESI positiv, Smeilus CB-TS-0 in DCM/MeOH, 29/08/14
$^1$H and $^{13}$C assignment of compound 7

$^1$H of compound 7
$^{13}$C of compound 7

APT of compound 7
H,H-COSY of compound 7

Edited HSQC of compound 7
HMBC of compound 7

HRMS of compound 7 (C_{46}H_{38}O_{5}N_{4}Na, m/z = 677.27)