

Supplementary Materials

Palladium-catalyzed β -C(sp³)–H bond arylation of tertiary aldehydes facilitated by 2-pyridone ligands

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I. Starting materials

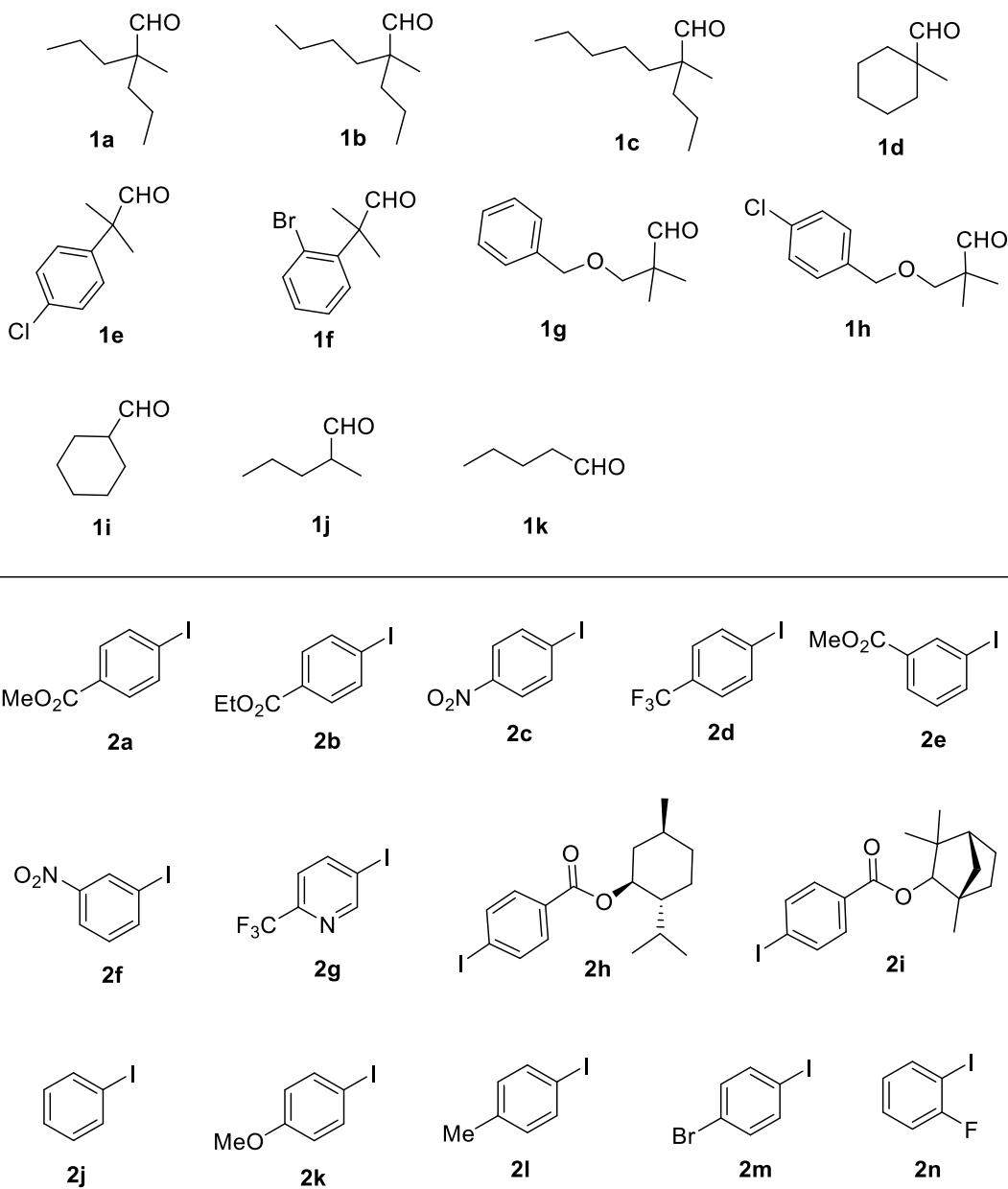


Figure S1. Aliphatic aldehydes and aryl iodides

II. ^1H and ^{13}C NMR Spectra

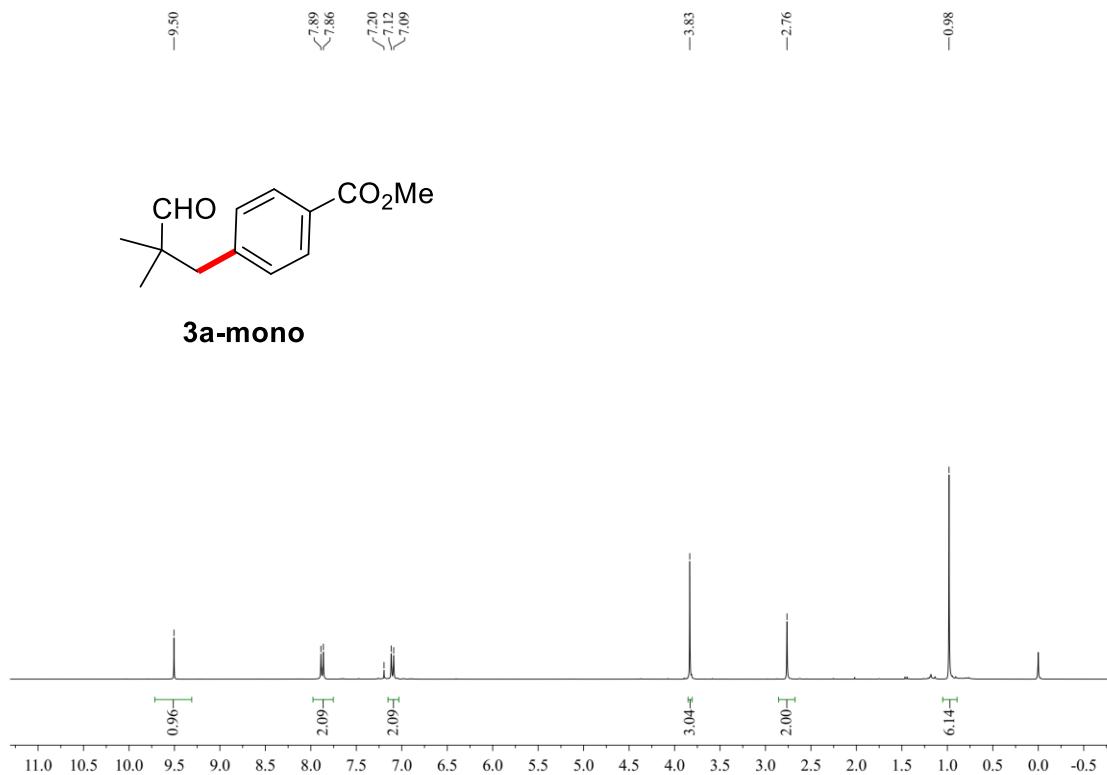


Figure S2 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3a-mono**

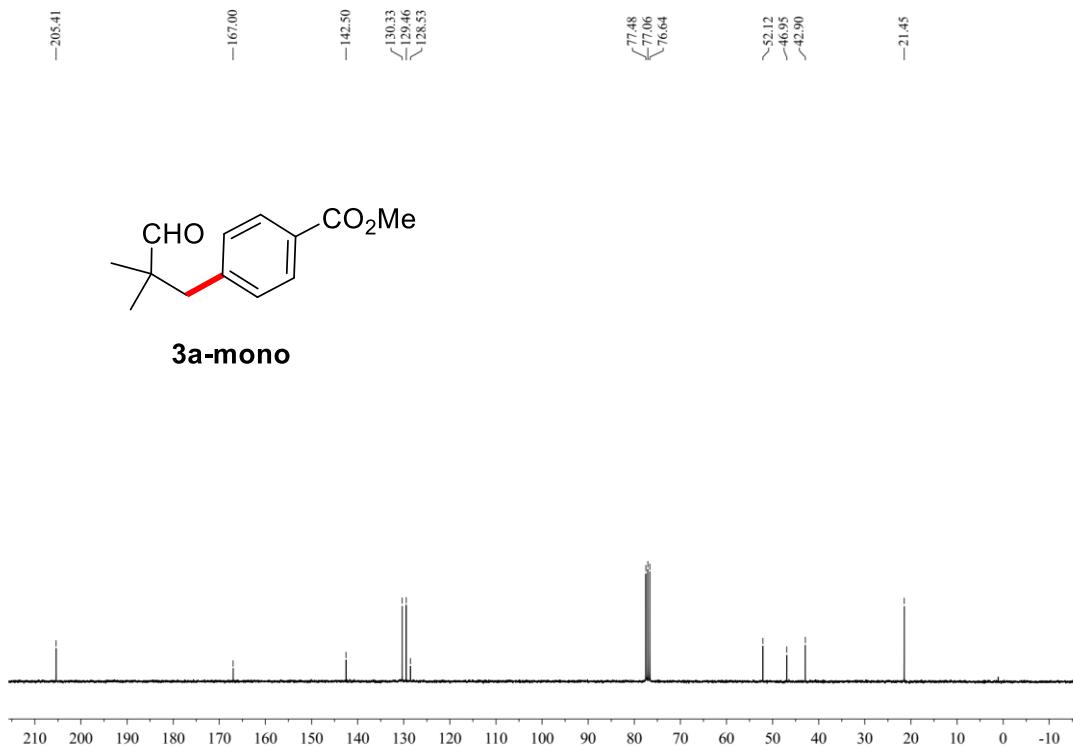


Figure S3 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3a-mono**

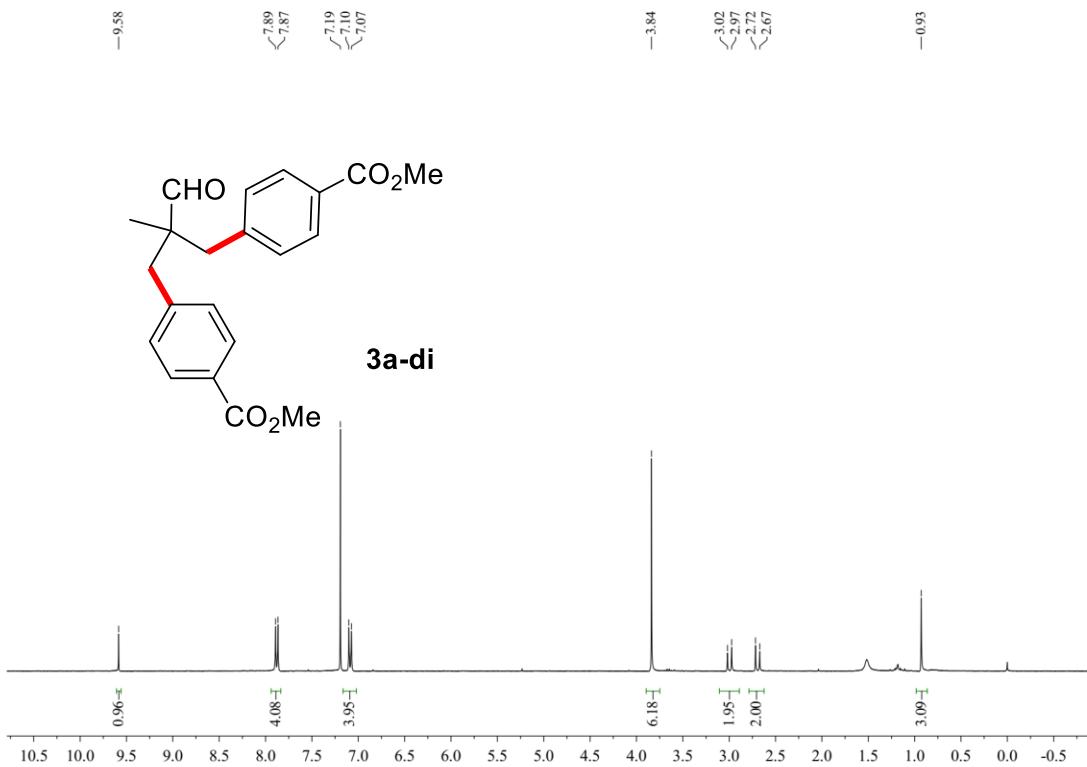


Figure S4 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3a-di**

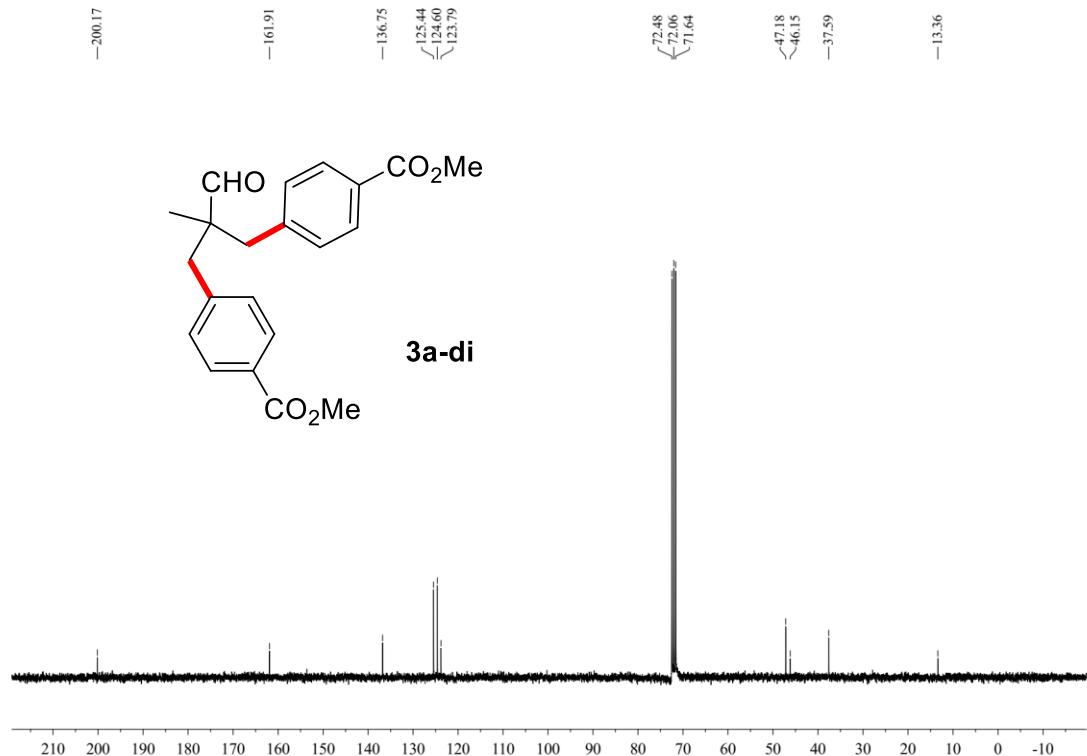


Figure S5 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3a-di**

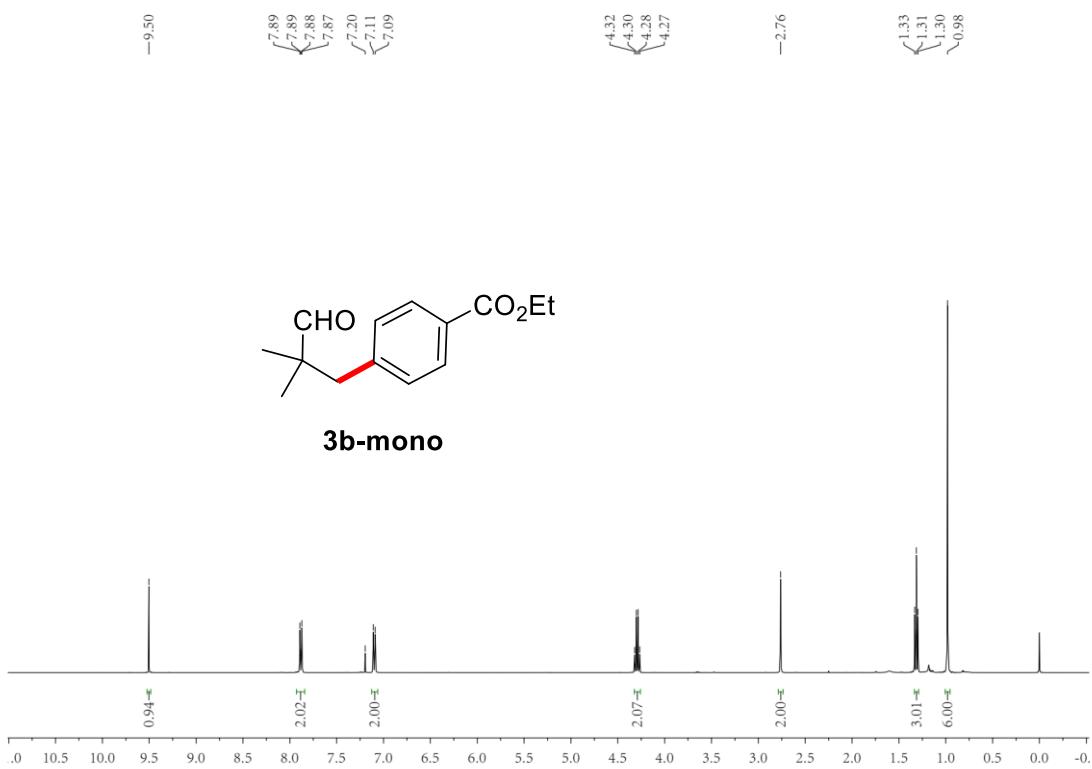


Figure S6 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3b-mono**

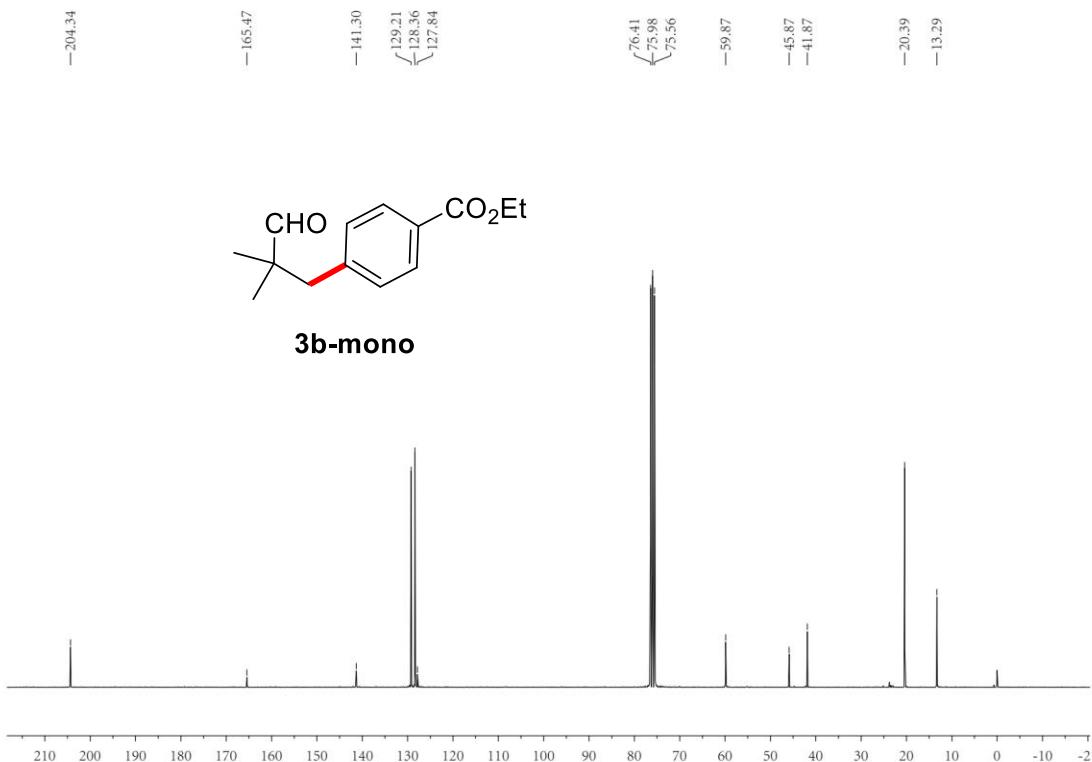


Figure S7 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3b-mono**

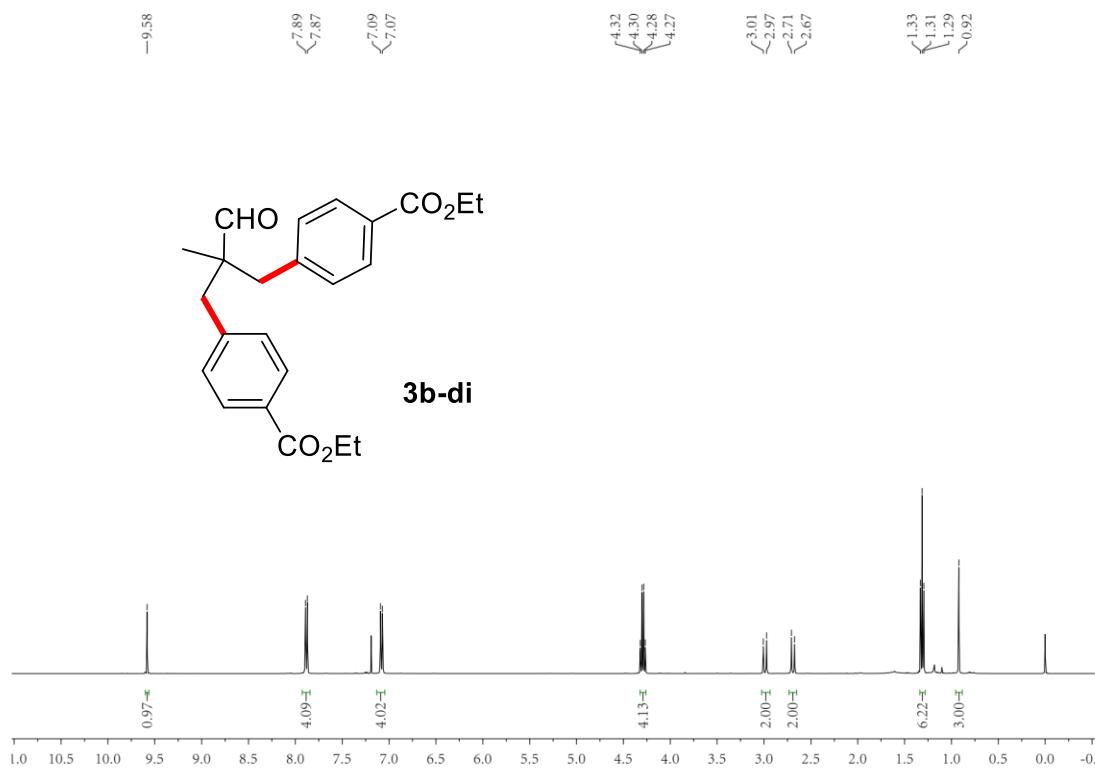


Figure S8 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3b-di**

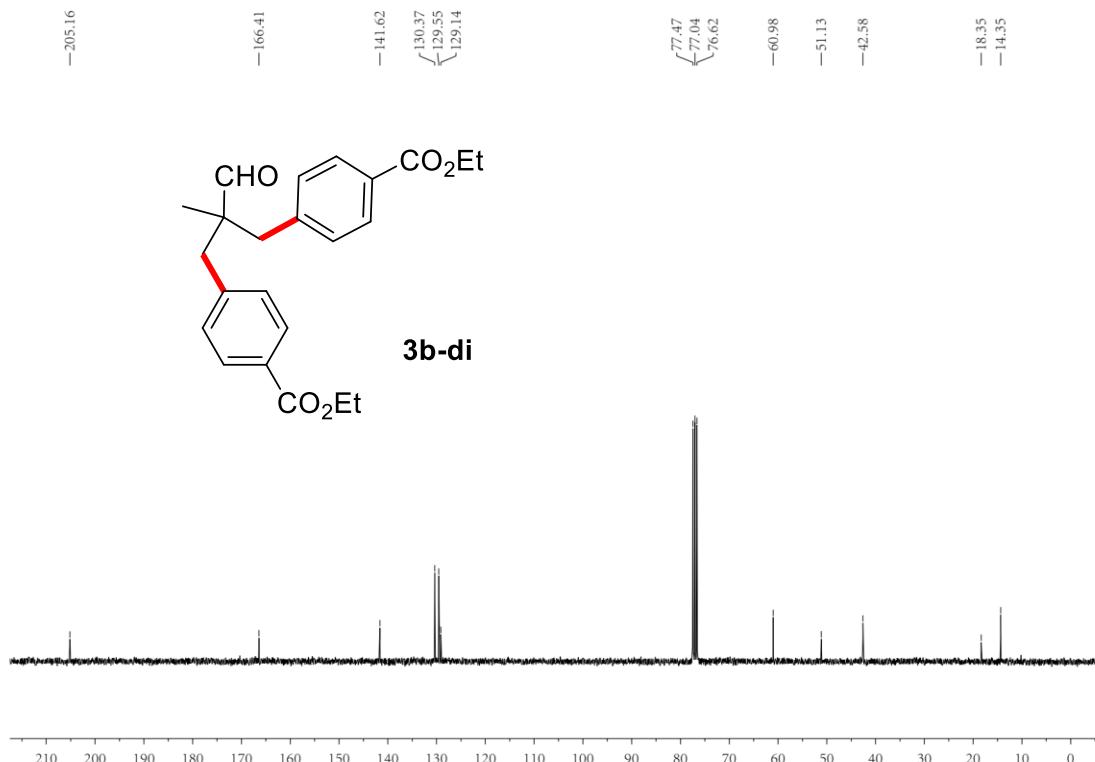


Figure S9 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3b-di**

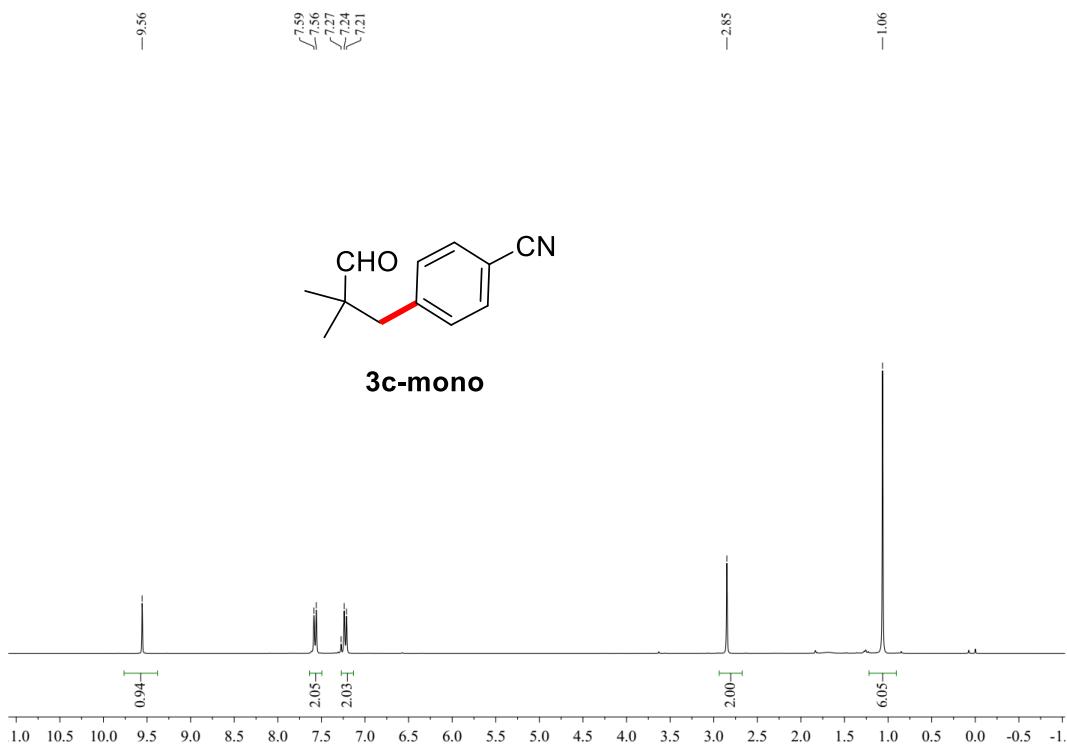


Figure S10 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3c-mono**

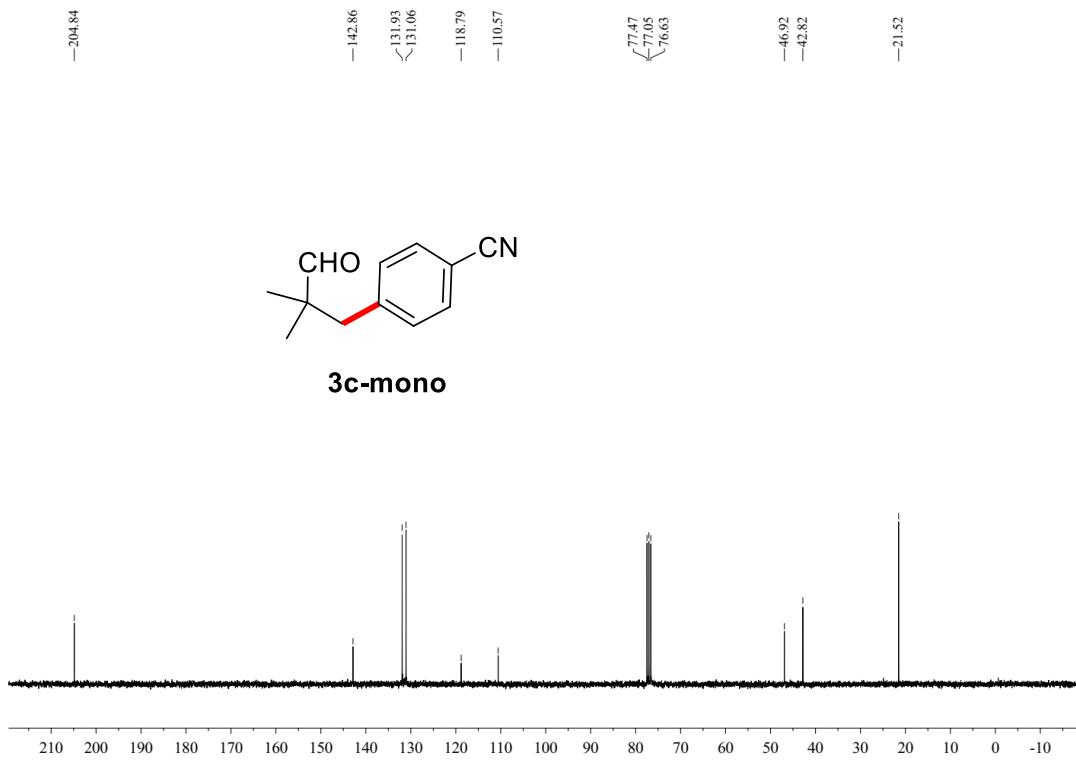


Figure S11 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3c-mono**

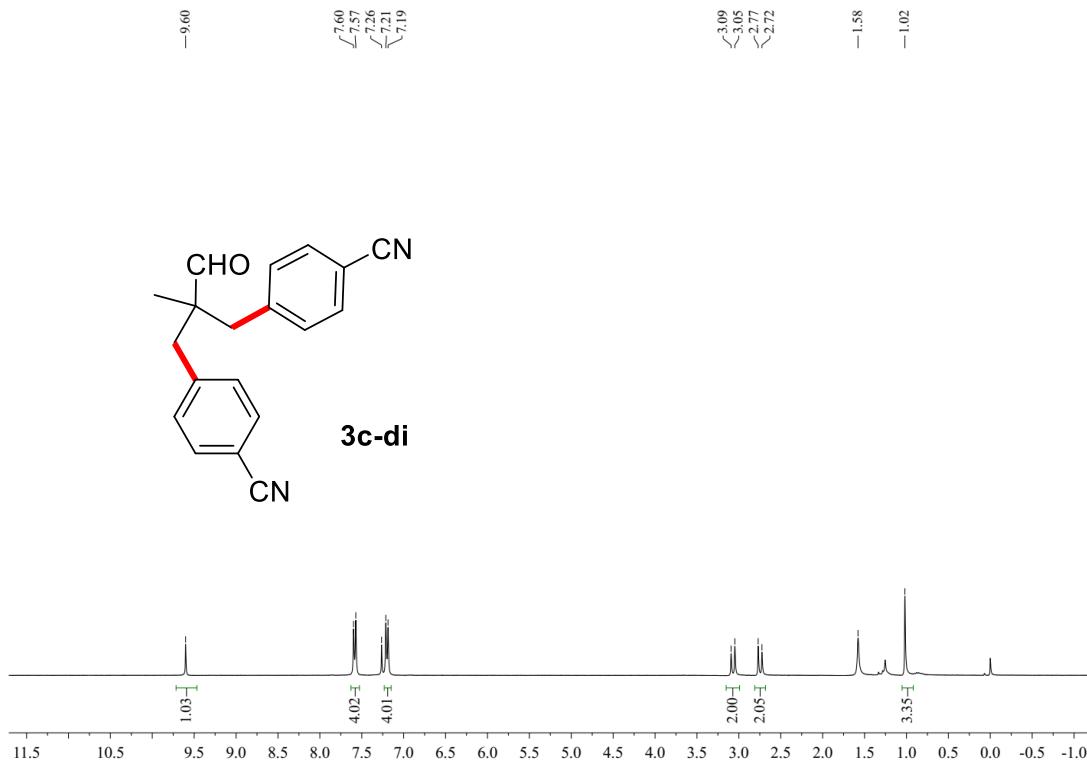


Figure S12 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3c-di**

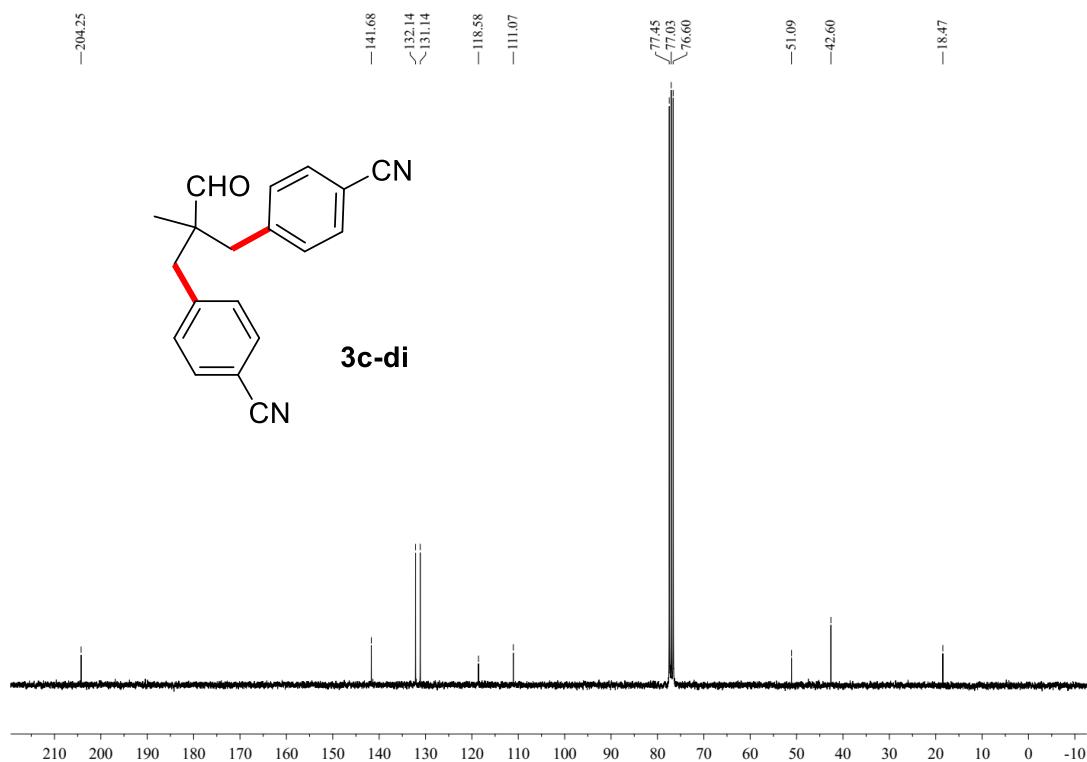


Figure S13 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3c-di**

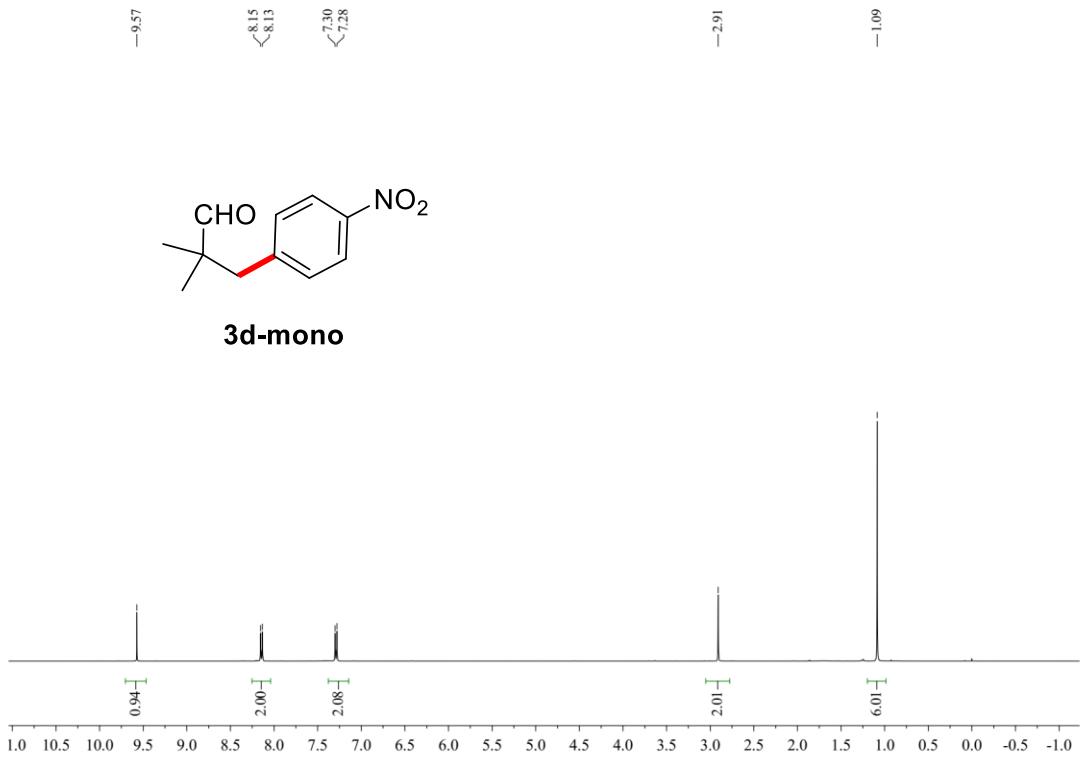


Figure S14 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3d-mono**

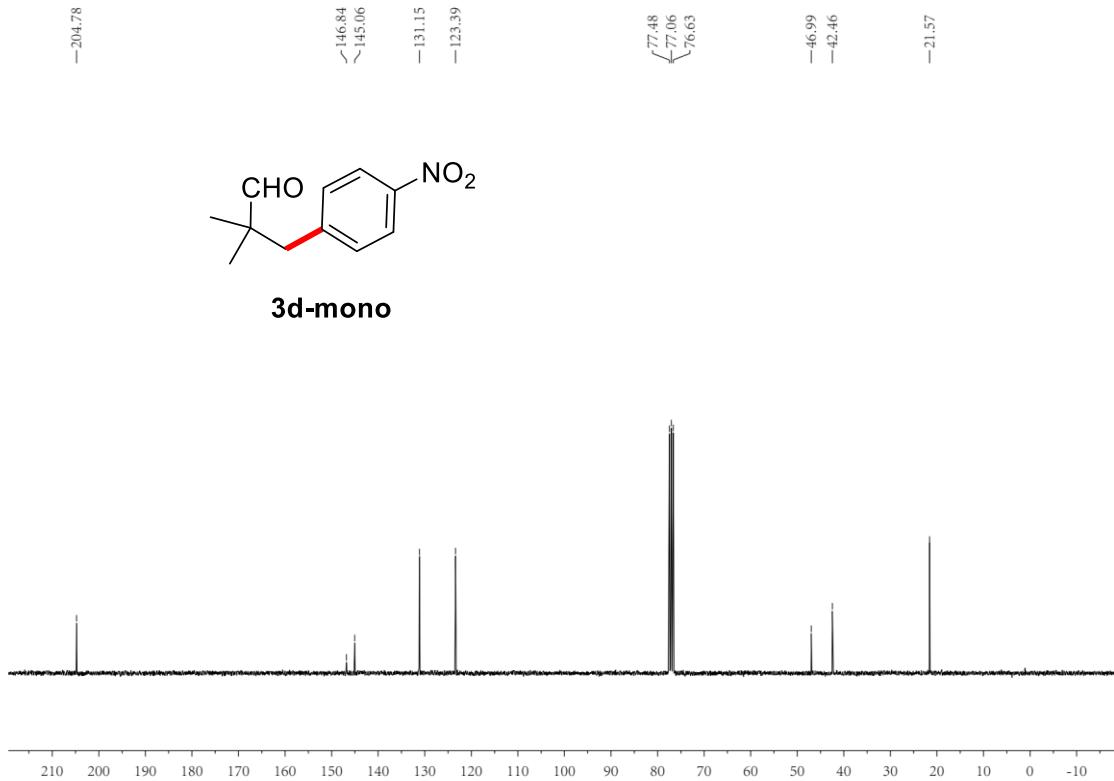


Figure S15 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3d-mono**

¹H NMR chemical shifts (δ , ppm): -9.56, <8.10, <8.07, <7.21, <7.19, 3.09, <3.04, <2.77, <2.73, -0.99.

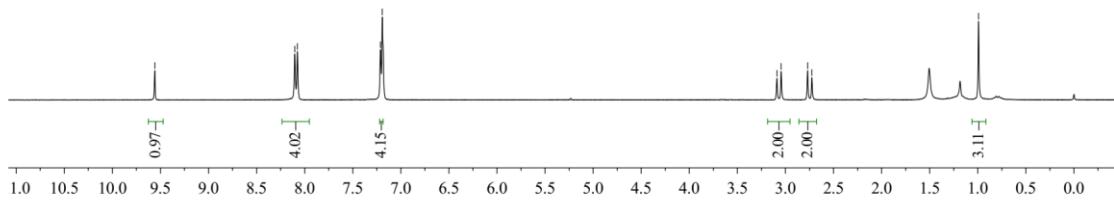
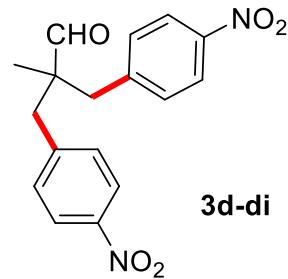


Figure S16 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3d-di**

¹³C NMR chemical shifts (δ , ppm): -204.10, -147.09, -143.74, -131.26, -123.61, 77.46, 77.04, 76.61, -51.15, -42.30, -18.54.

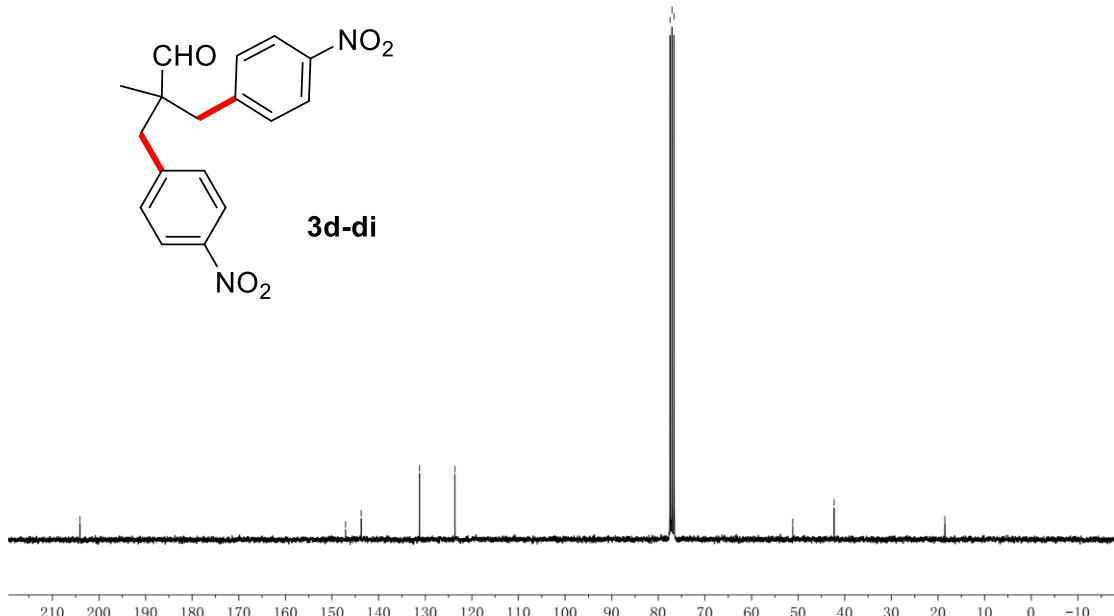
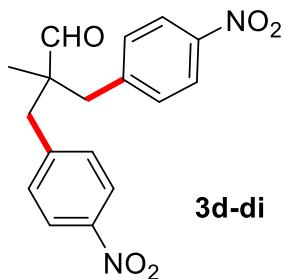


Figure S17 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3d-di**

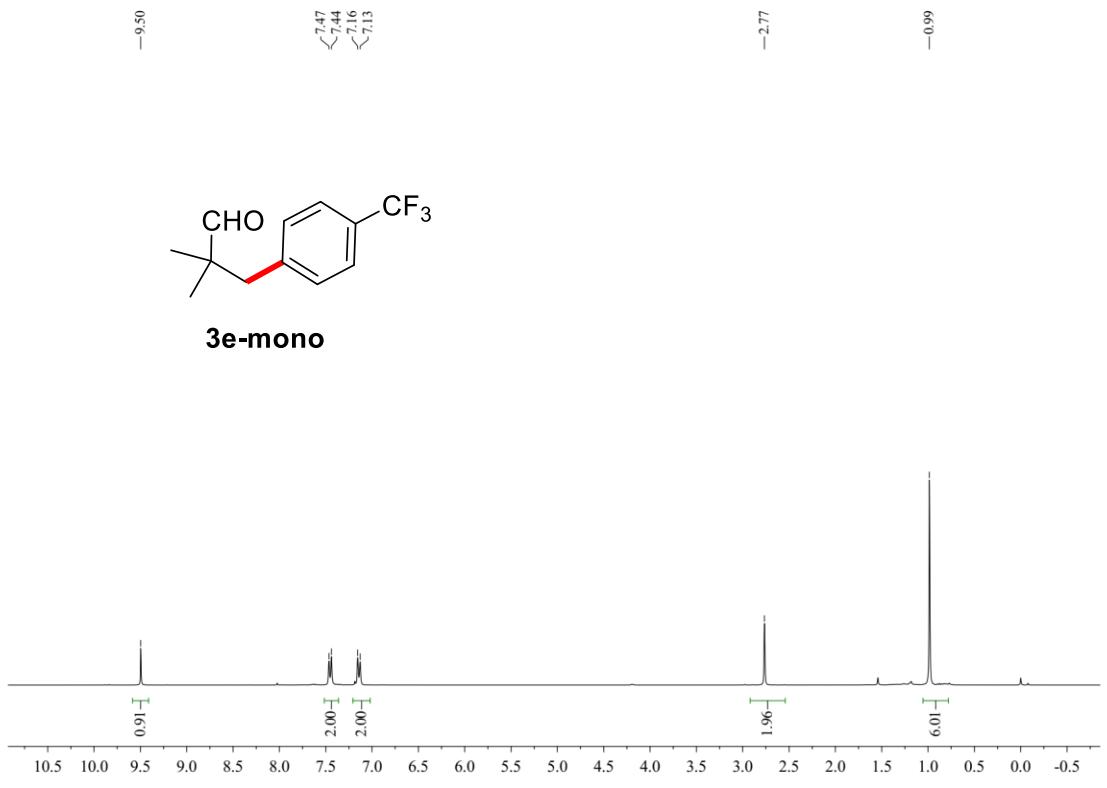


Figure S18 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3e-mono**

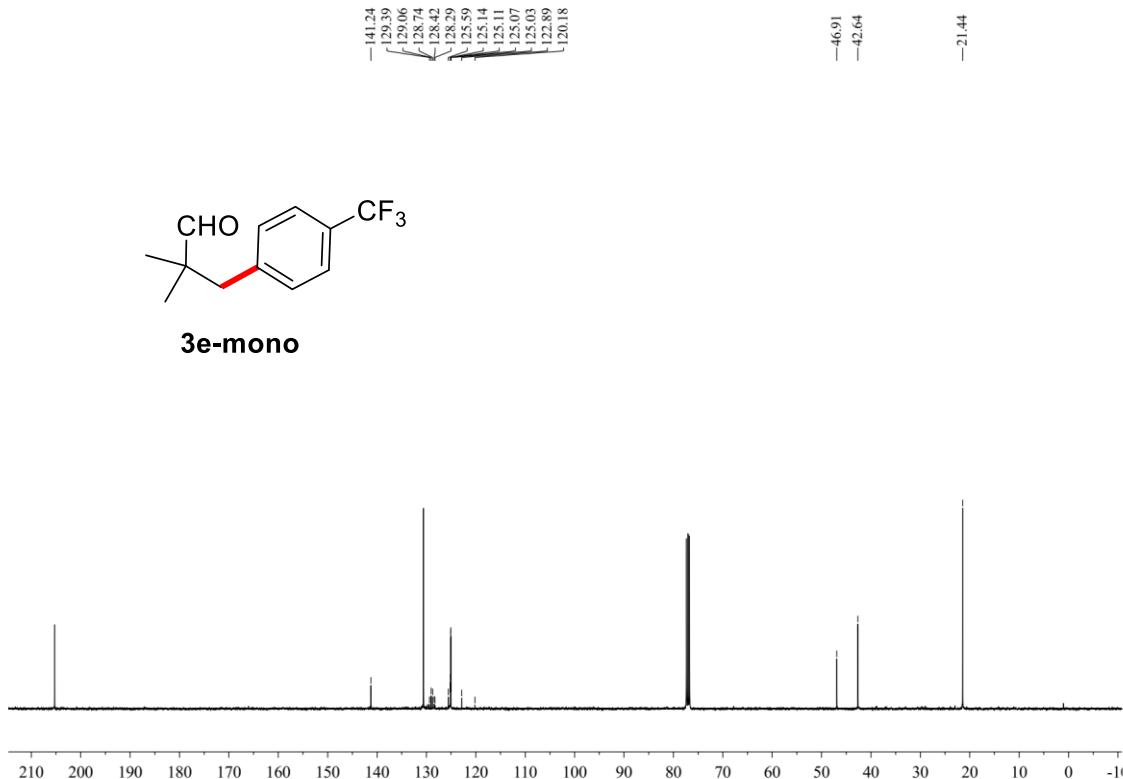


Figure S19 ^{13}C NMR spectrum (101MHz, CDCl_3 , 298K) of **3e-mono**

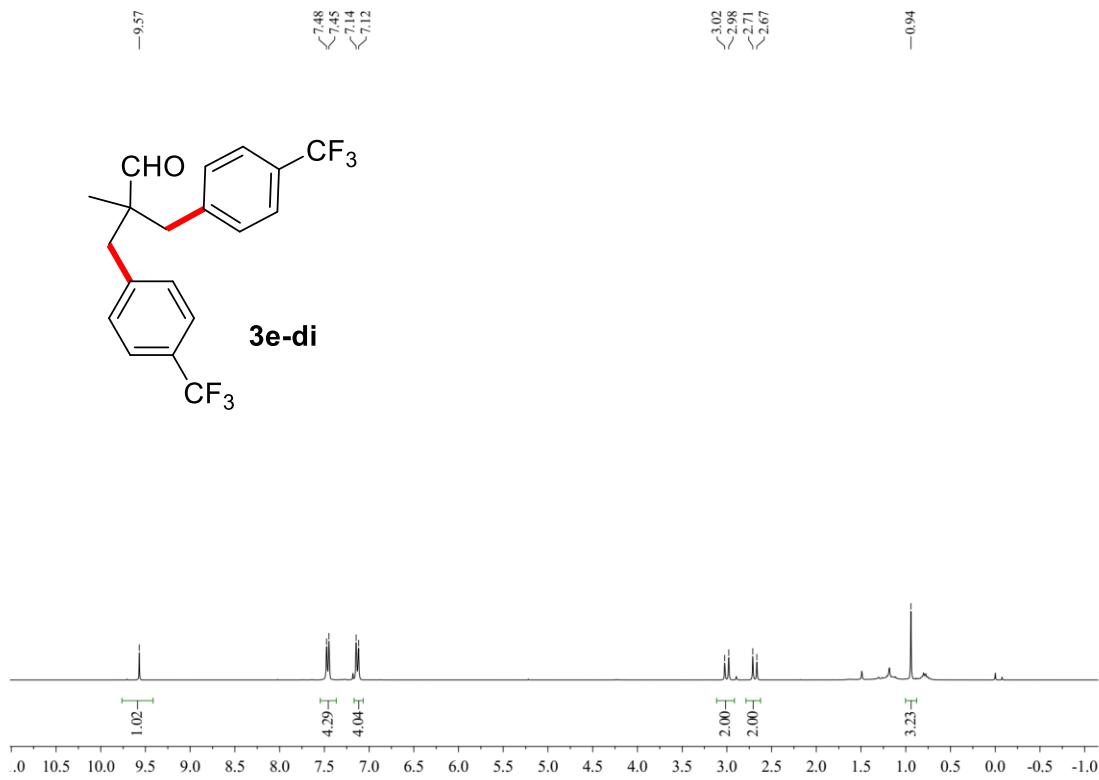


Figure S20 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3e-di**

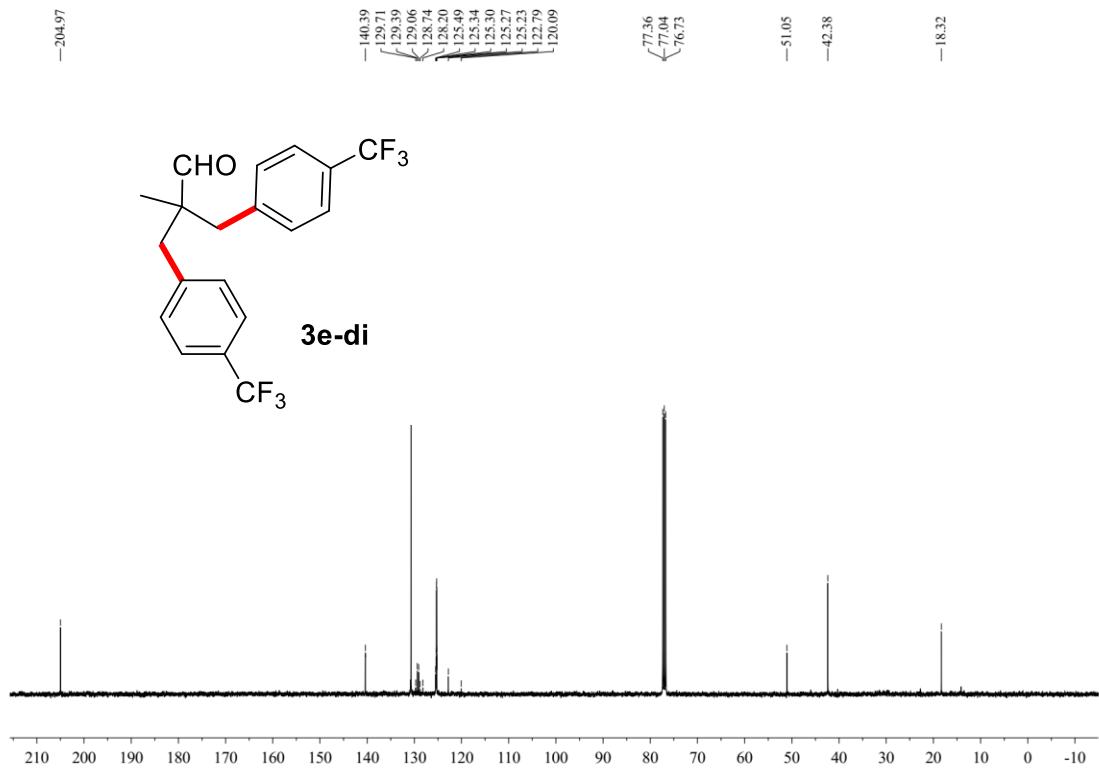


Figure S21 ^{13}C NMR spectrum (101MHz, CDCl_3 , 298K) of **3e-di**

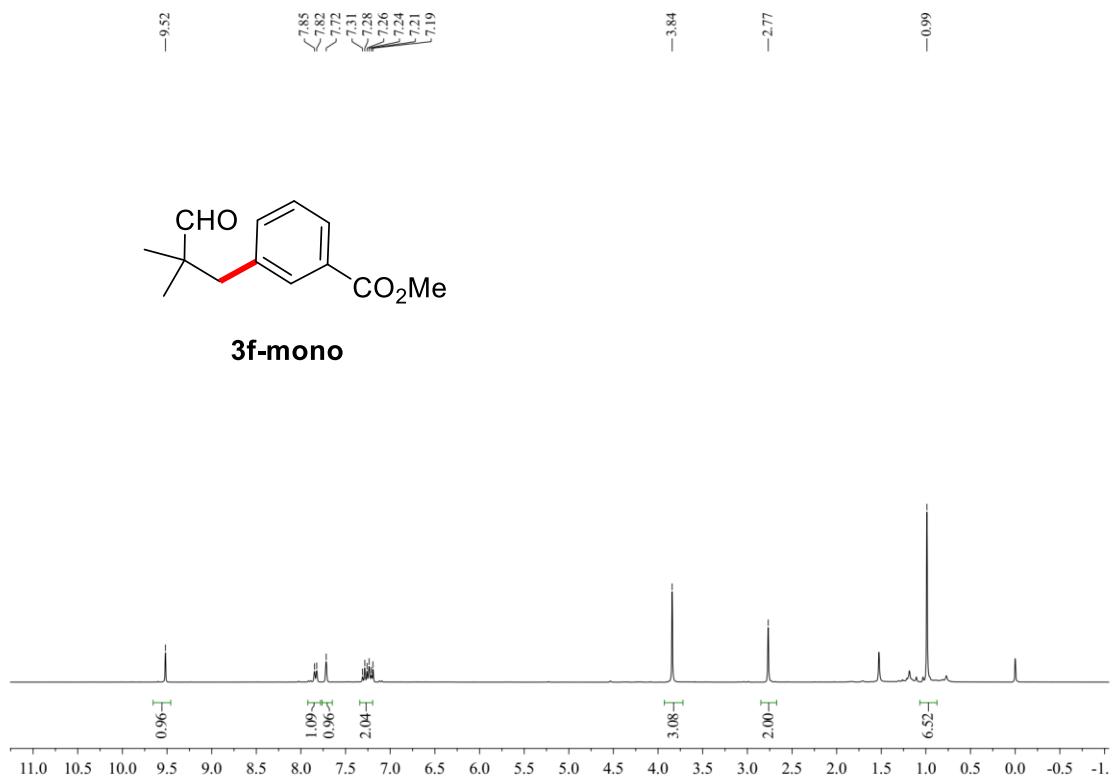


Figure S22 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3f-mono**

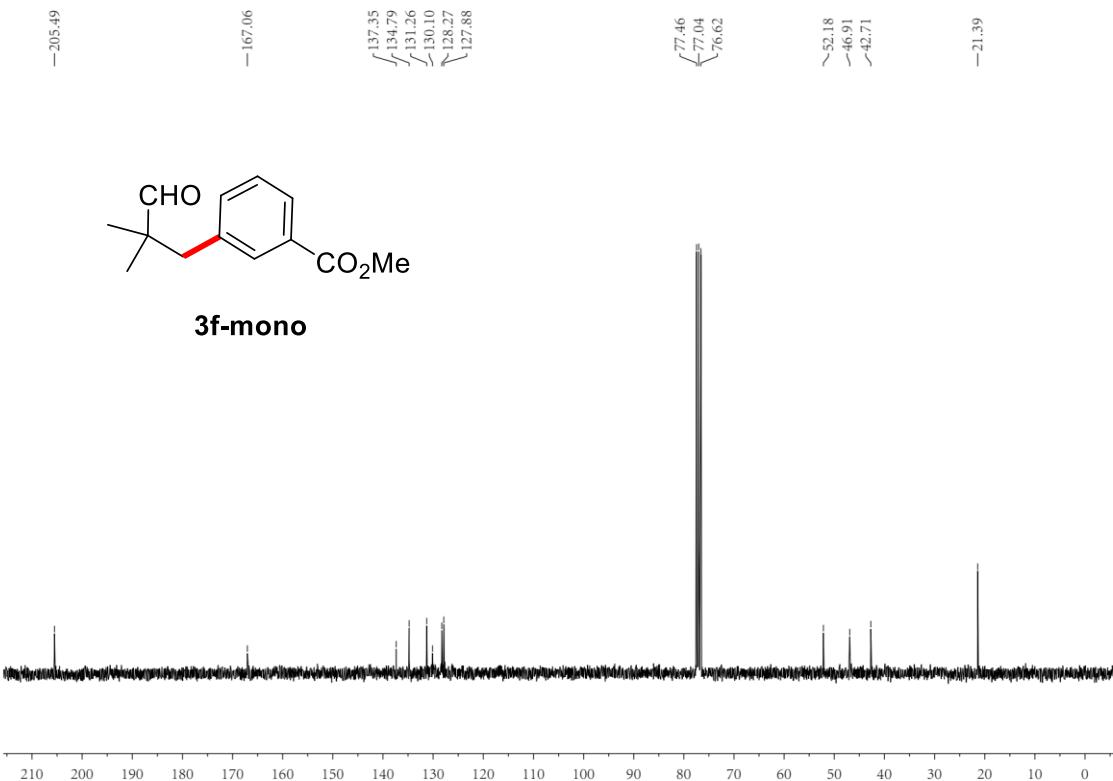


Figure S23 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3f-mono**

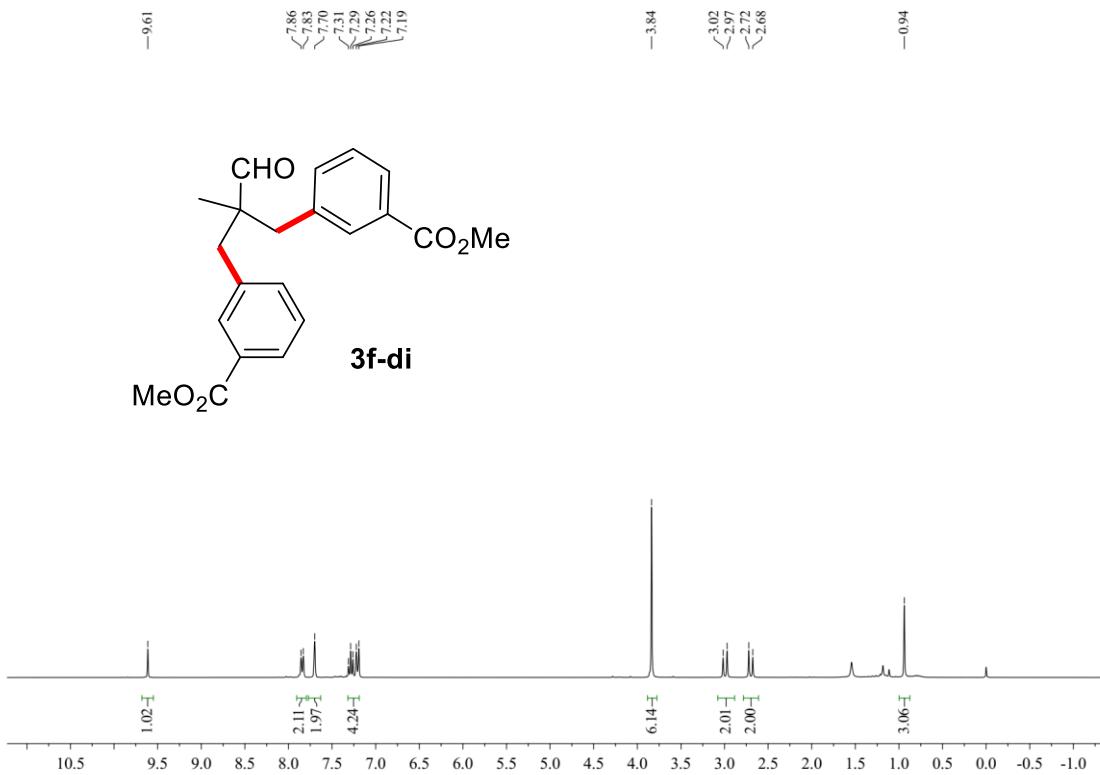


Figure S24 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3f-di**

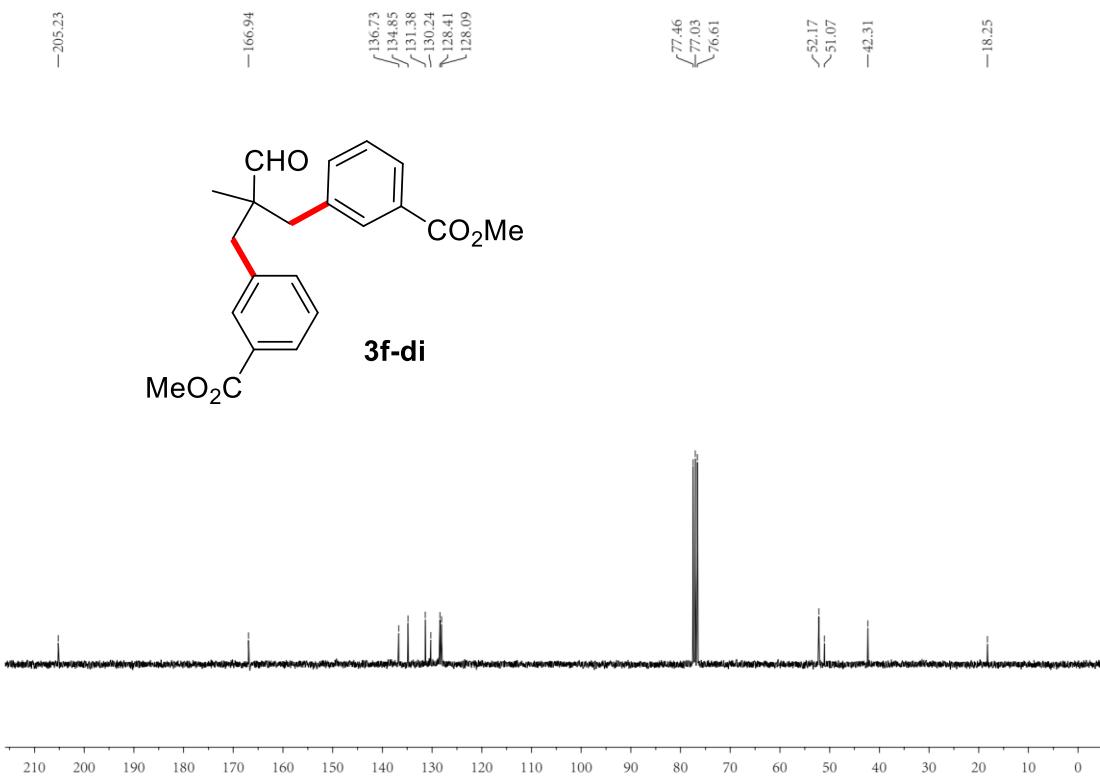


Figure S25 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3f-di**

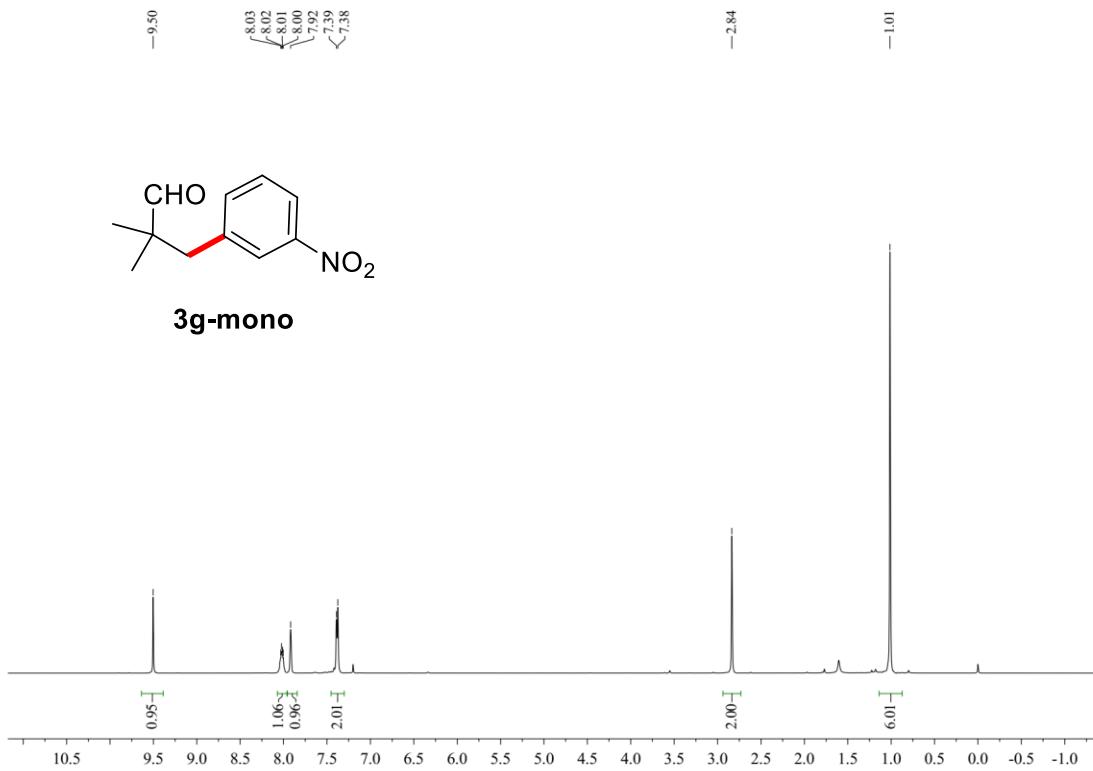


Figure S26 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3g-mono**

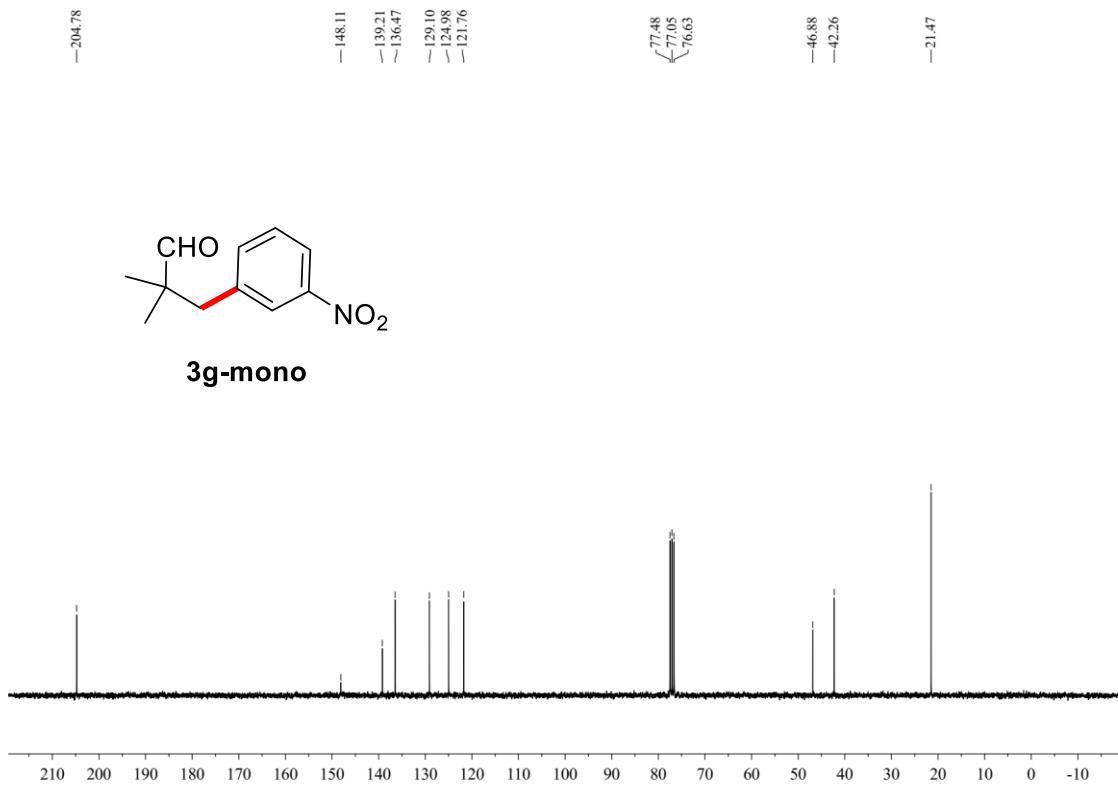


Figure S27 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3g-mono**

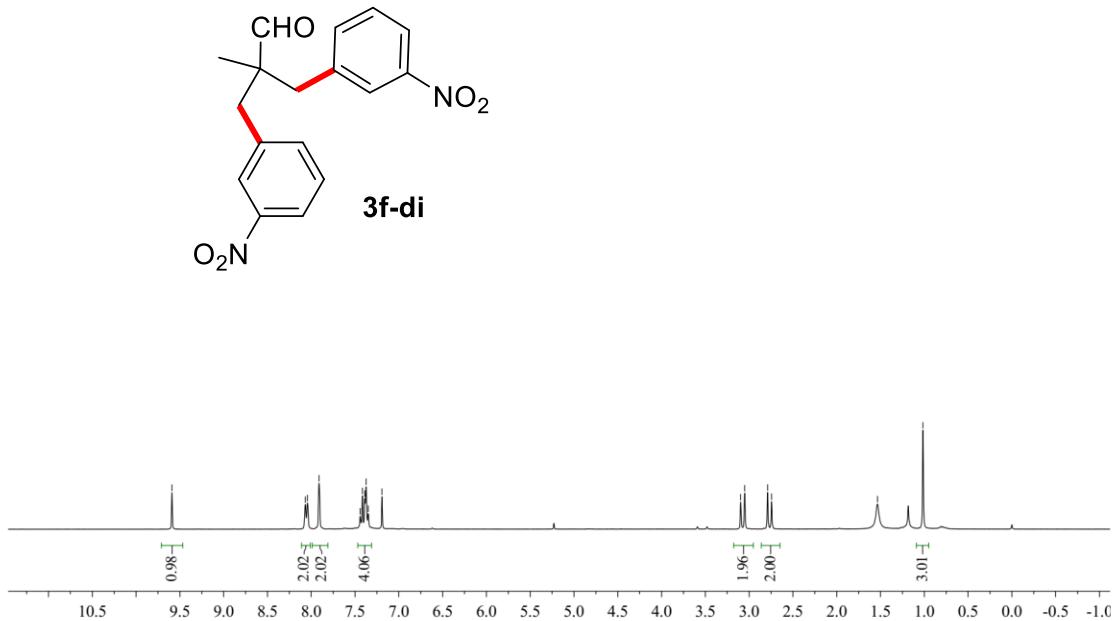
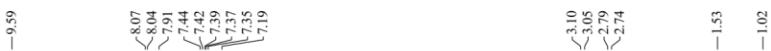


Figure S28 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3g-di**

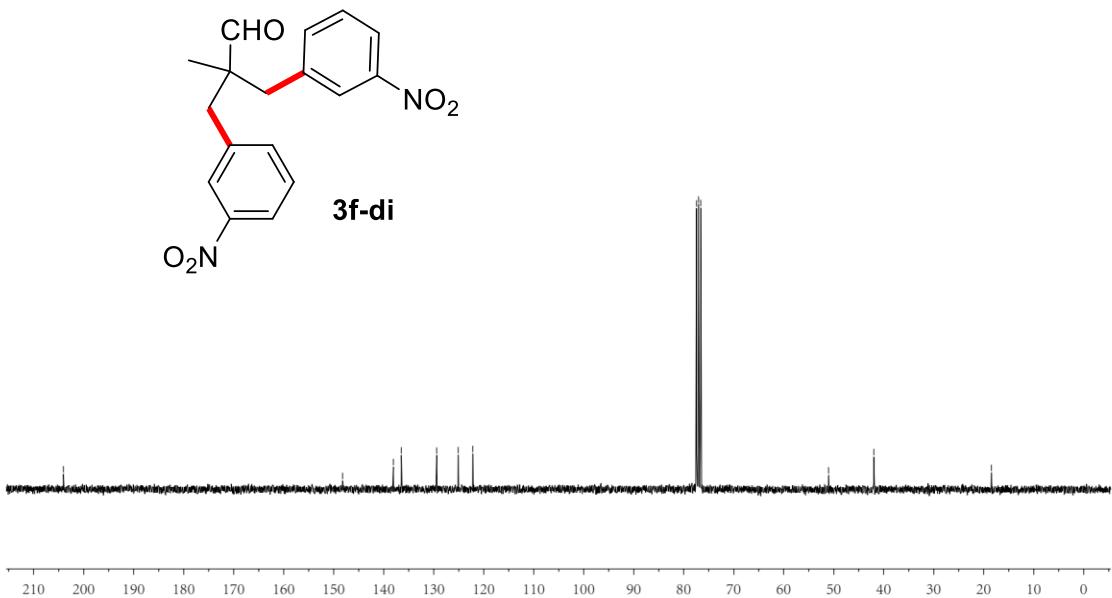


Figure S29 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3g-di**

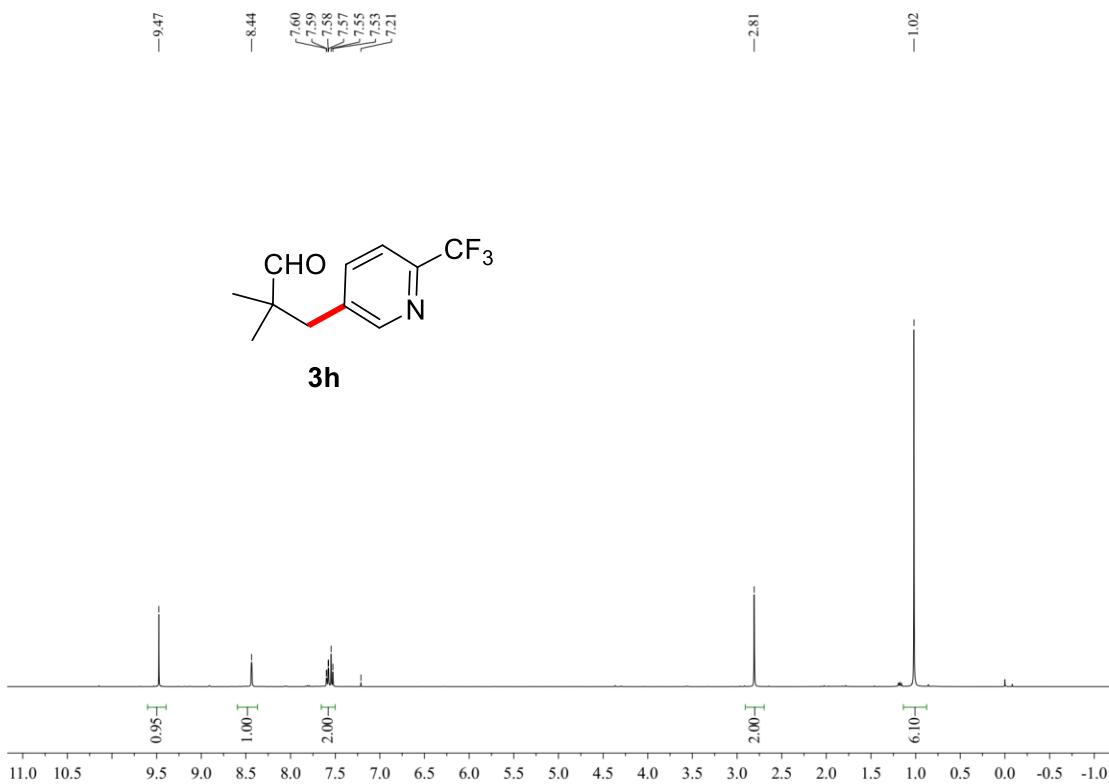


Figure S30 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3h**

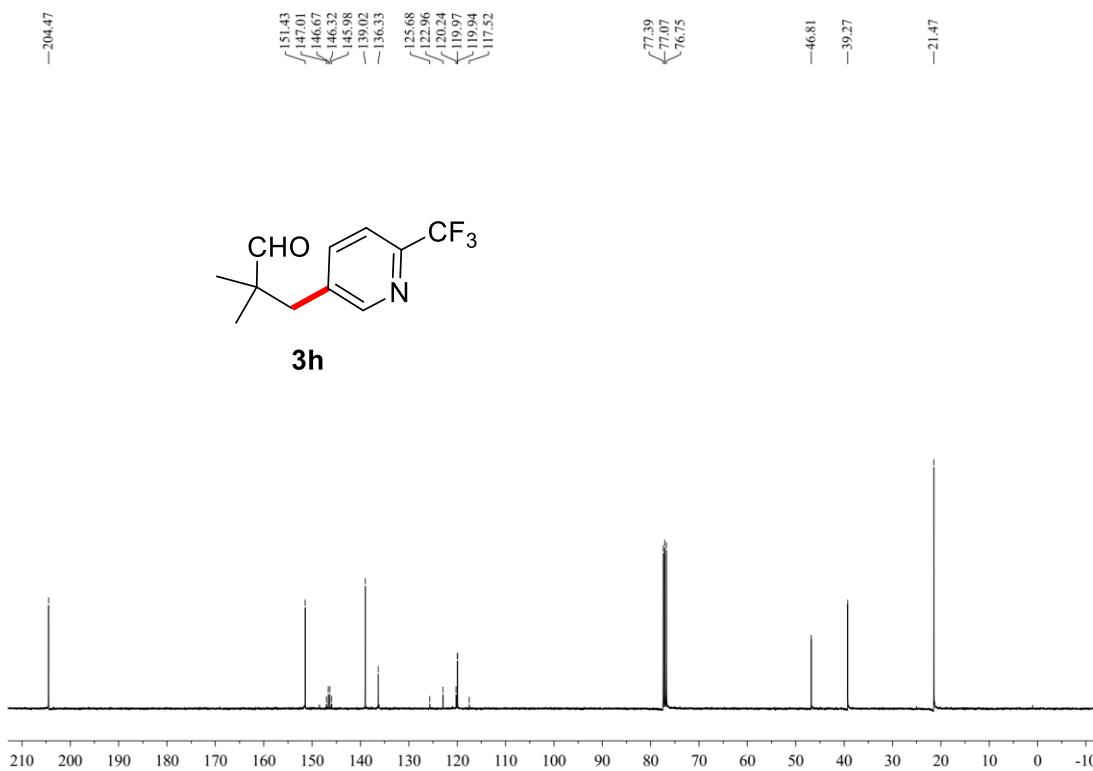


Figure S31 ^{13}C NMR spectrum (101MHz, CDCl_3 , 298K) of **3h**

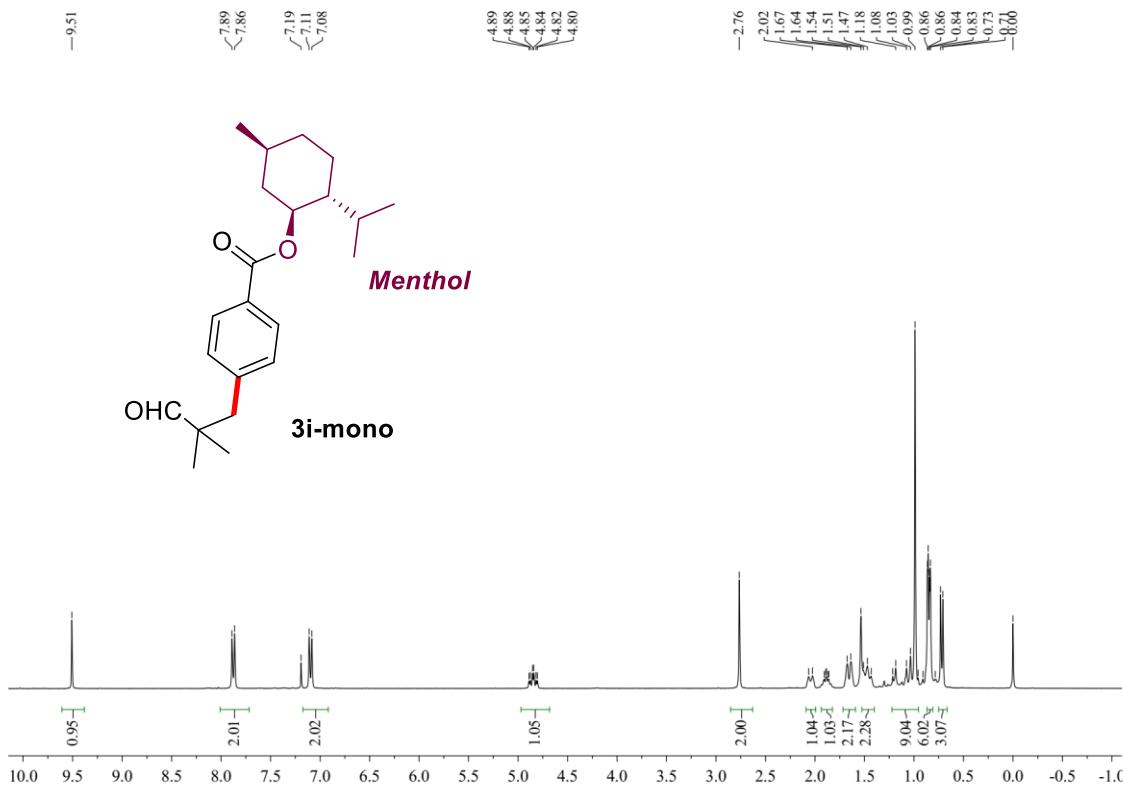


Figure S32 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3i-mono**

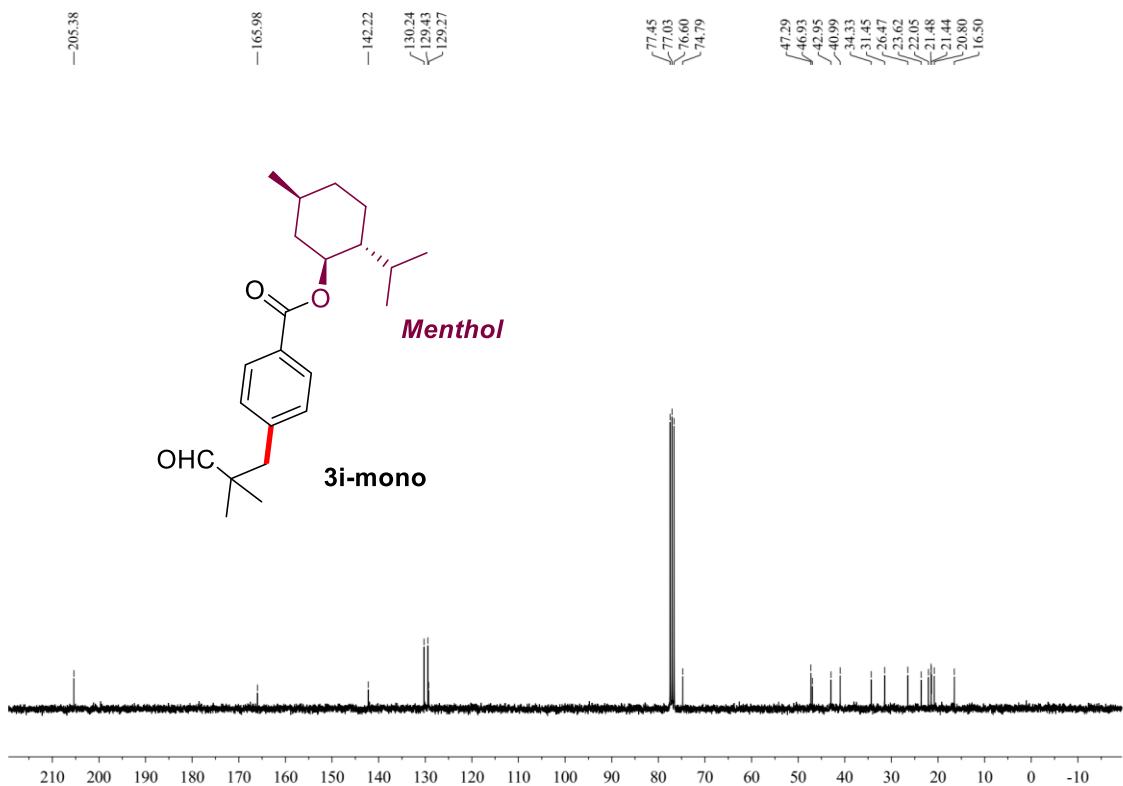


Figure S33 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3i-mono**

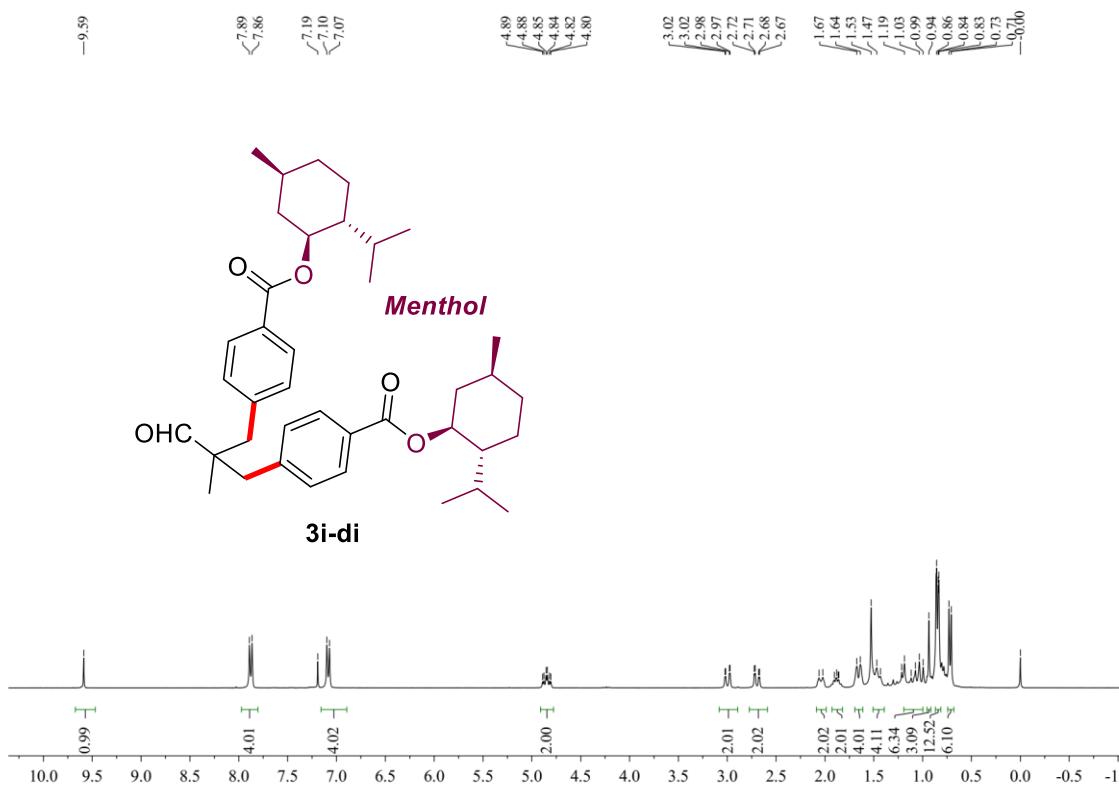


Figure S34 ¹H NMR spectrum (300MHz, CDCl₃, 298K) of **3i-di**

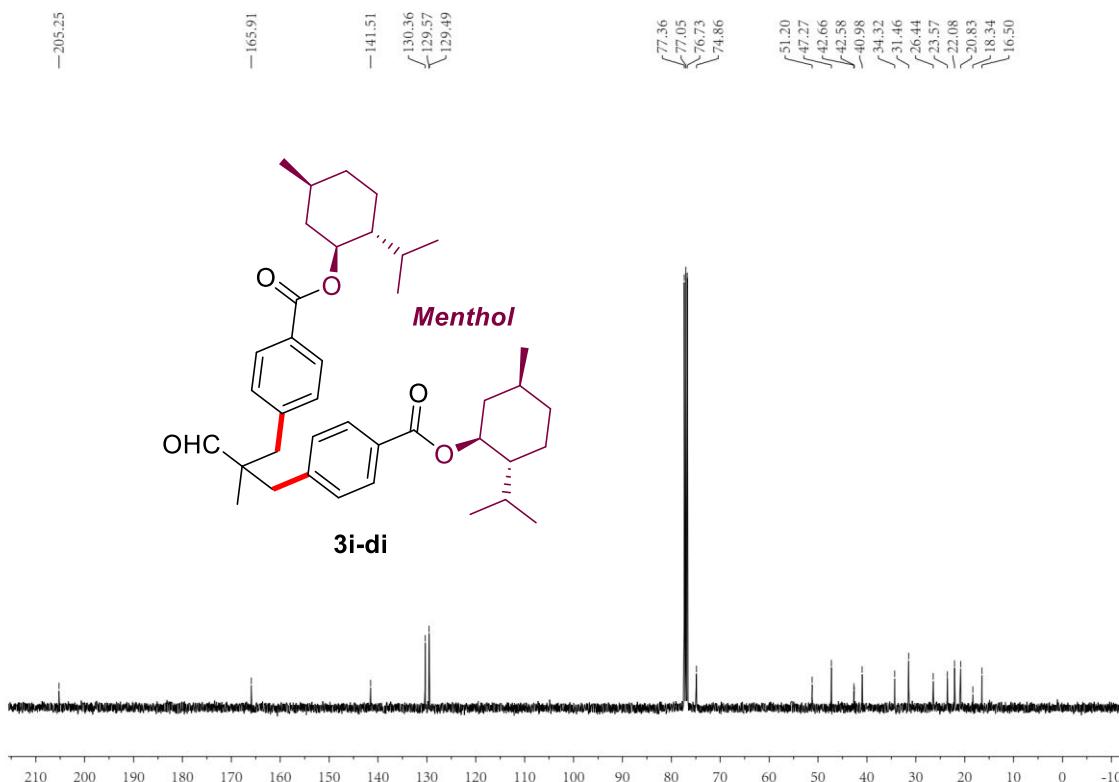


Figure S35 ¹³C NMR spectrum (101MHz, CDCl₃, 298K) of **3i-di**

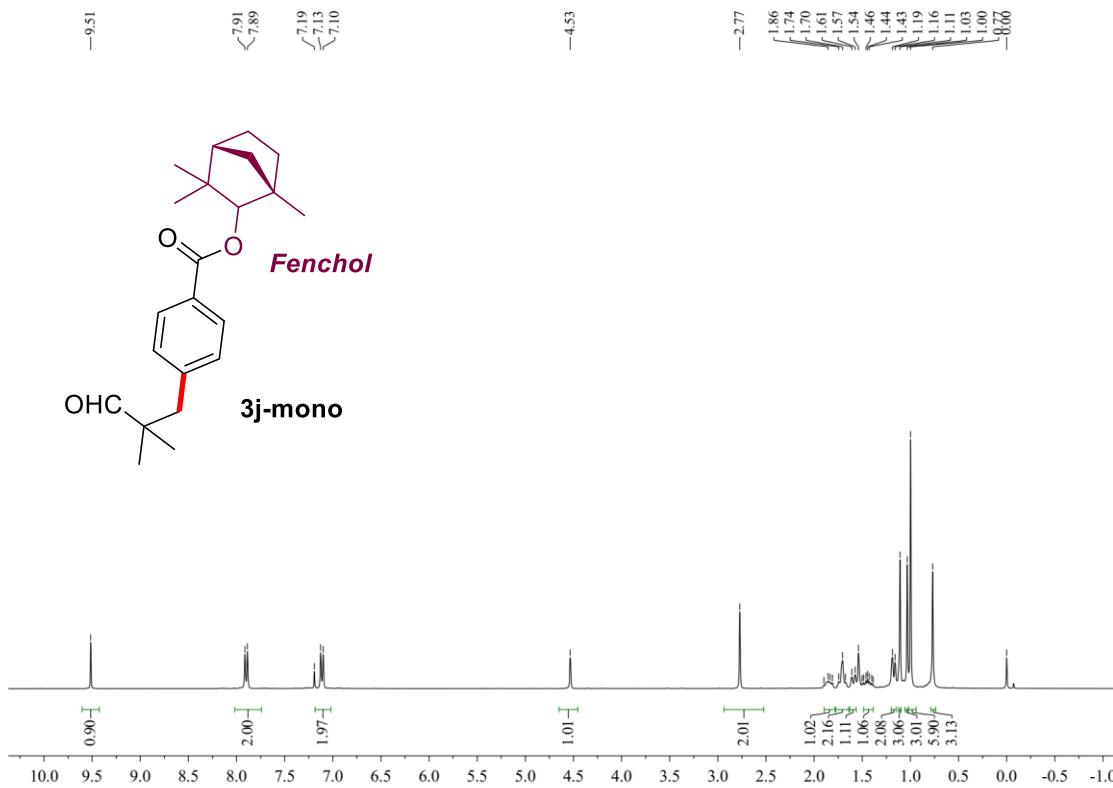


Figure S36 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3j-mono**

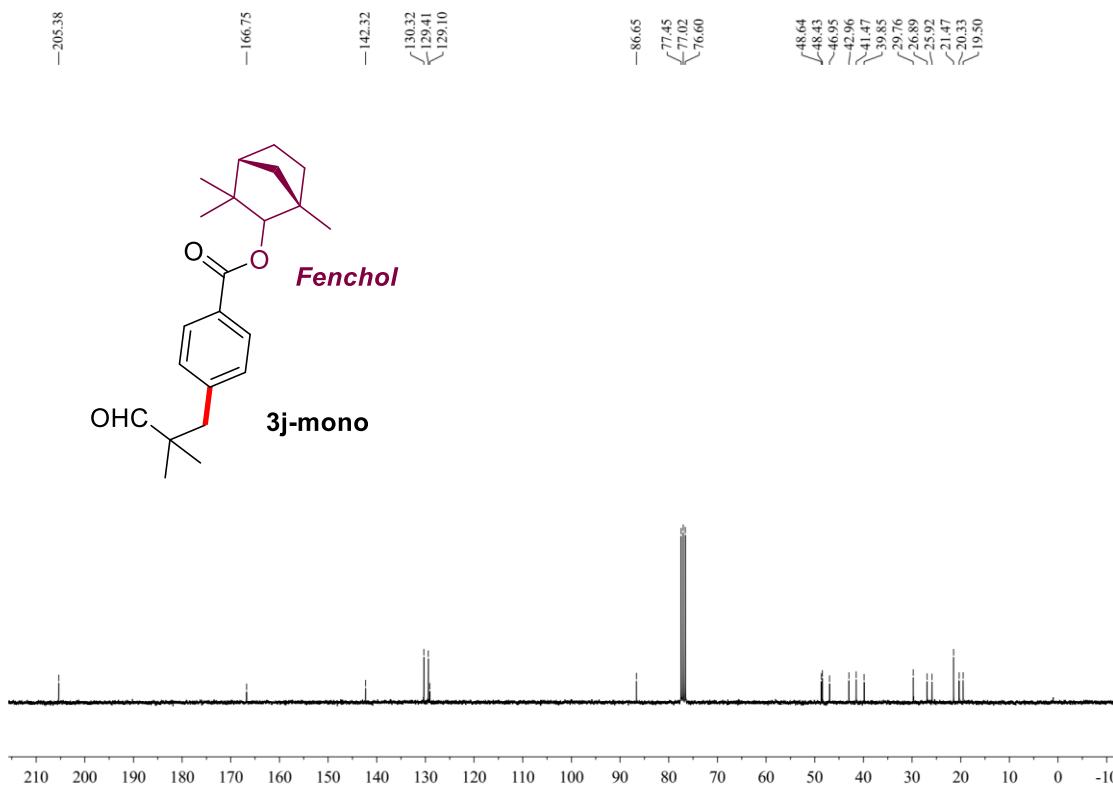


Figure S37 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3j-mono**

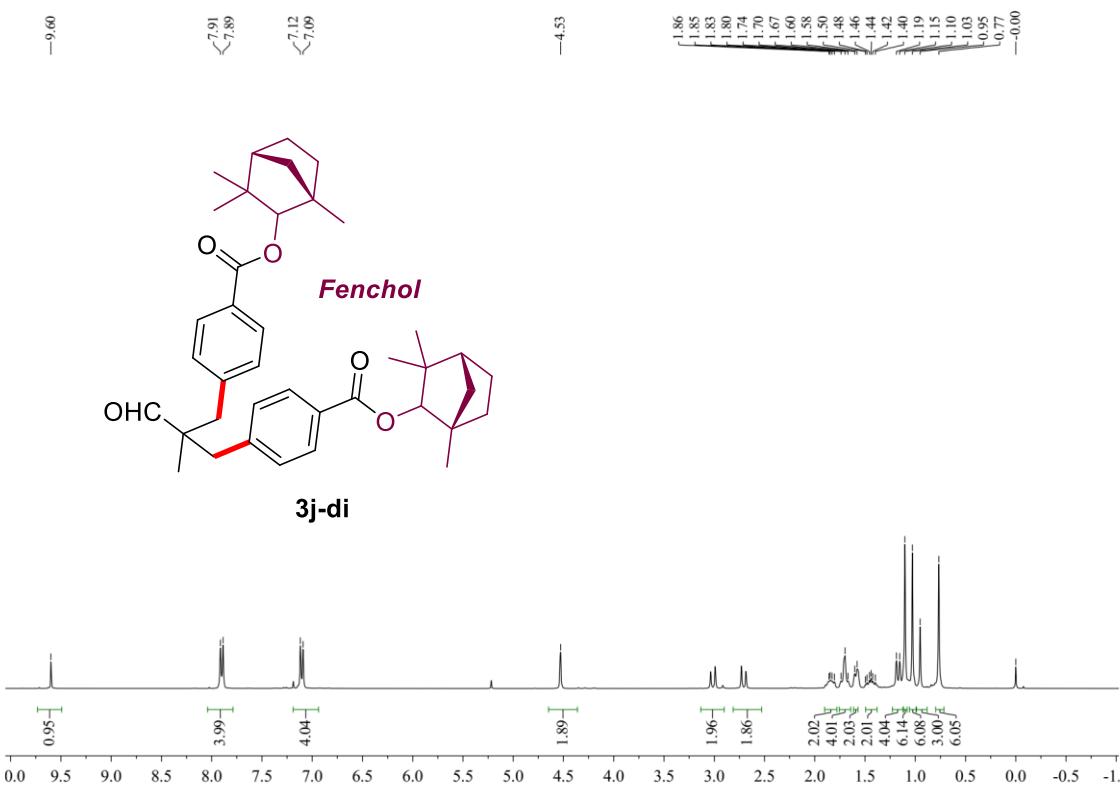


Figure S38 ¹H NMR spectrum (300MHz, CDCl₃, 298K) of 3j-di

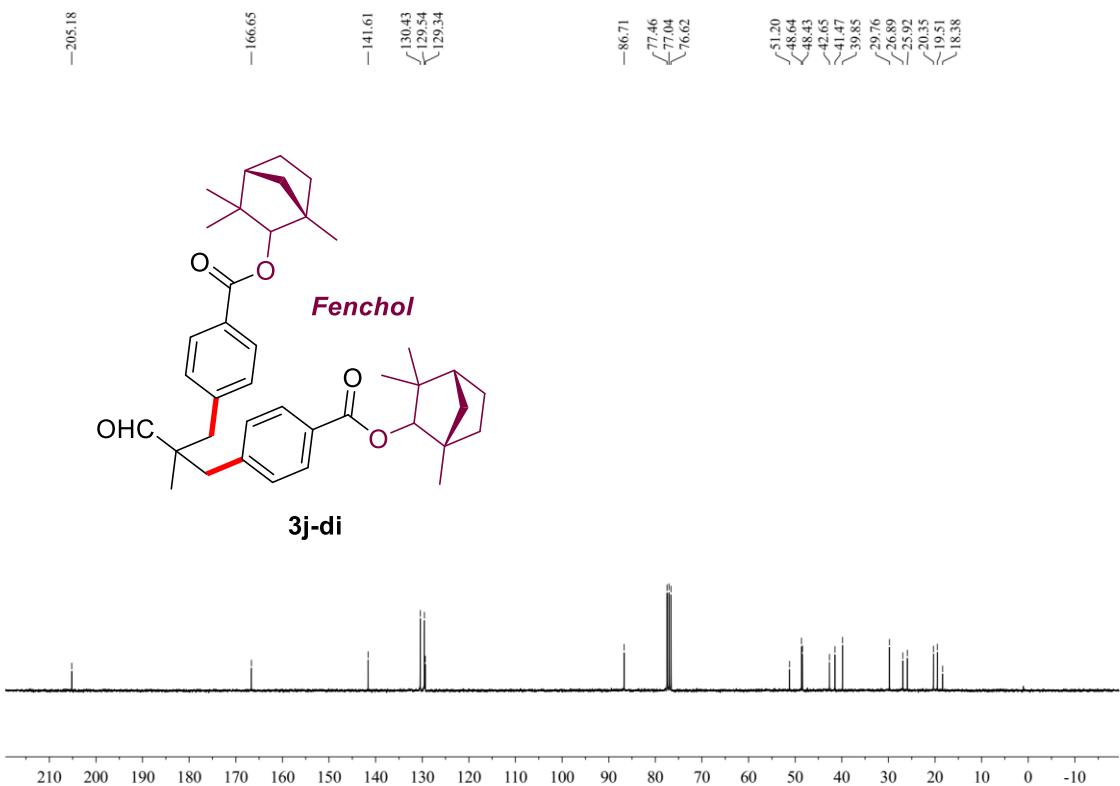


Figure S39 ¹³C NMR spectrum (75MHz, CDCl₃, 298K) of 3j-di

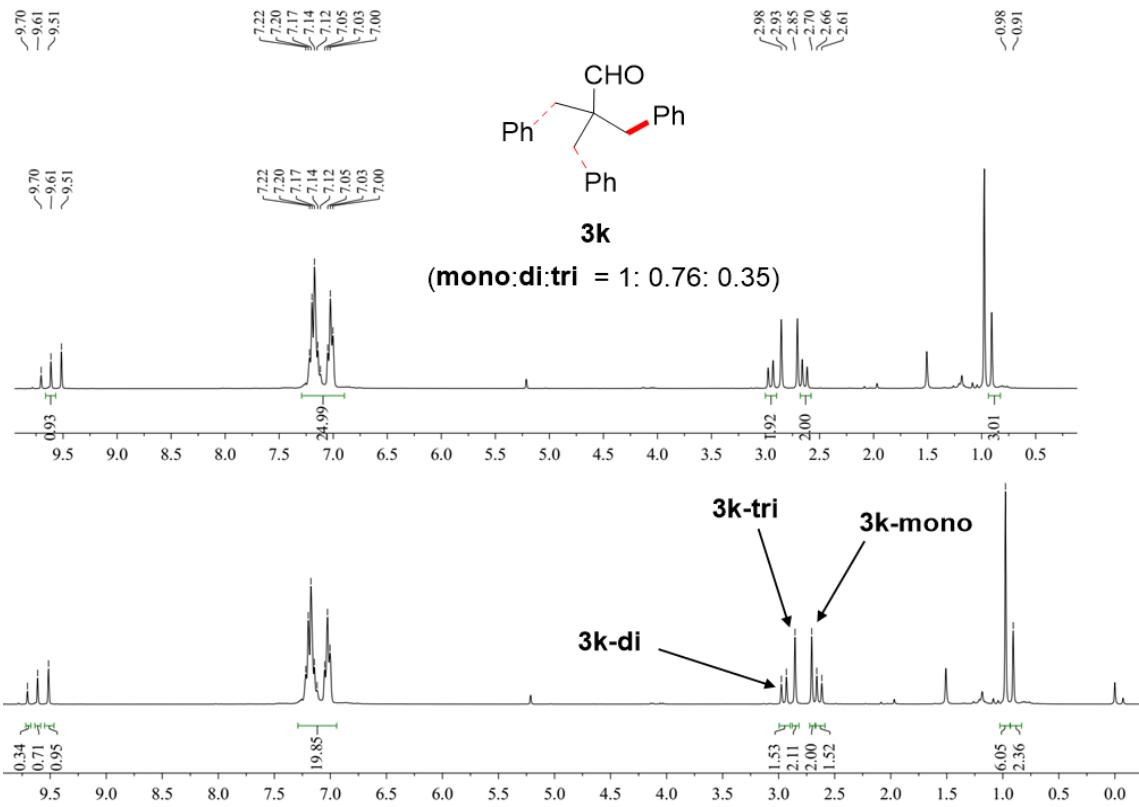


Figure S40 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3k**

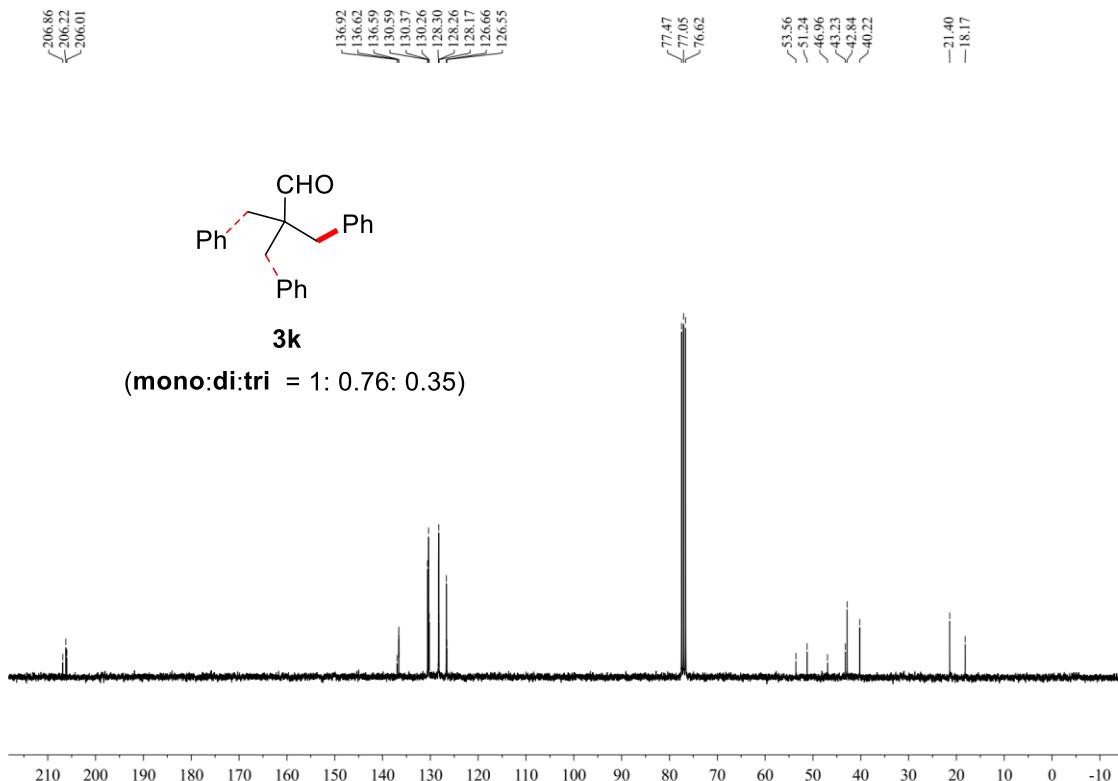
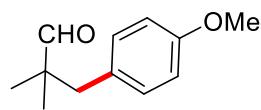


Figure S41 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3k**

—9.50
 7.19
 6.95
 6.92
 6.75
 6.72



3l-mono

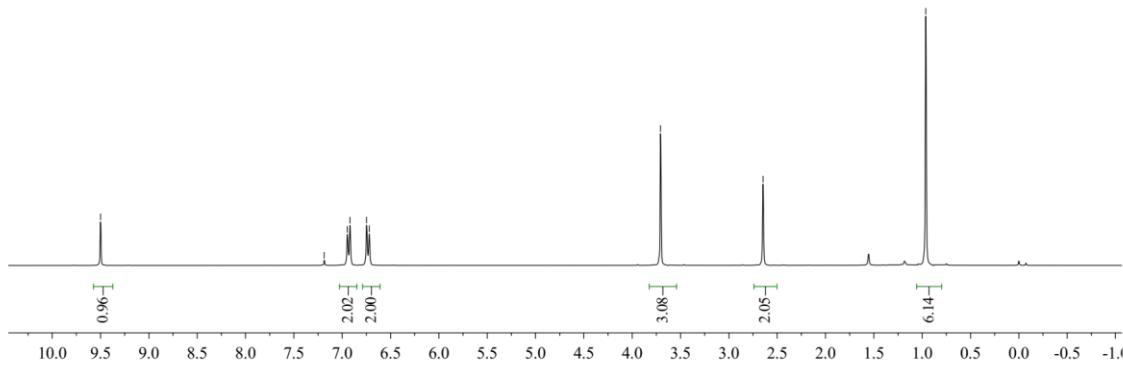
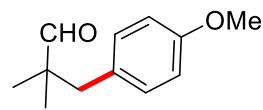


Figure S42 ¹H NMR spectrum (300MHz, CDCl₃, 298K) of **3l-mono**

—206.24
 —158.32
 —131.18
 —128.90
 —113.58
 —77.47
 —77.05
 —76.62
 —55.22
 —47.04
 —42.38
 —21.33



3l-mono

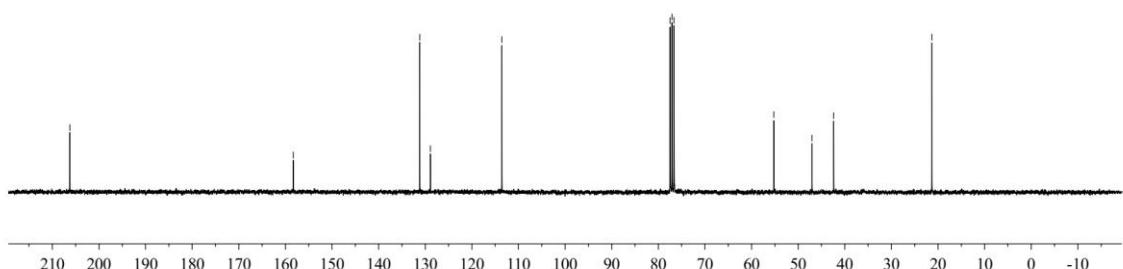


Figure S43 ¹³C NMR spectrum (75MHz, CDCl₃, 298K) of **3l-mono**

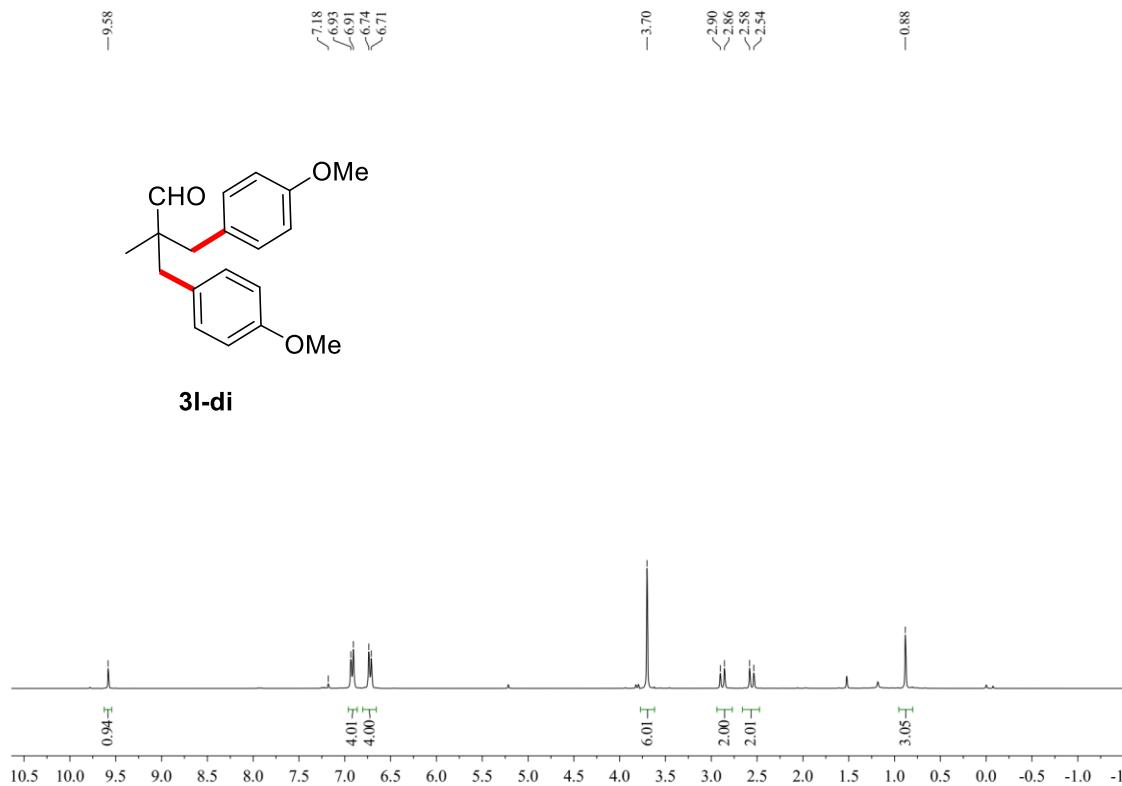
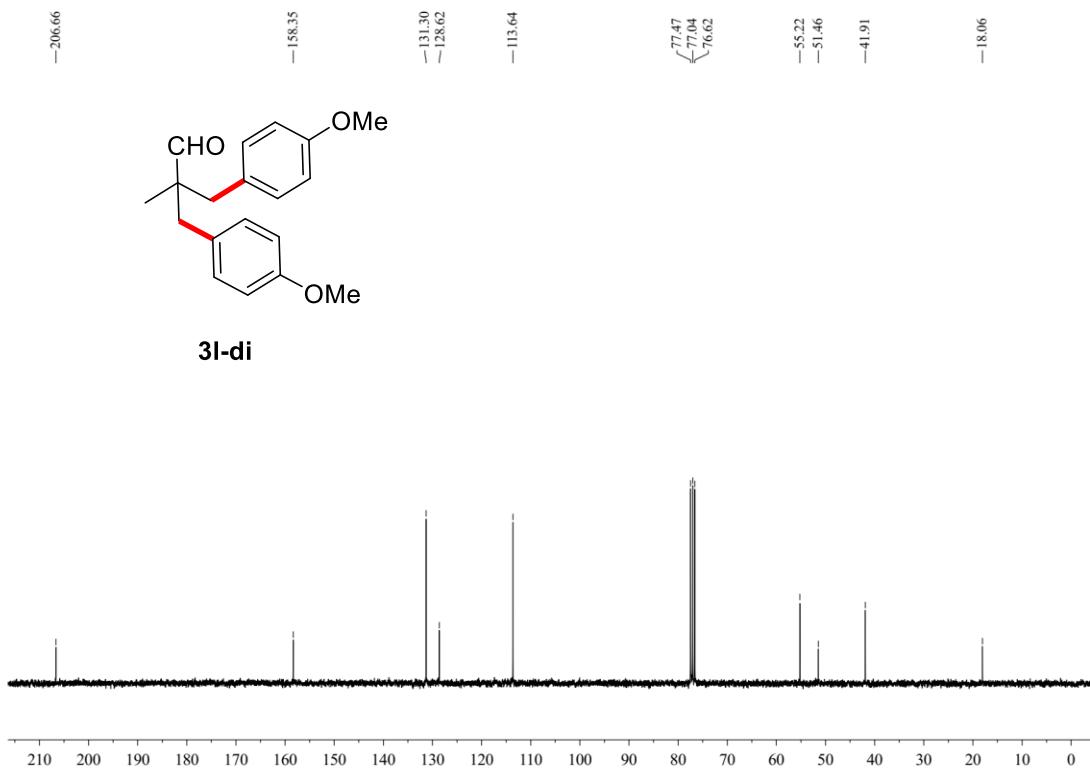


Figure S44 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3l-di**



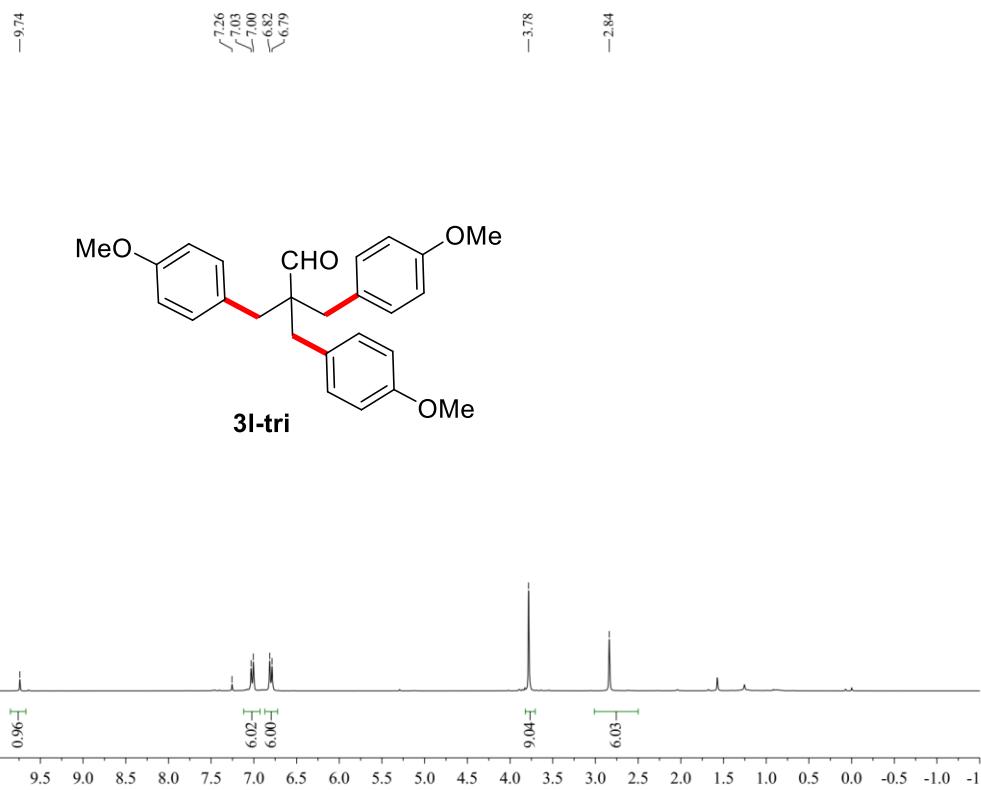


Figure S46 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3l-tri**

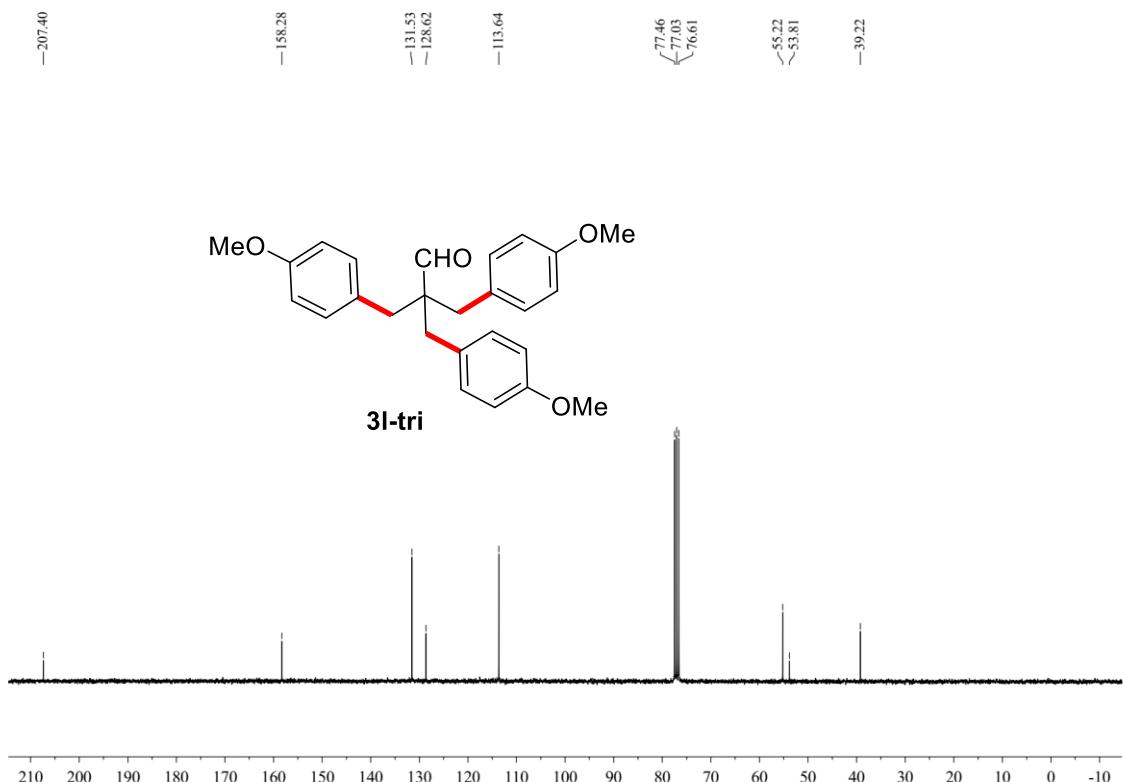


Figure S47 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3l-tri**

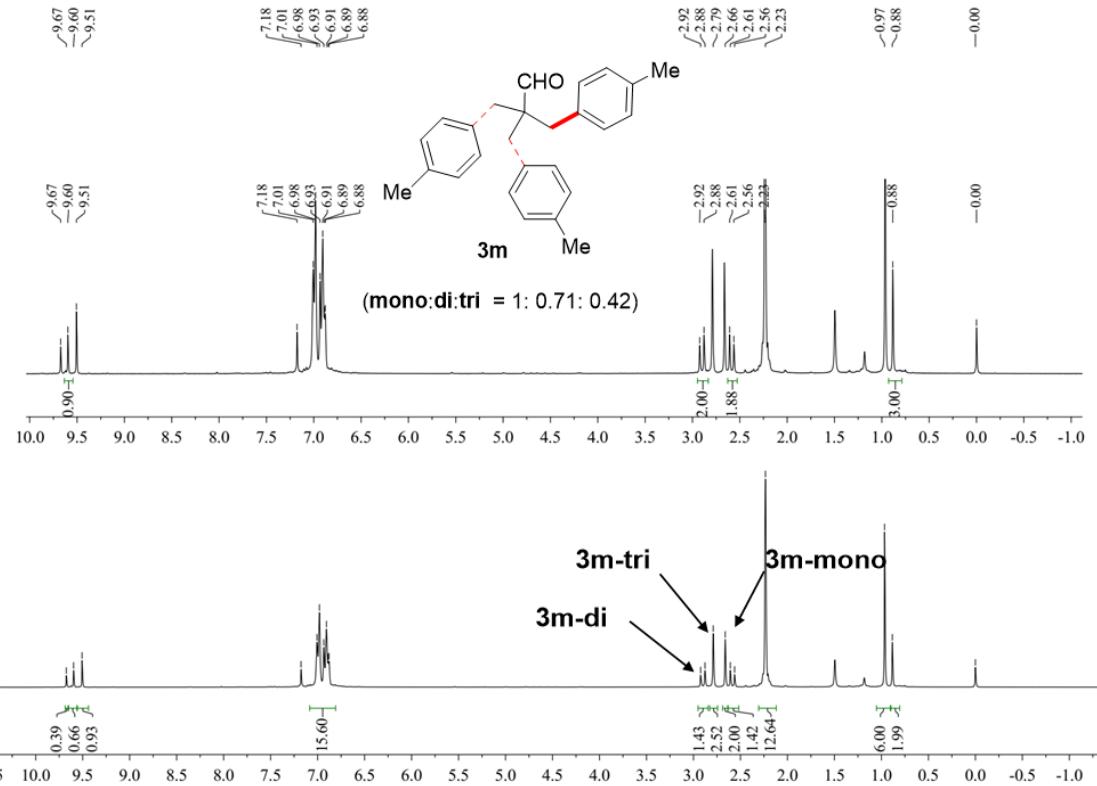


Figure S48 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3m**

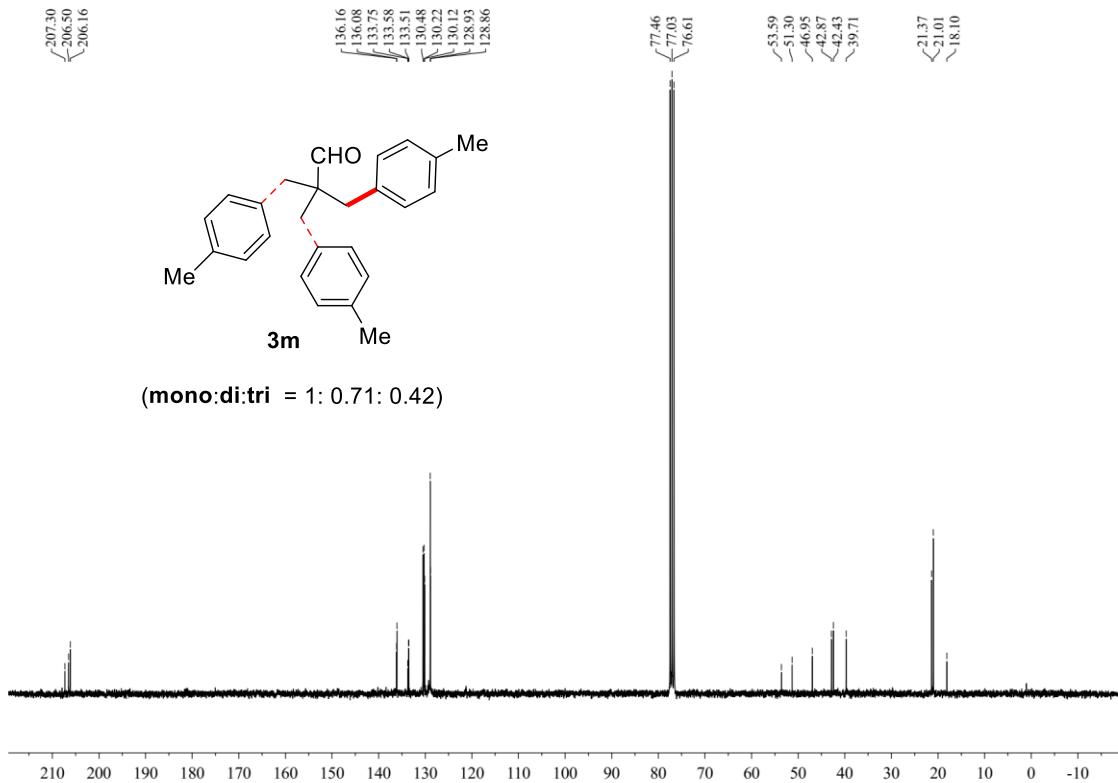


Figure S49 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3m**

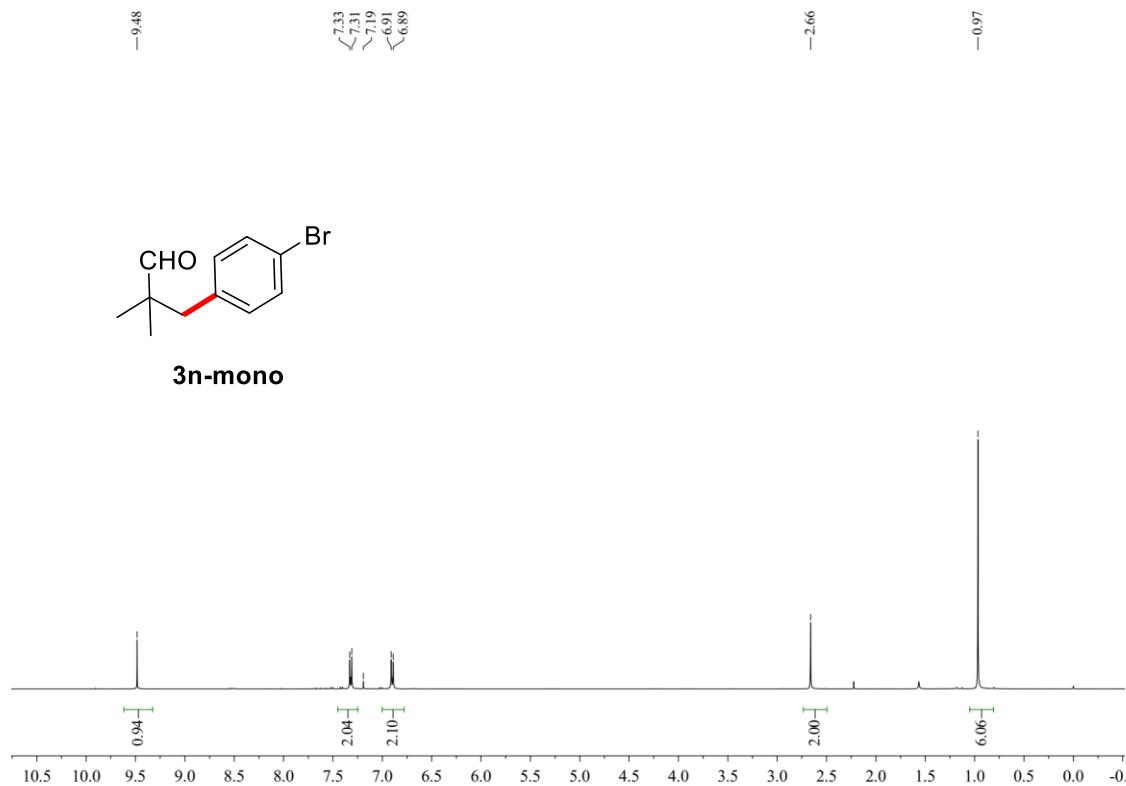


Figure S50 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3n-mono**

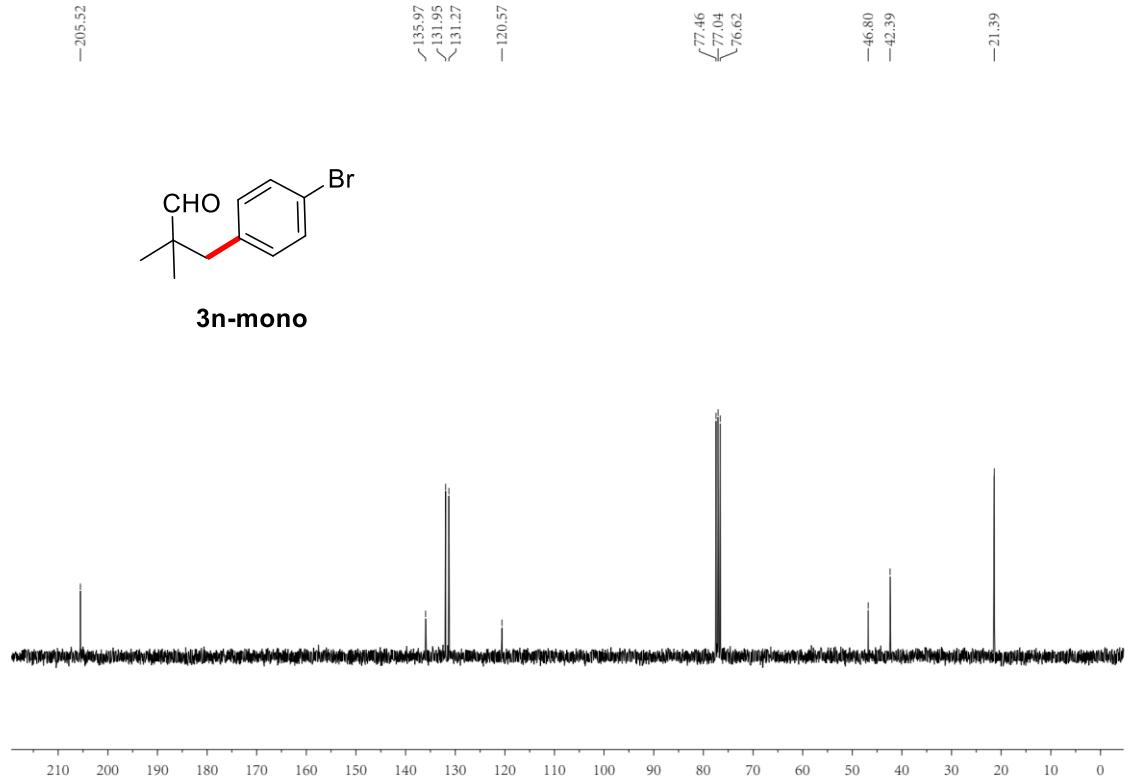


Figure S51 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3n-mono**

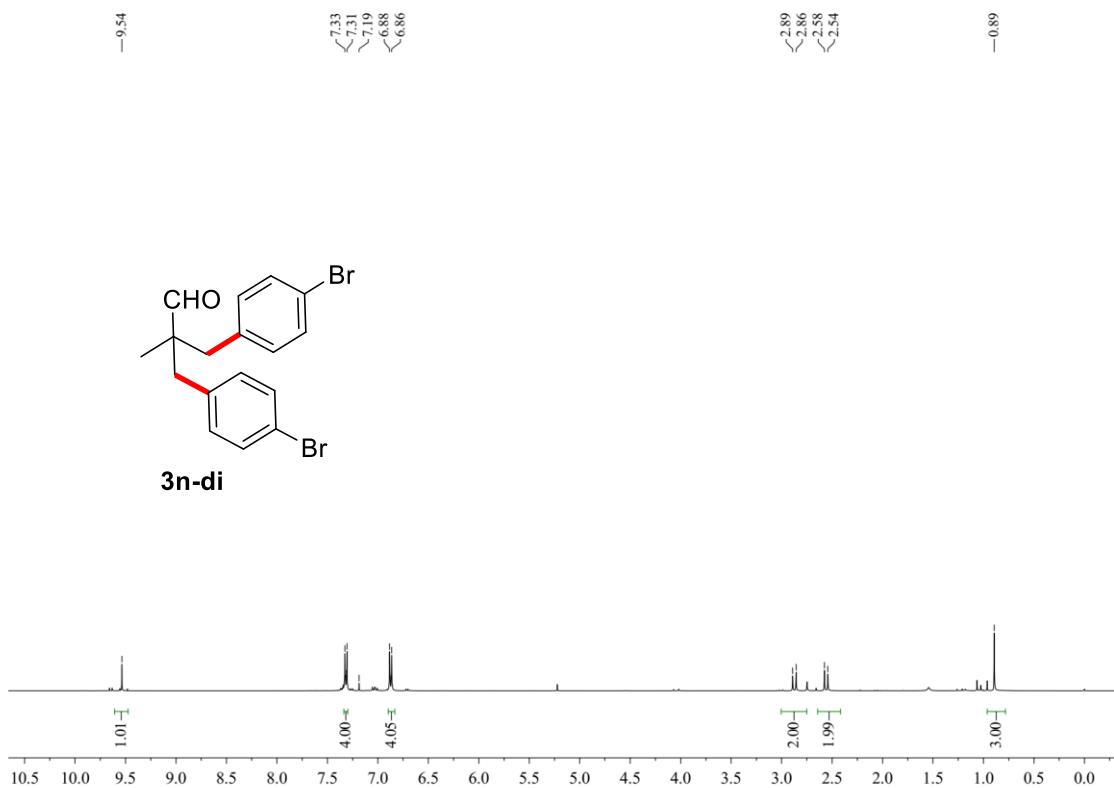


Figure S52 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3n-di**

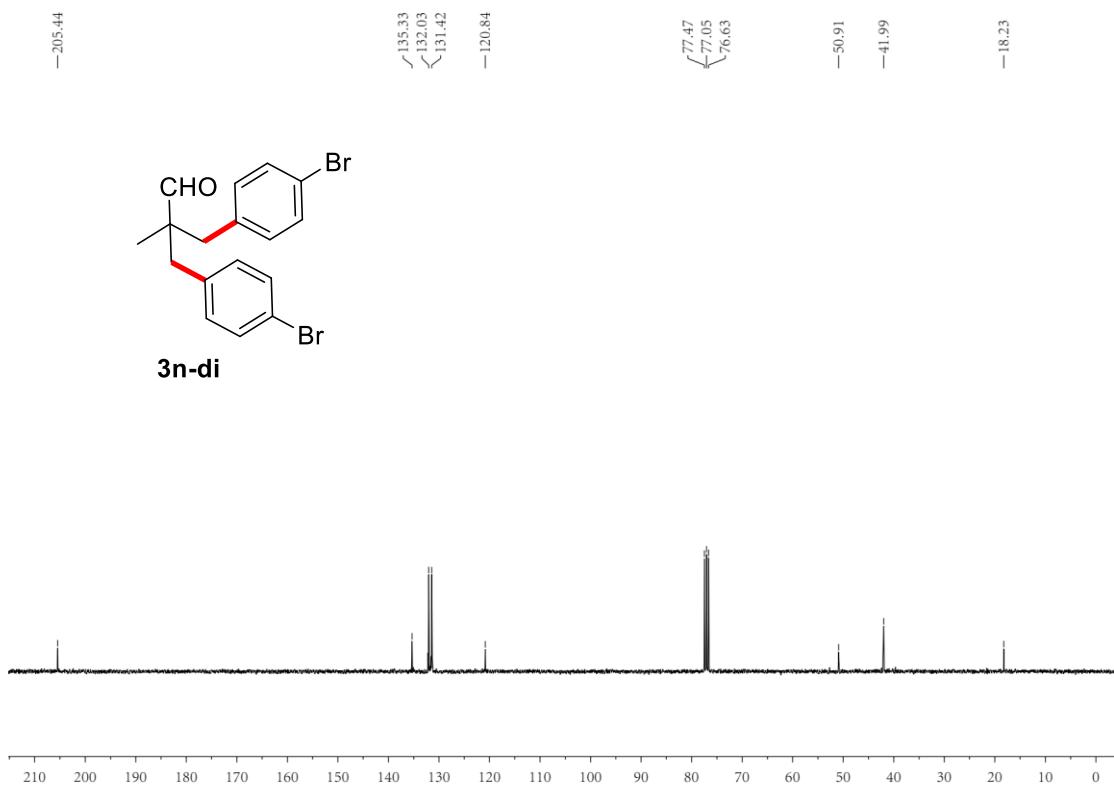


Figure S53 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3n-di**

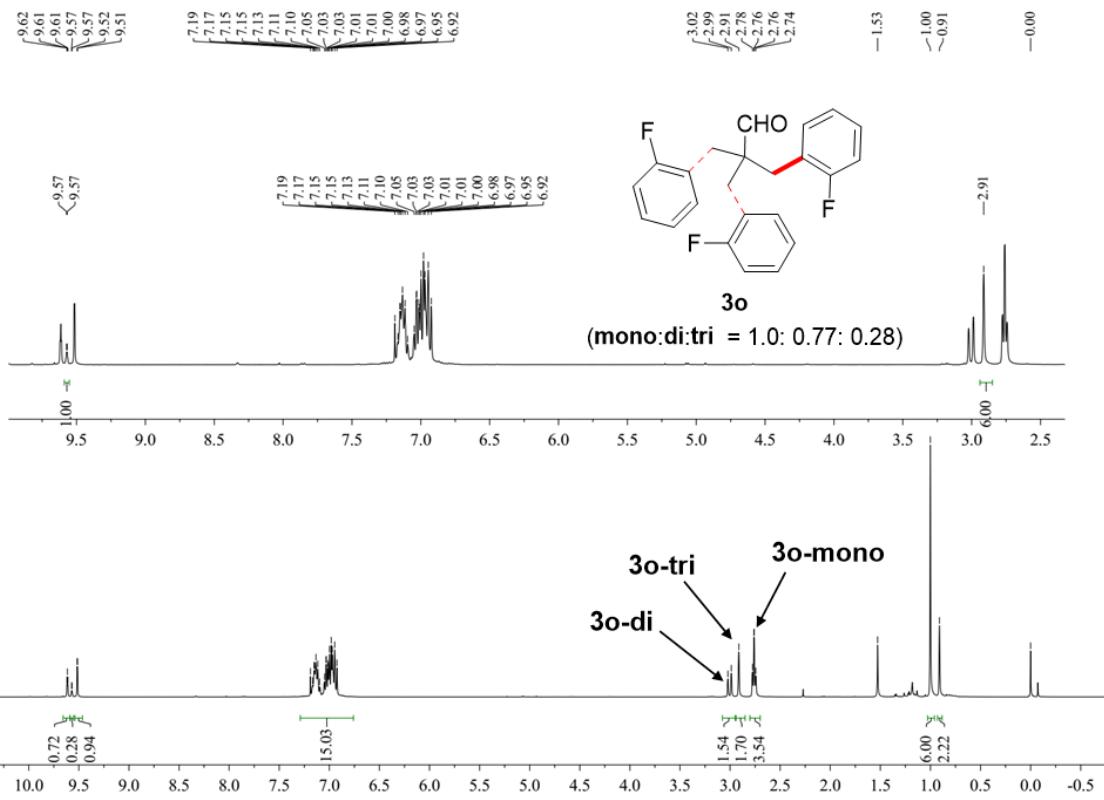


Figure S54 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3o**

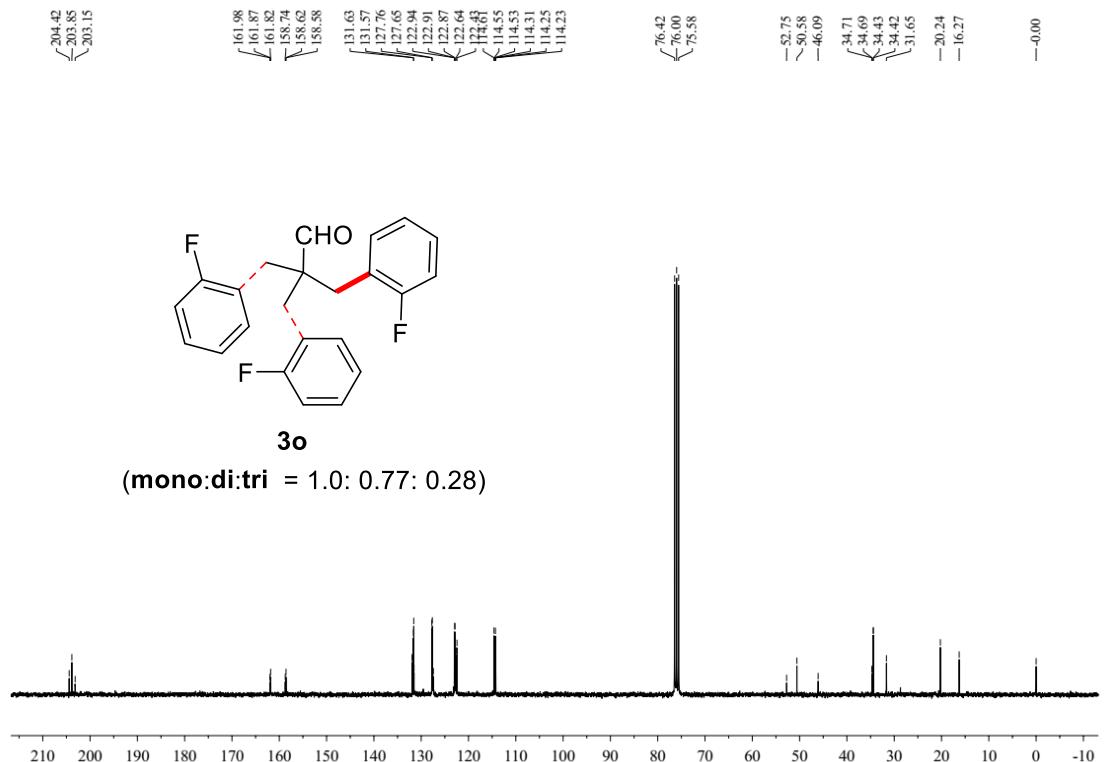


Figure S55 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3o**

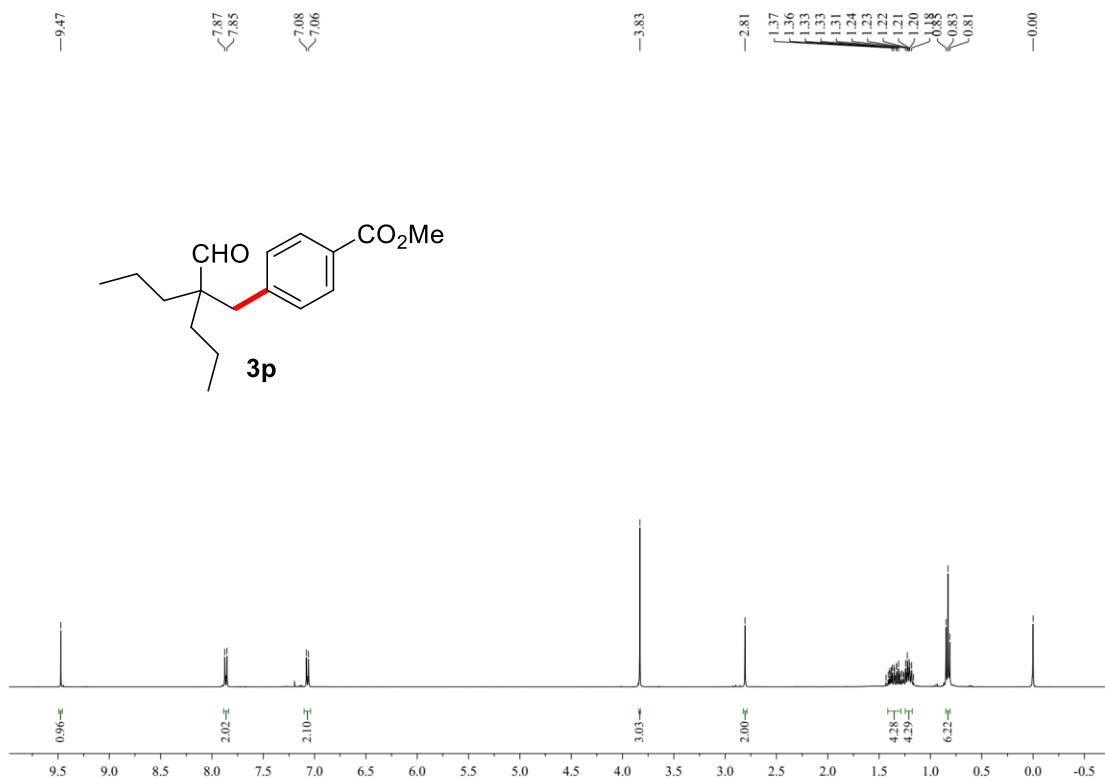


Figure S56 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3p**

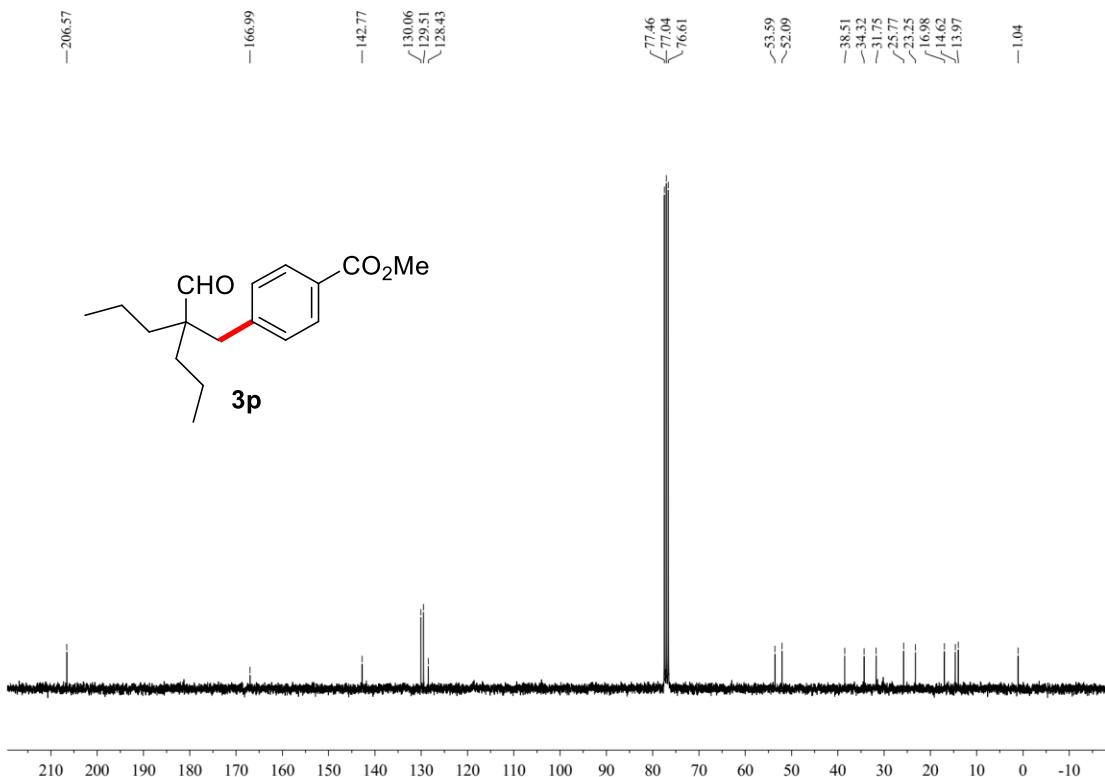


Figure S57 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3p**

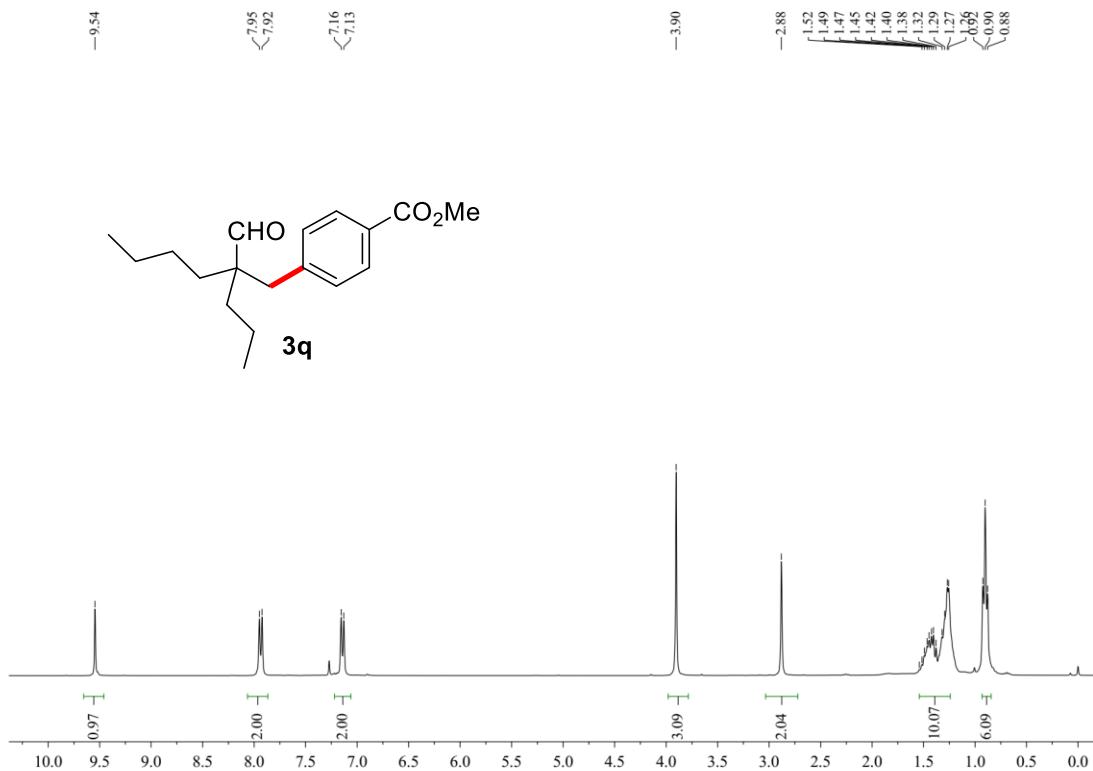


Figure S58 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3q**

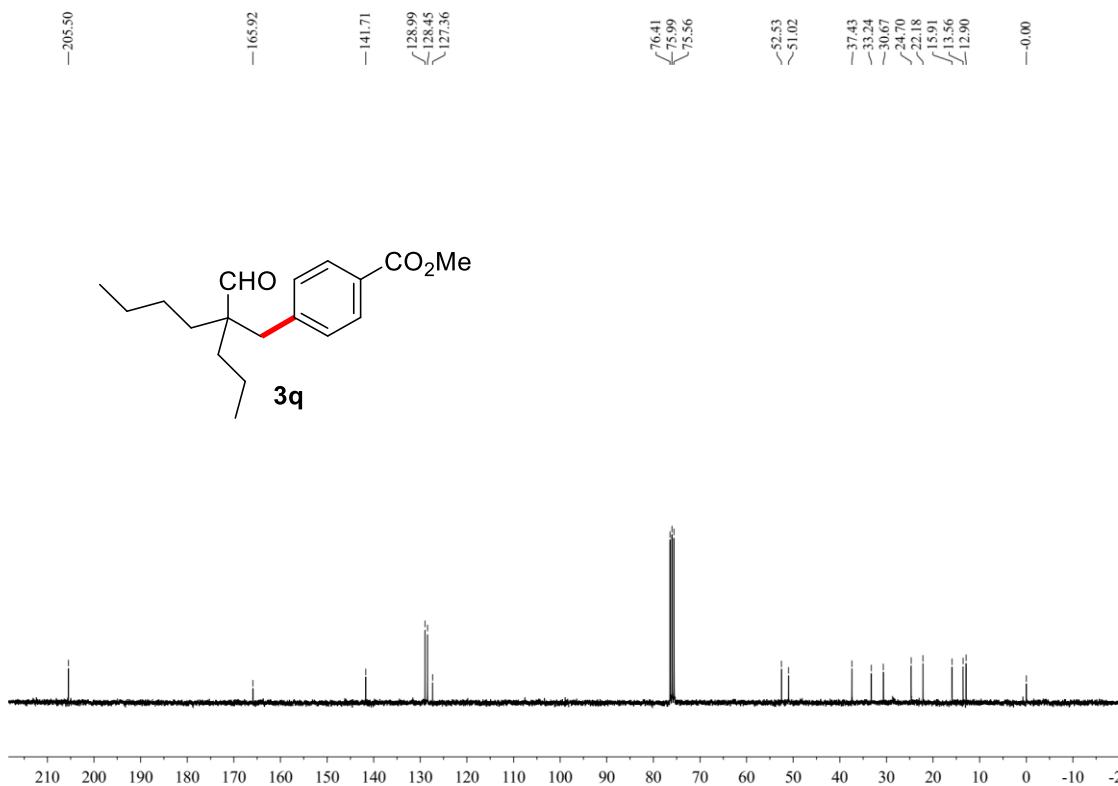


Figure S58 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3q**

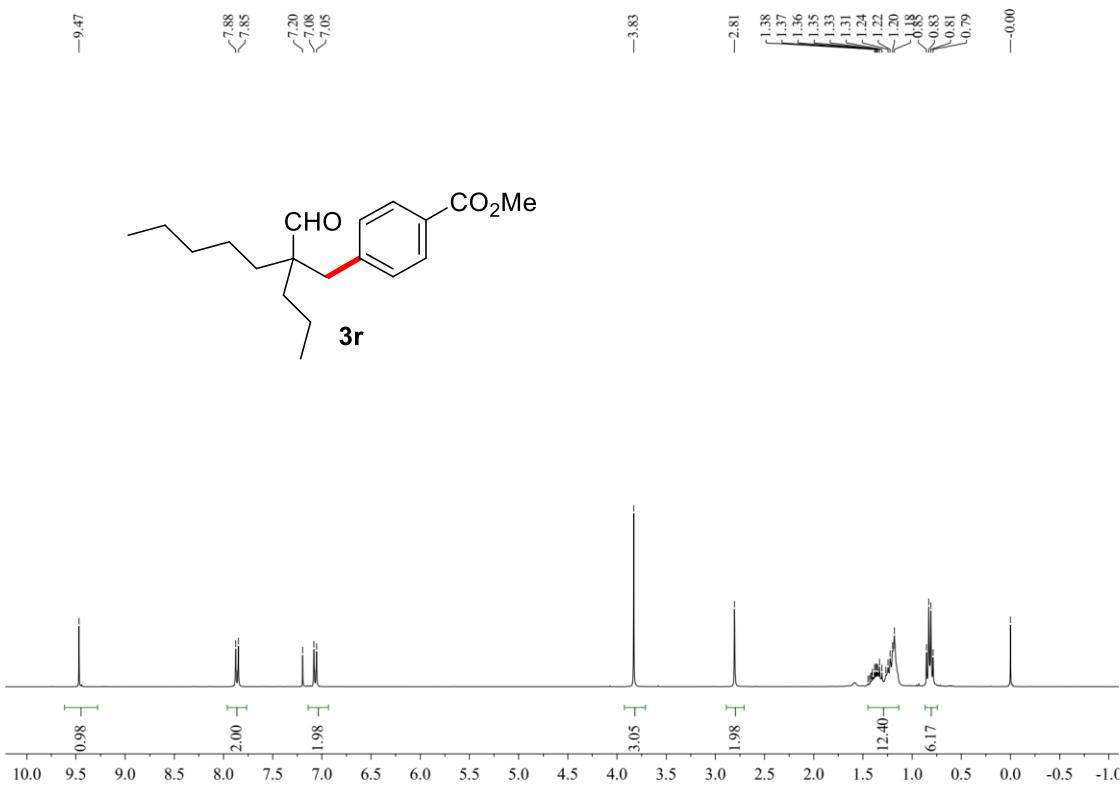


Figure S60 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3r**

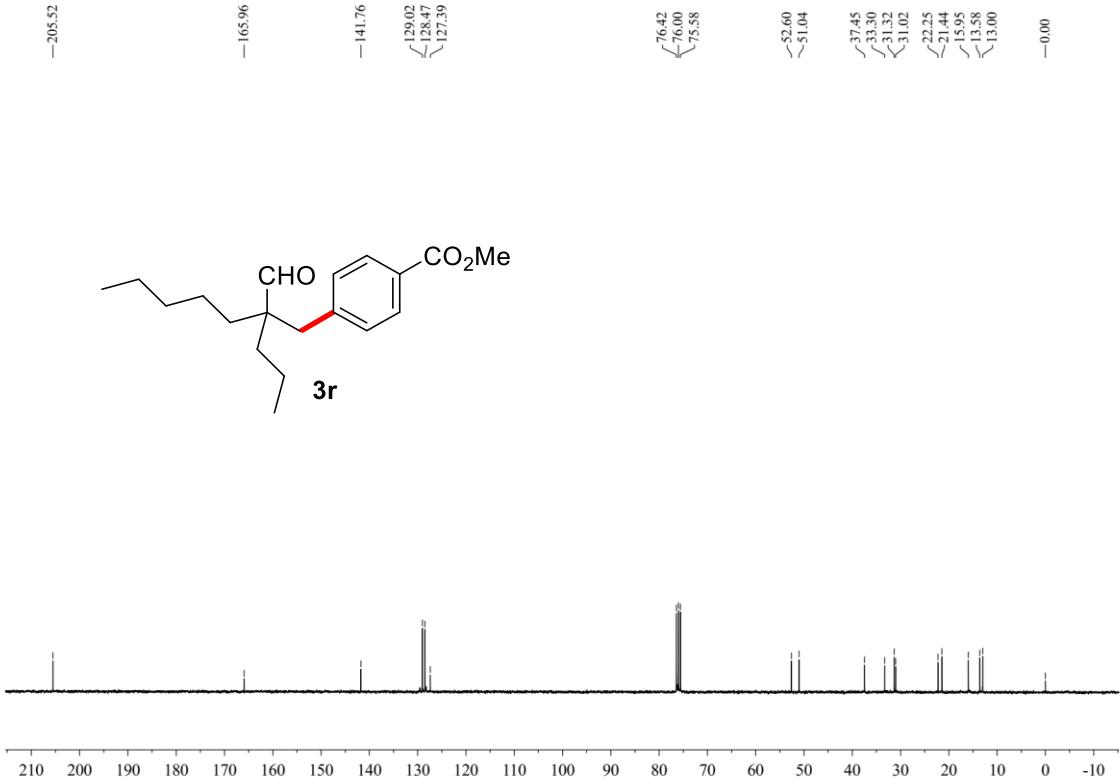


Figure S61 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3r**

—9.46 <7.87
 —7.85 <7.19
 <7.07 <7.04

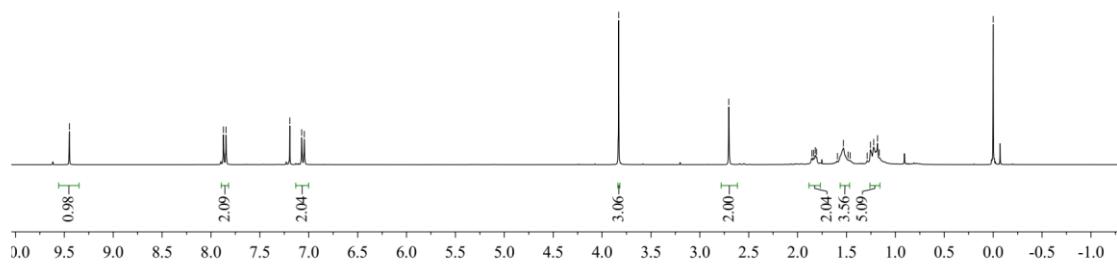
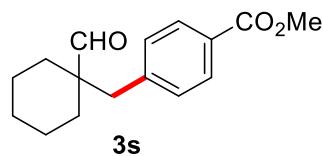


Figure S62 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3s**

—205.78
 —165.94
 —140.74
 <129.25
 <128.38
 <127.52
 —76.42
 —76.00
 —75.57
 —51.04
 —49.67
 —42.25
 ~30.14
 ~24.47
 ~21.58
 —0.00

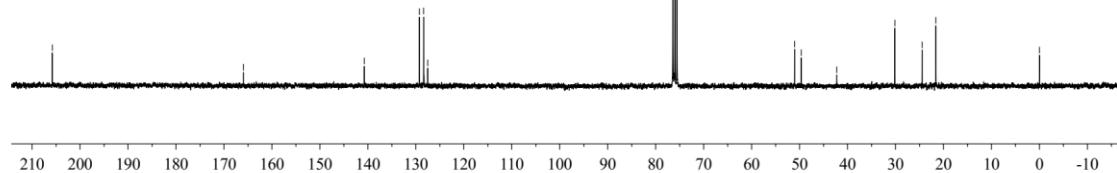
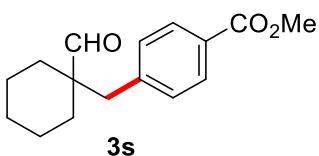


Figure S63 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3s**

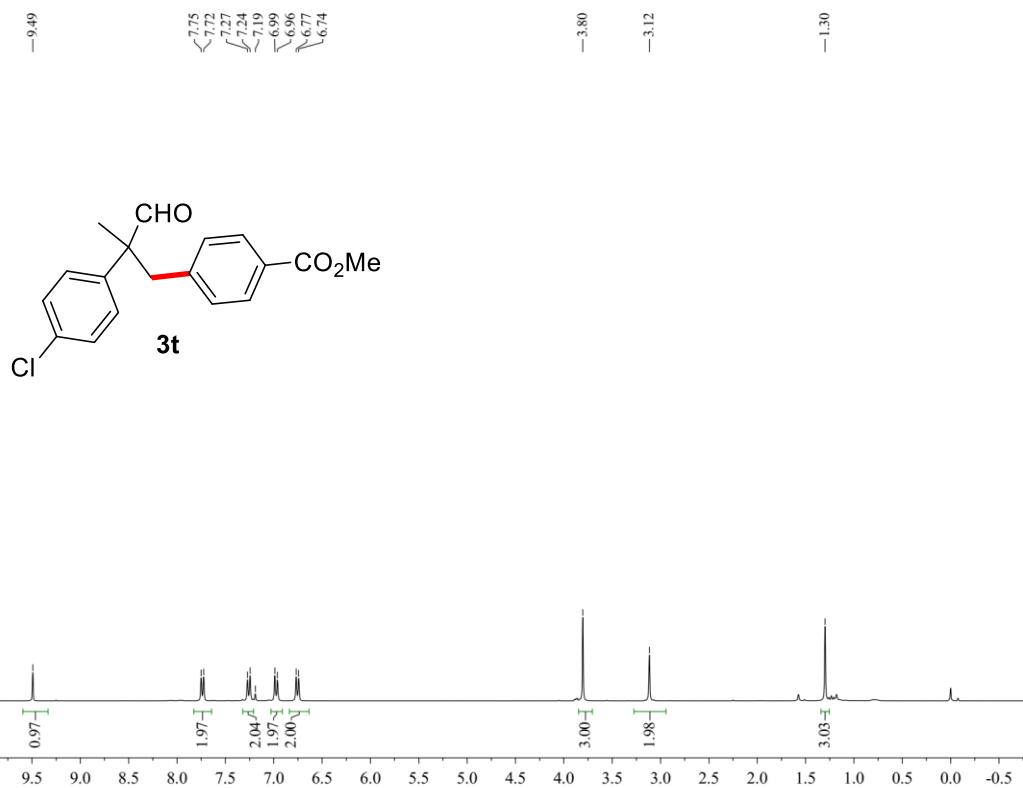


Figure S64 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3t**

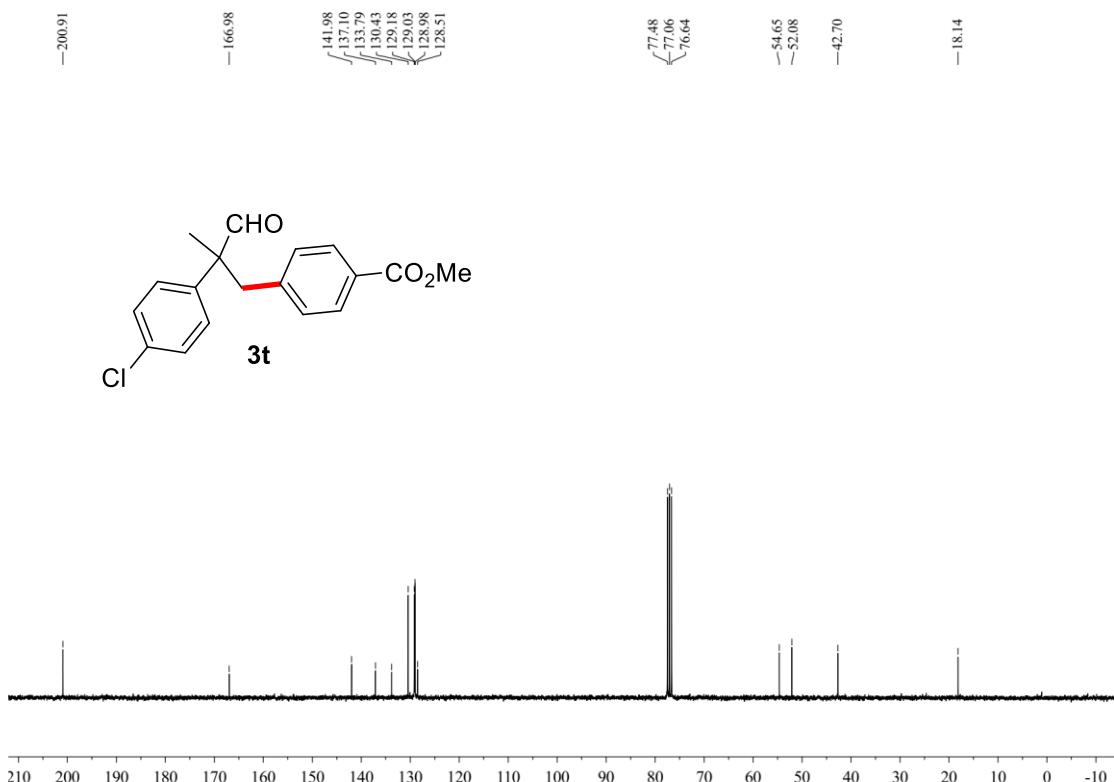


Figure S65 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3t**

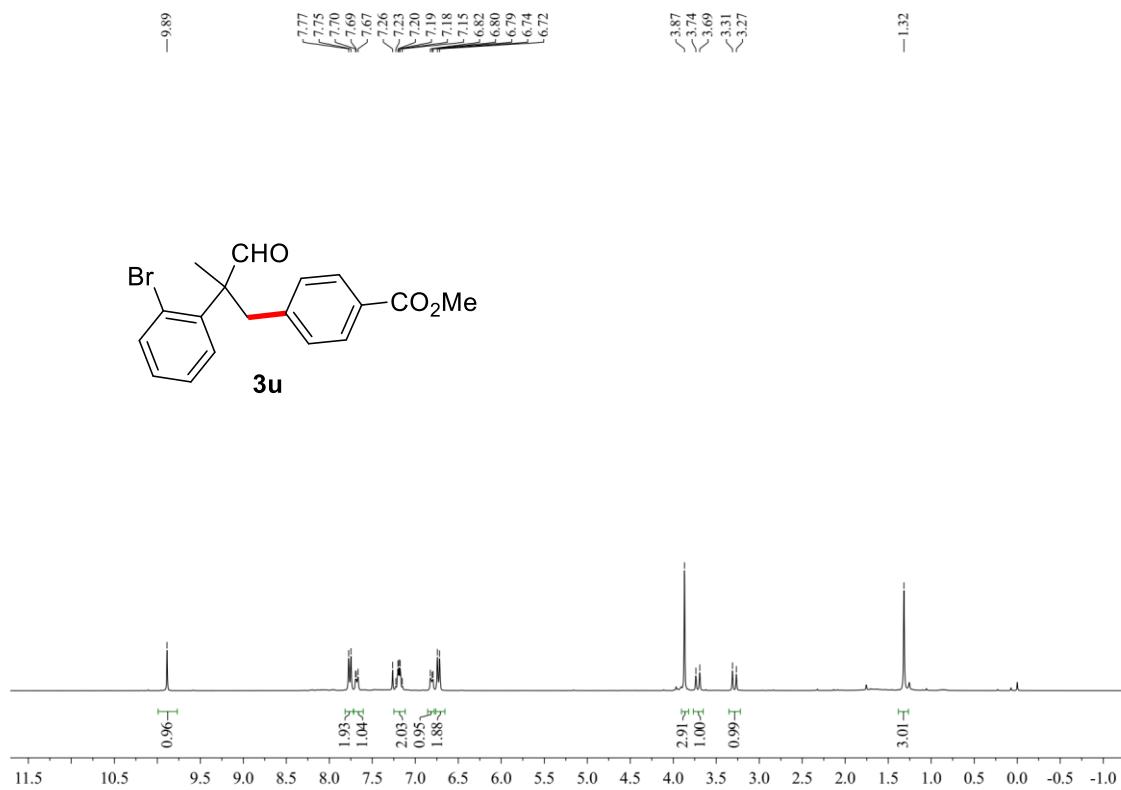


Figure S66 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3u**

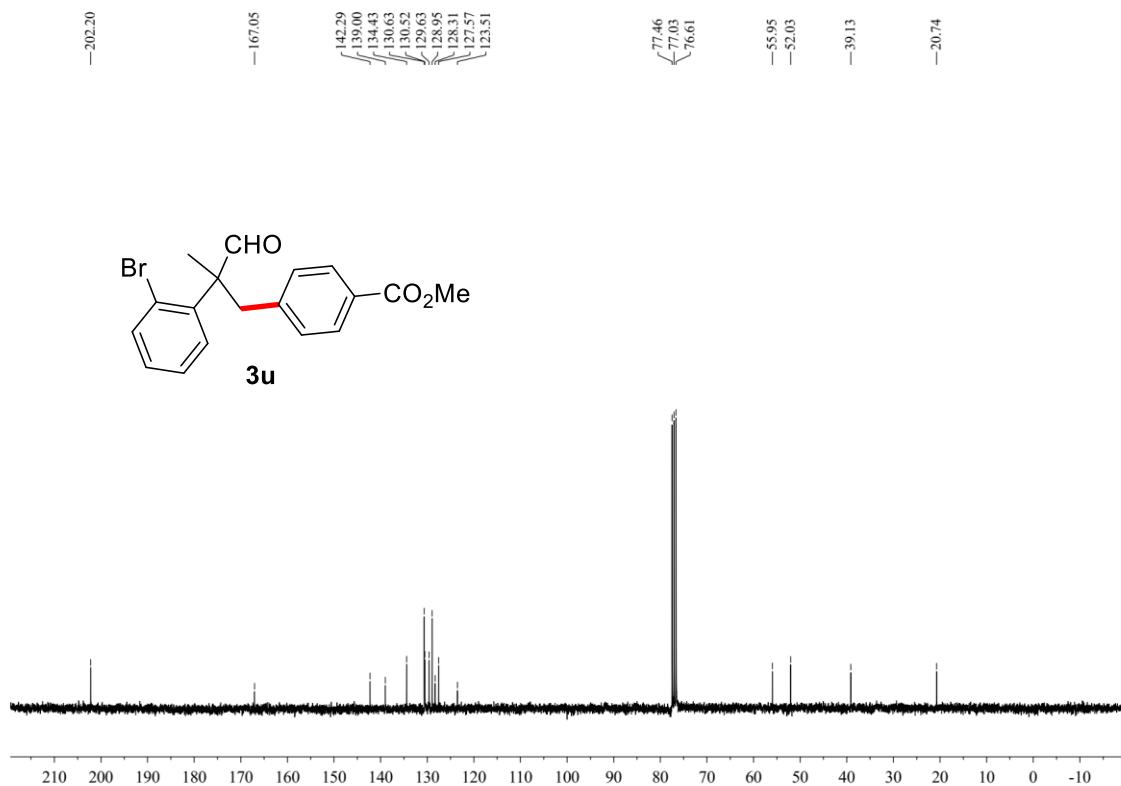


Figure S67 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3u**

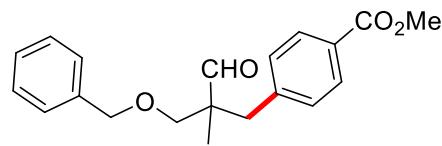
-9.58

7.85
7.82
7.29
7.27
7.25
7.24
7.24
7.23
7.18
7.10
7.07

-4.42

-3.82
-3.35
-3.32
-3.26
-3.23
-2.99
-2.95
-2.82
-2.77

-0.90



3v-mono

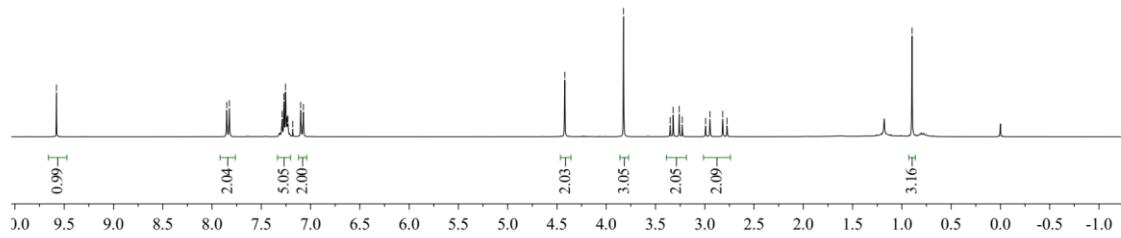


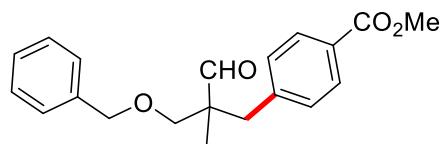
Figure S68 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3v-mono**

-204.65

-167.02
-142.20
-137.71
-130.46
-129.45
-128.49
-127.87
-127.72

77.50
77.07
76.65
73.40
72.12

52.10
51.12
-37.74
-16.70



3v-mono

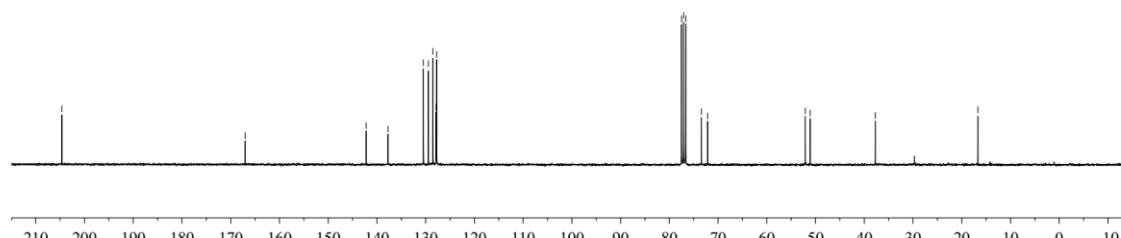


Figure S69 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3v-mono**

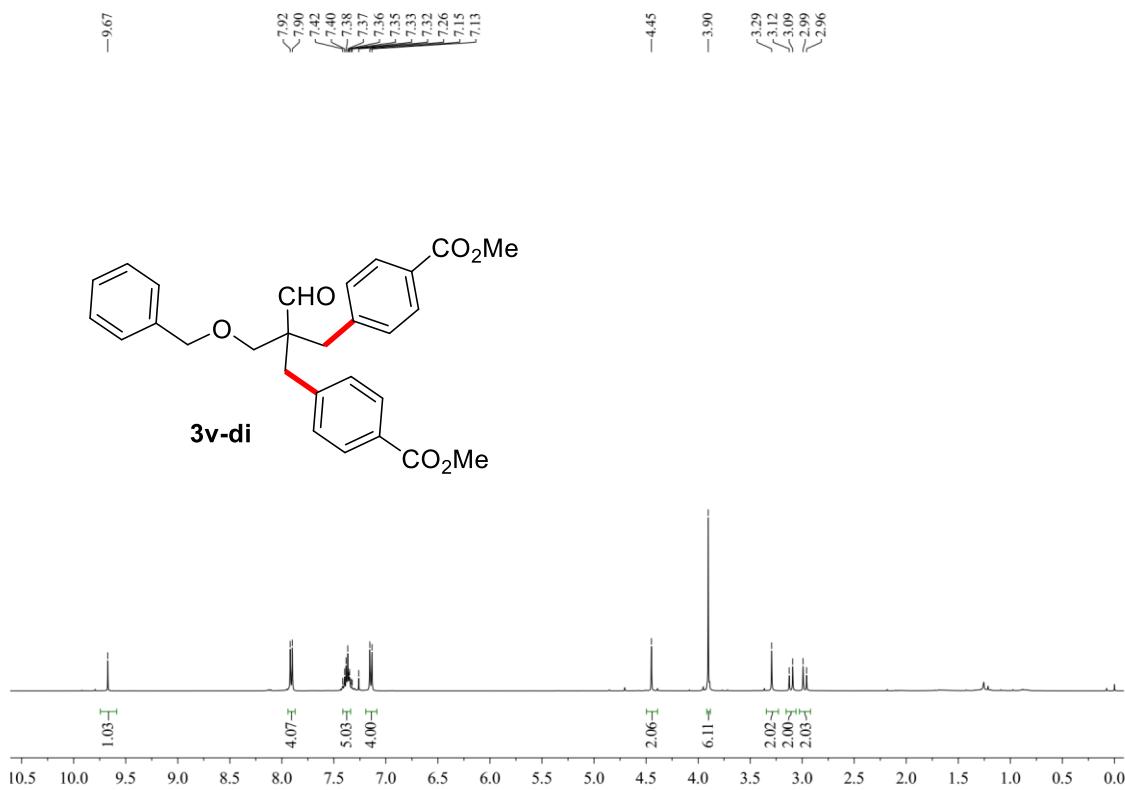


Figure S70 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3v-di**

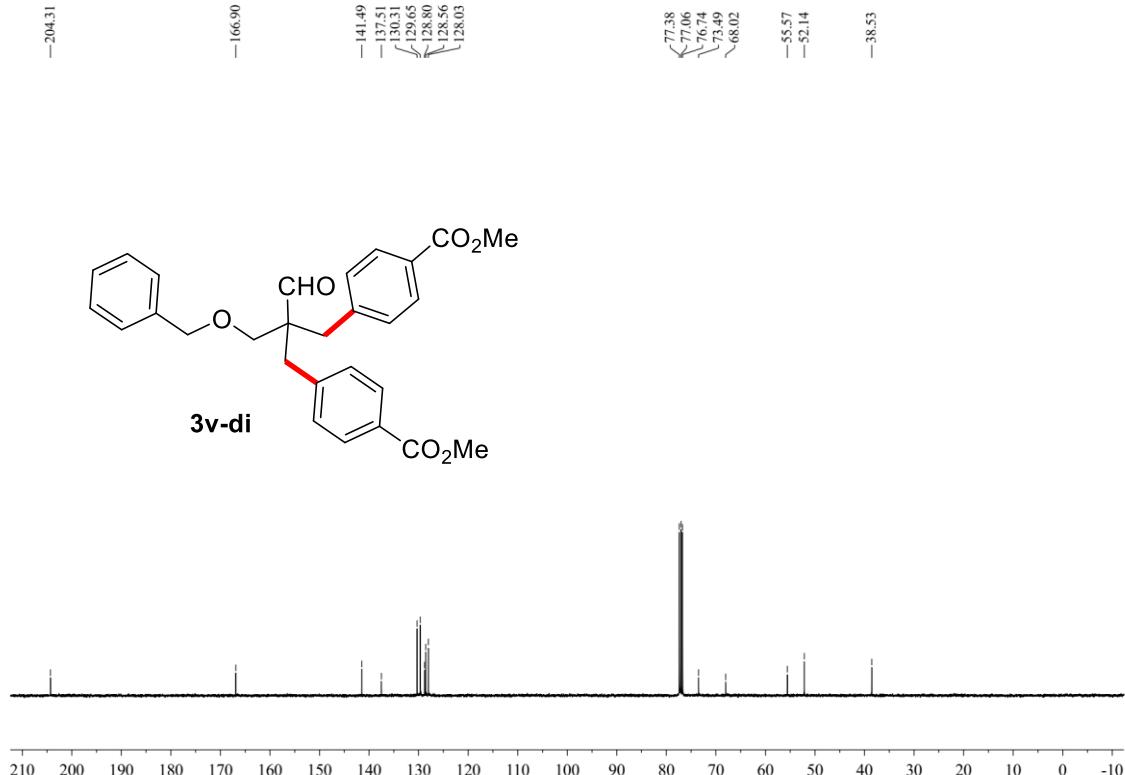
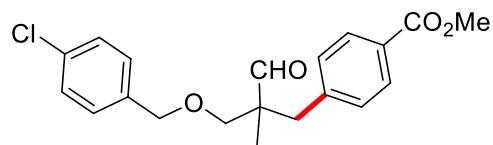


Figure S71 ^{13}C NMR spectrum (101MHz, CDCl_3 , 298K) of **3v-di**



3w-mono

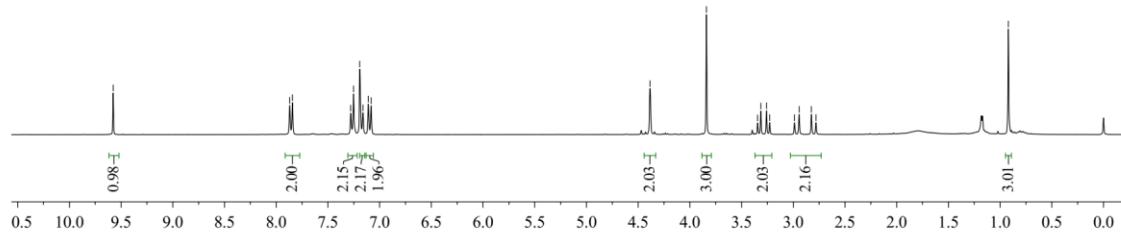
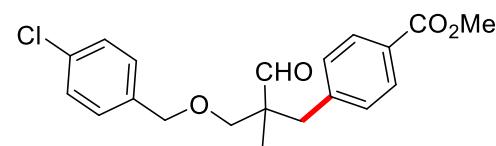


Figure S72 ^1H NMR spectrum (300MHz, CDCl_3 , 298K) of **3w-mono**



3w-mono

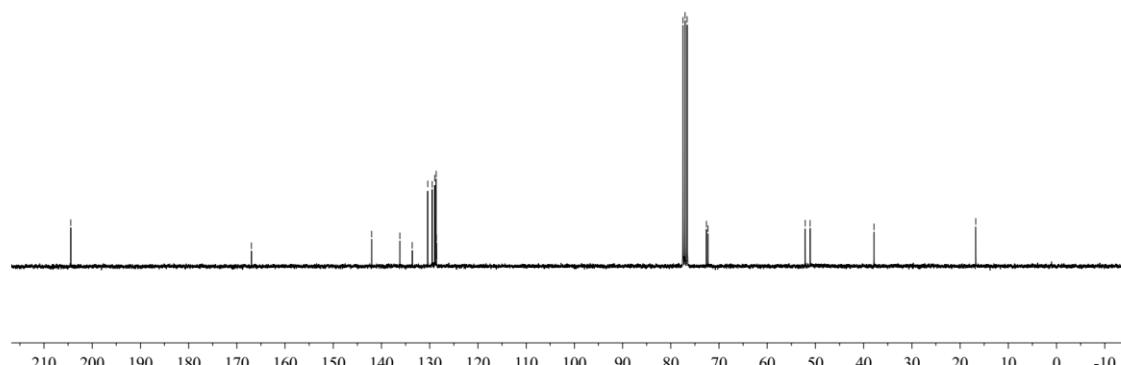


Figure S73 ^{13}C NMR spectrum (75MHz, CDCl_3 , 298K) of **3w-mono**

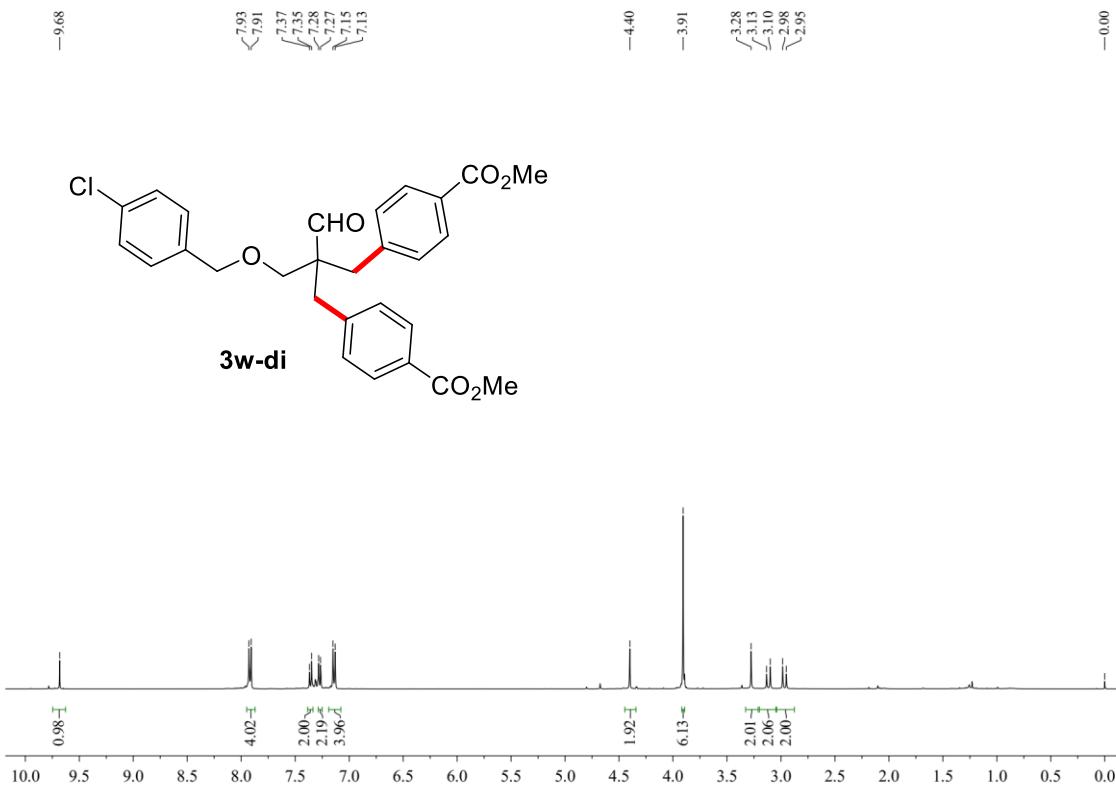


Figure S74 ^1H NMR spectrum (400MHz, CDCl_3 , 298K) of **3w-di**

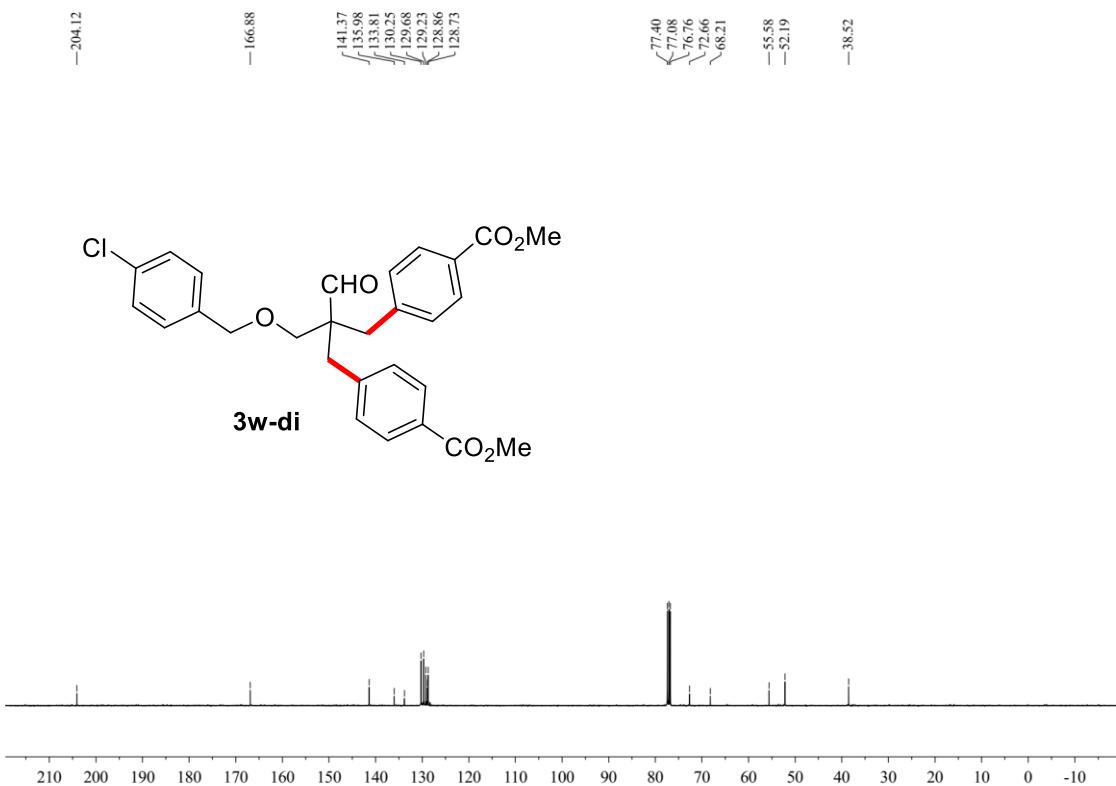


Figure S75 ^1H NMR spectrum (101MHz, CDCl_3 , 298K) of **3w-di**