Supplementary Information

Synthesis of thioesters through copper-catalyzed coupling of aldehydes with thiols in water

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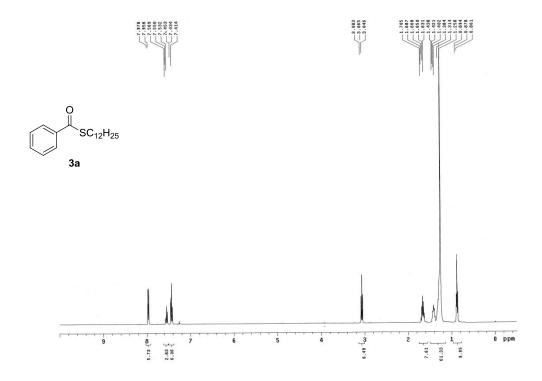
E-mail: cfalee@dragon.nchu.edu.tw

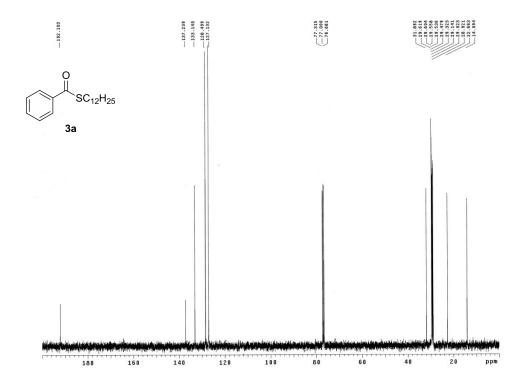
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1. General information for NMR measurement

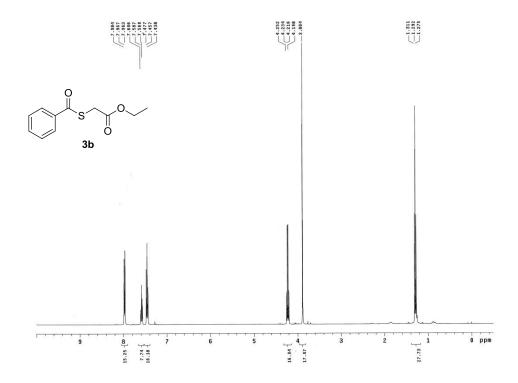
Proton and carbon nuclear magnetic resonance spectra (1 H and 13 C NMR) were recorded in CDCl₃. Chemical shifts (δ) are reported in ppm, and coupling constants (J) are given in Hz.

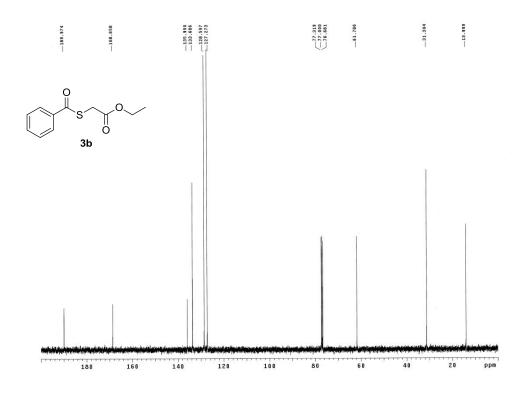
S-Dodecyl bezothioate (3a)



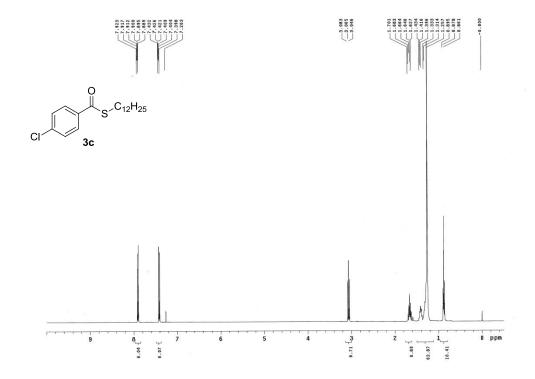


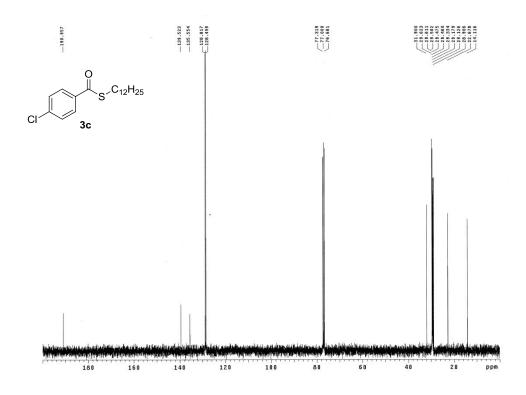
Ethyl 2-(benzoylthio)acetate (3b)



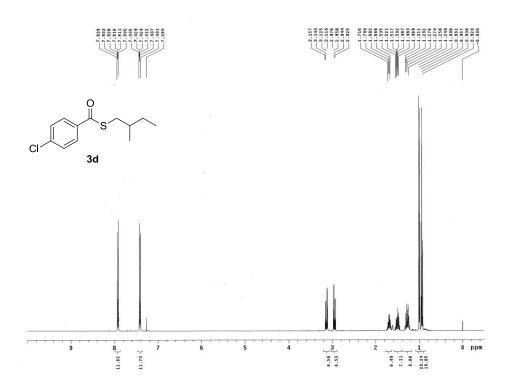


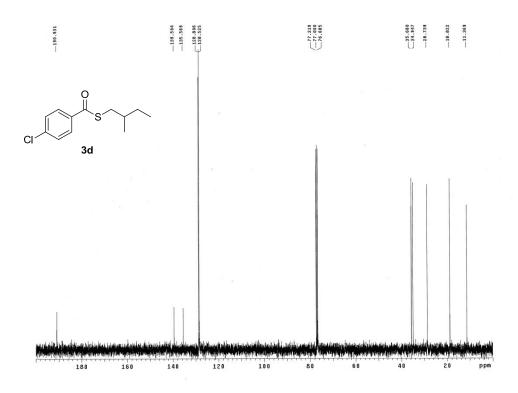
S-Dodecyl 4-chlorobezothioate (3c)



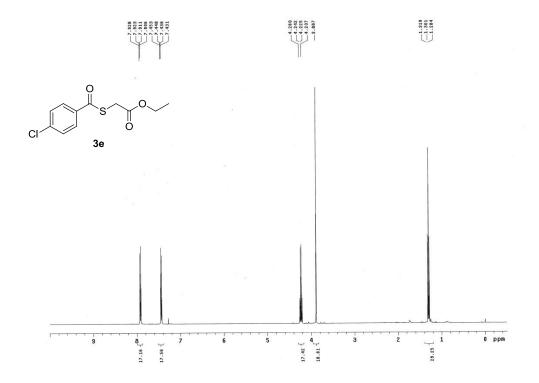


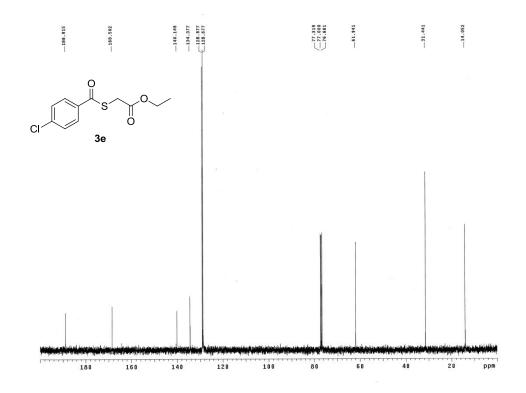
S-(2-Methyl-1-butyl) 4-chlorobenzothioate (3d)



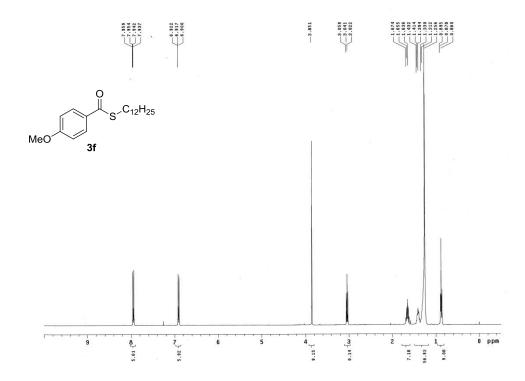


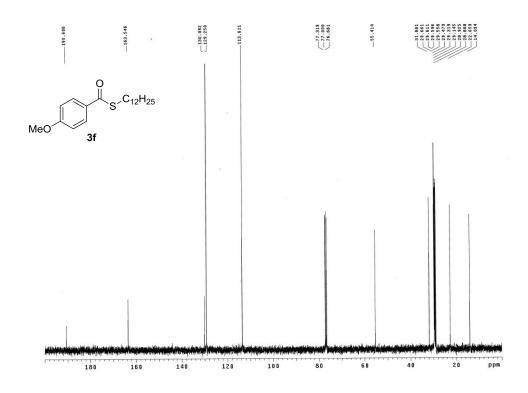
Ethyl 2-((4-chlorobenzoyl)thio)acetate (3e)



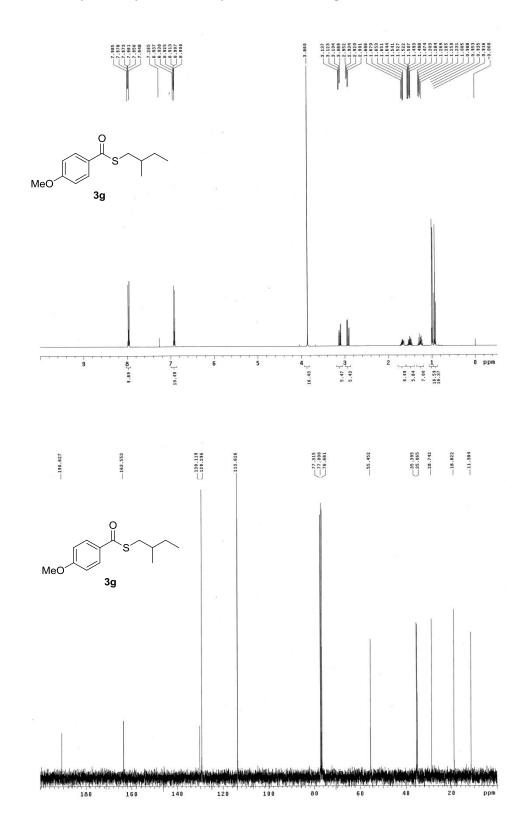


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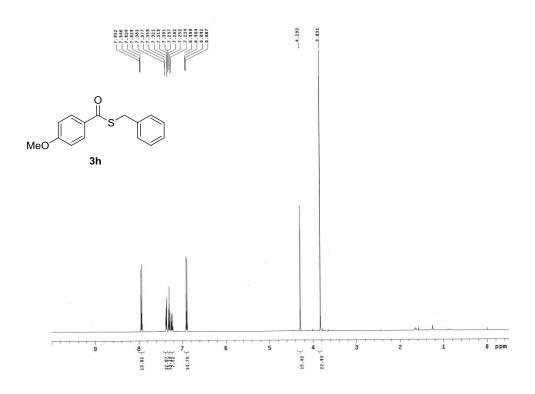


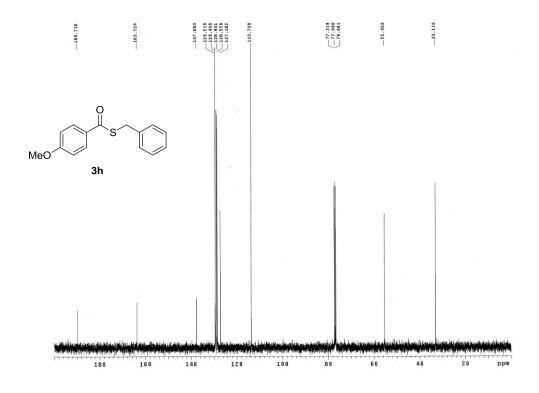


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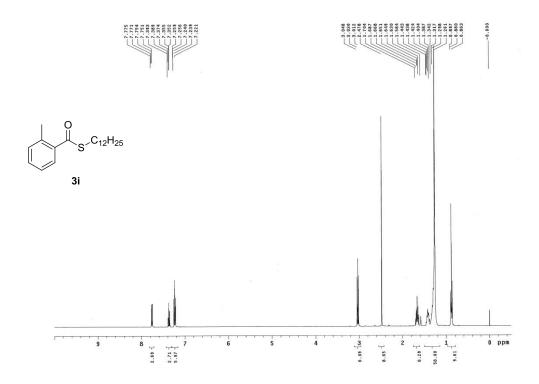


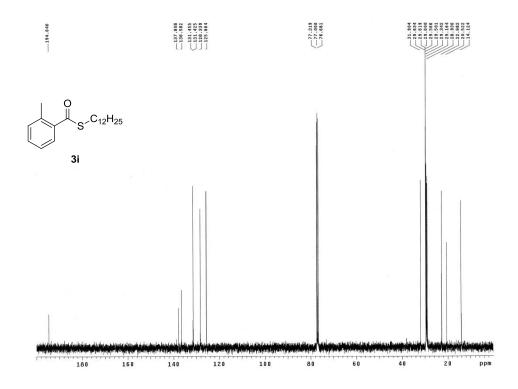
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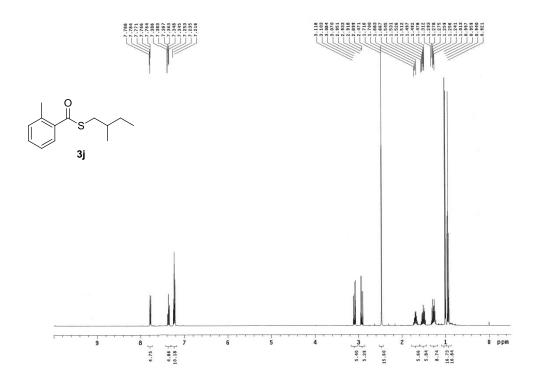


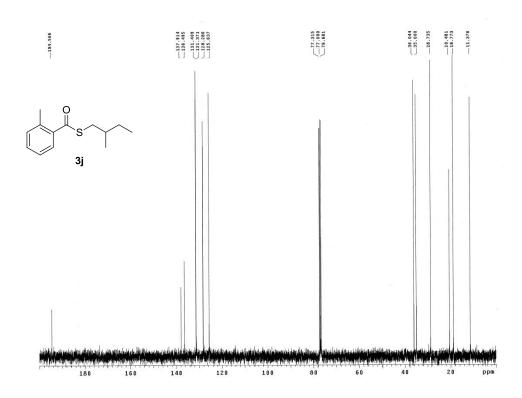
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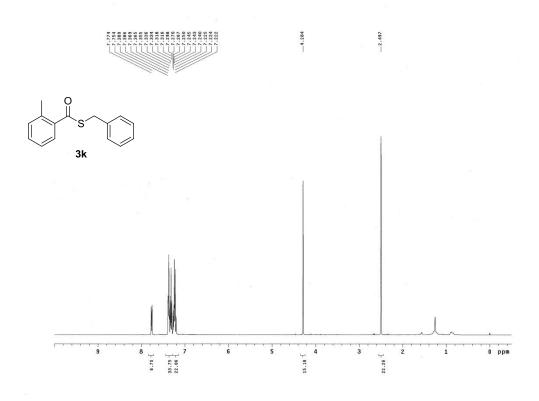


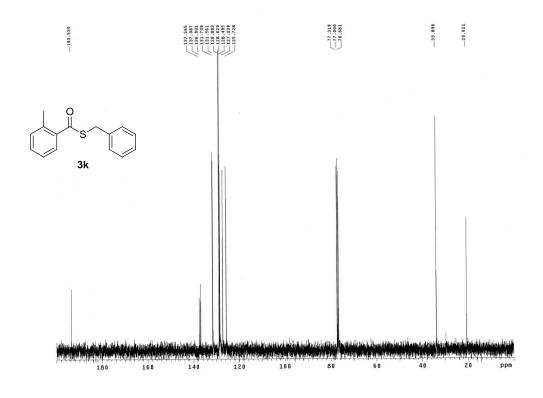
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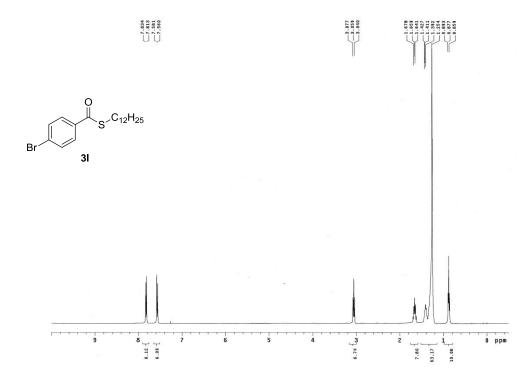


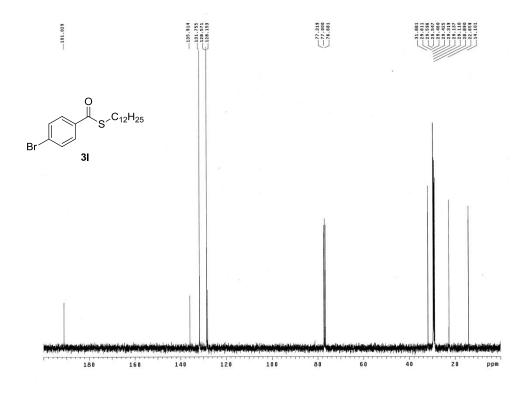
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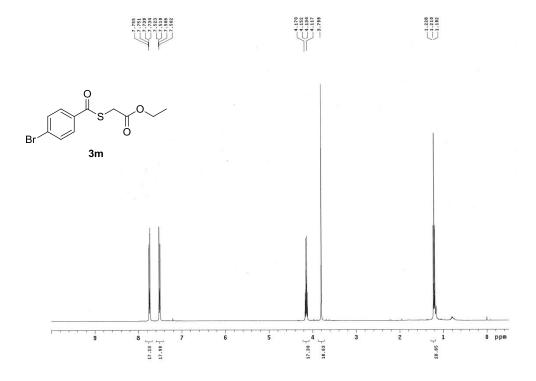


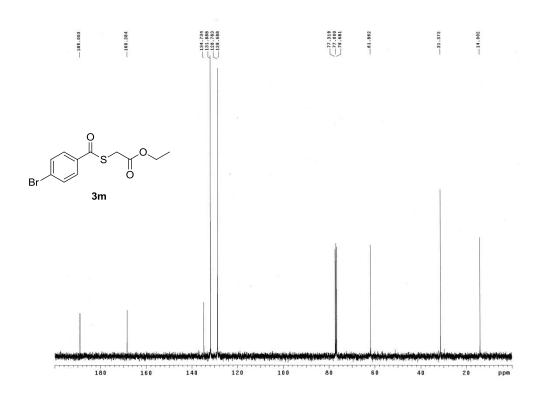
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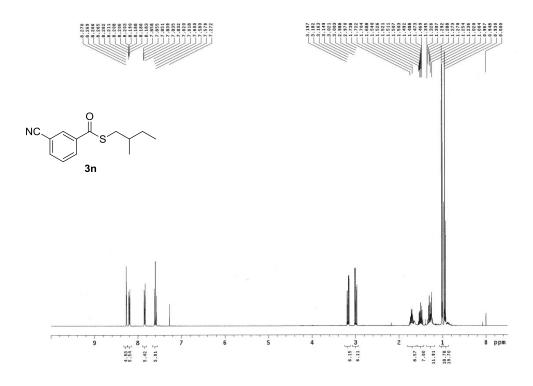


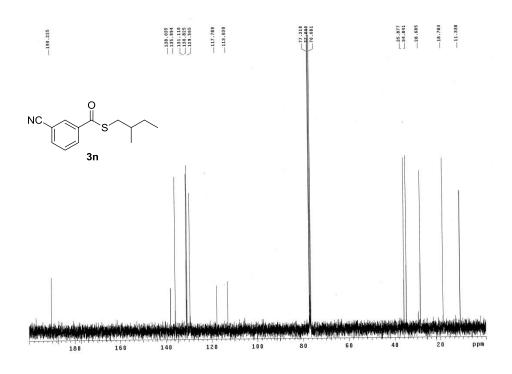
Ethyl 2-((4-bromobenzoyl)thio)acetate (3m)



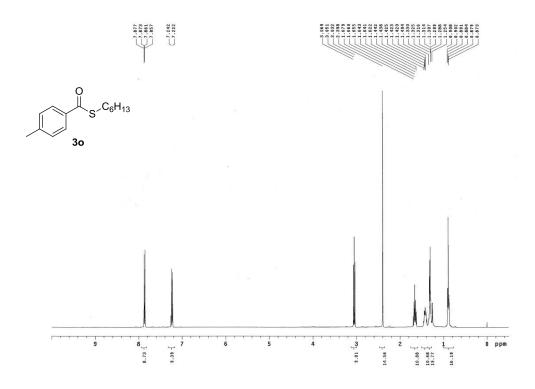


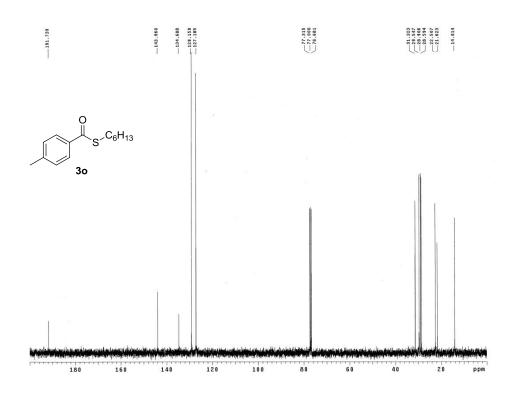
S-(2-Methyl-1-butyl) 3-cyanobenzothioate (3n)



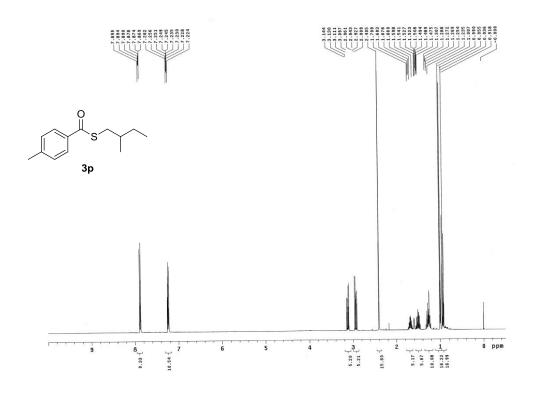


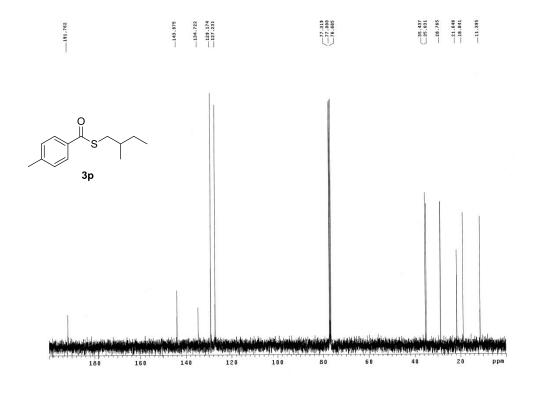
S-Hexyl 4-methylbenzothioate (30)



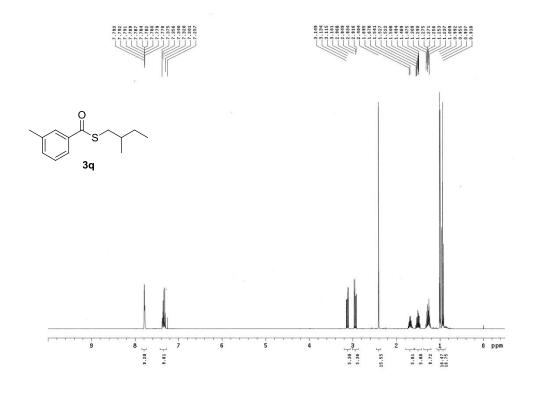


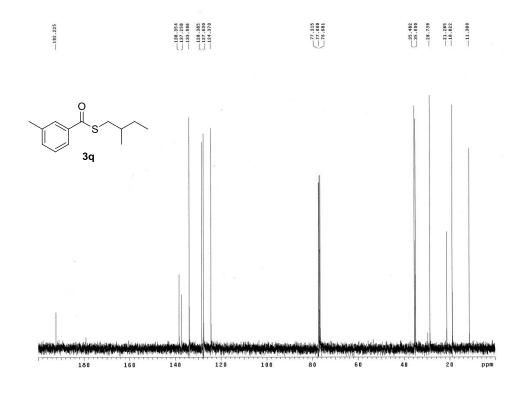
S-(2-Methyl-1-butyl) 4-methylbenzothioate (3p)



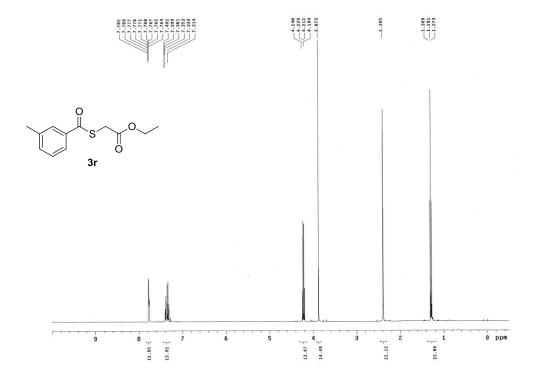


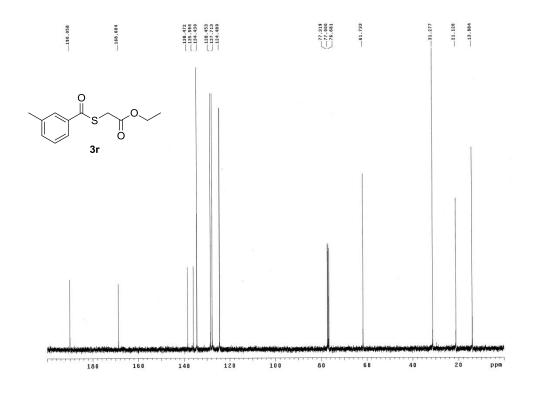
S-(2-Methyl-1-butyl) 3-methylbenzothioate (3q)



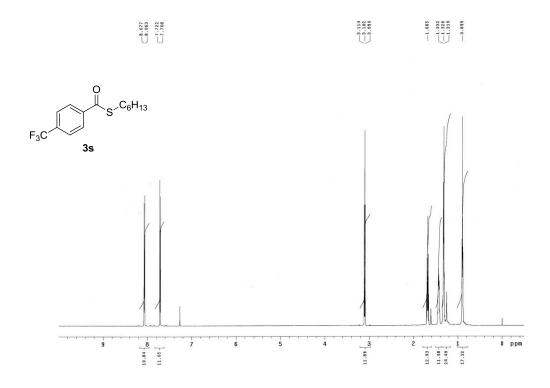


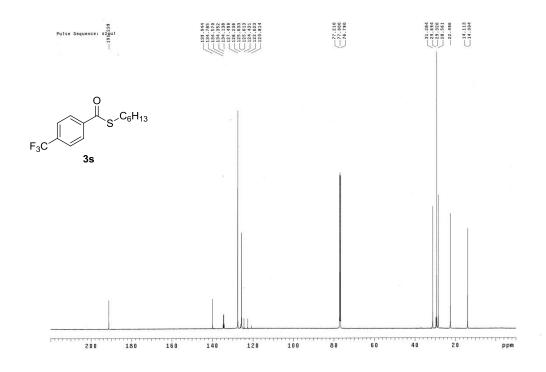
Ethyl 2-((3-methylbenzoyl)thio)acetate (3r)

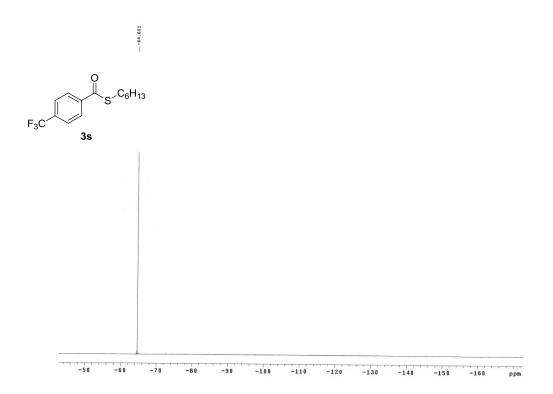




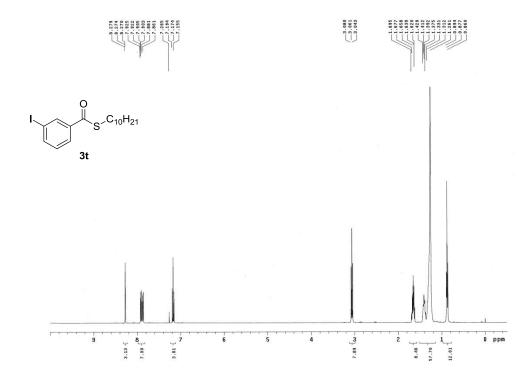
S-Hexyl 4-(trifluoromethyl)benzothioate (3s)

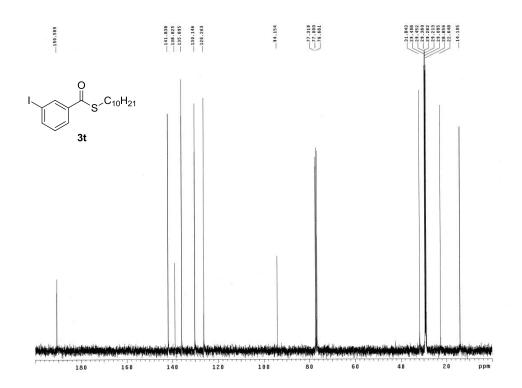




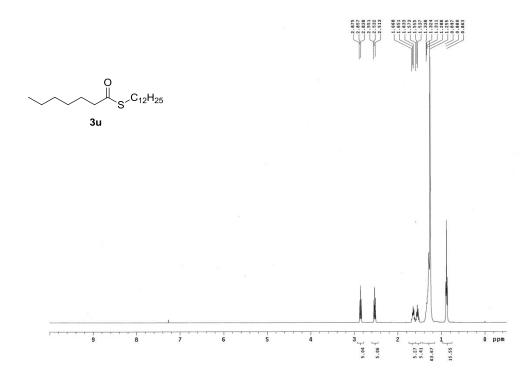


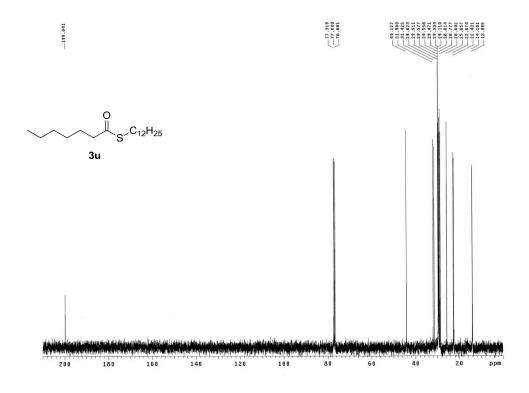
S-Decyl 3-iodobenzothioate (3t)



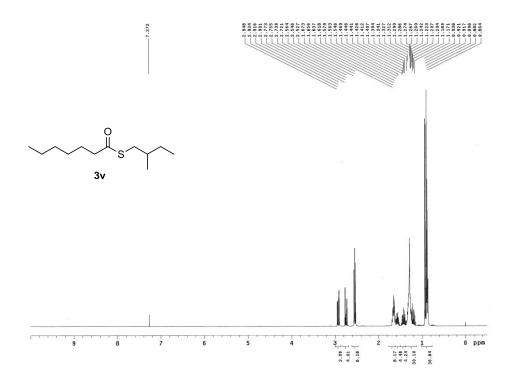


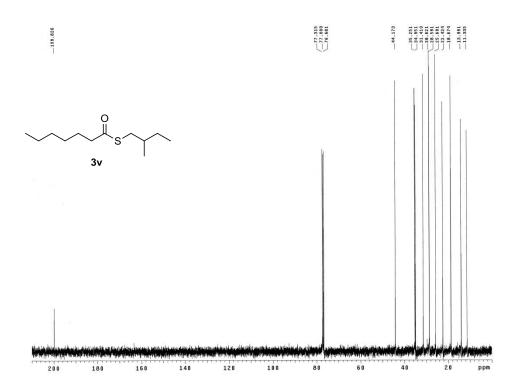
S-Dodecyl heptanethioate (3u)



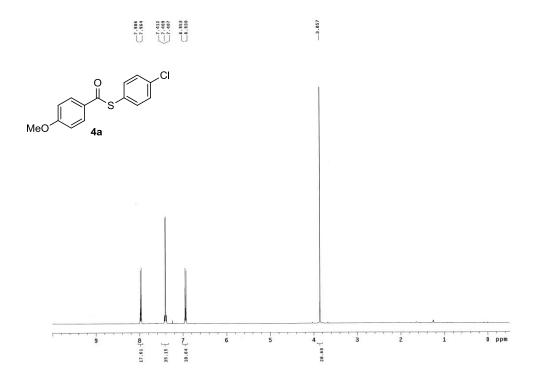


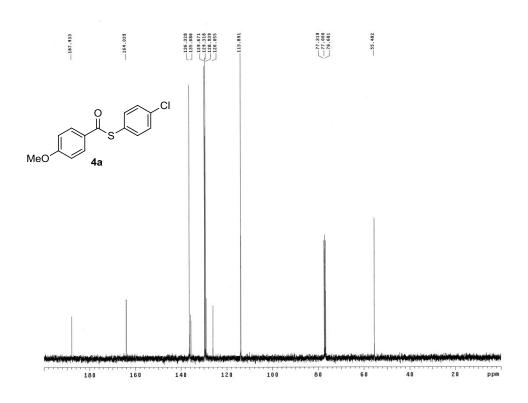
S-(2-Methyl-1-butyl) heptanethioate (3v)



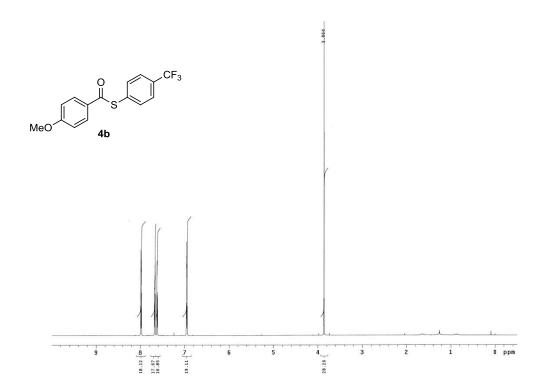


S-(4-Chlorophenyl) 4-methoxybenzothioate (4a)

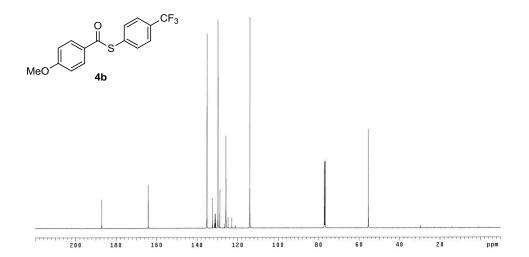


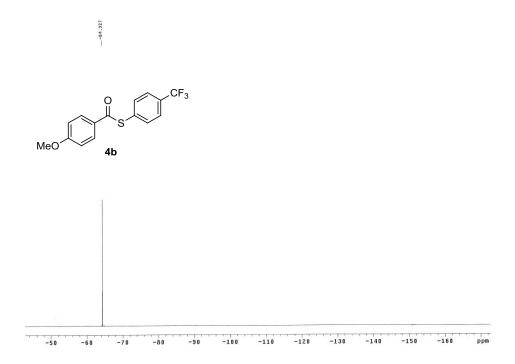


S-(4-(Trifluoromethyl)phenyl) 4-methoxybenzothioate (4b)

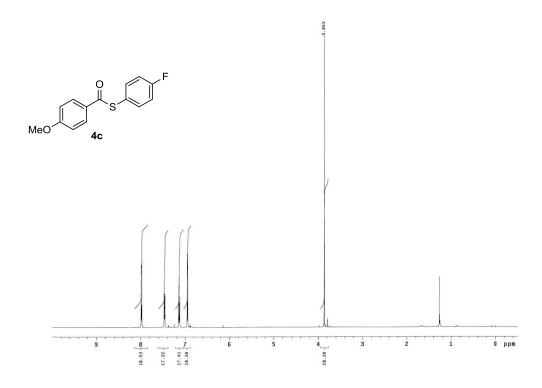


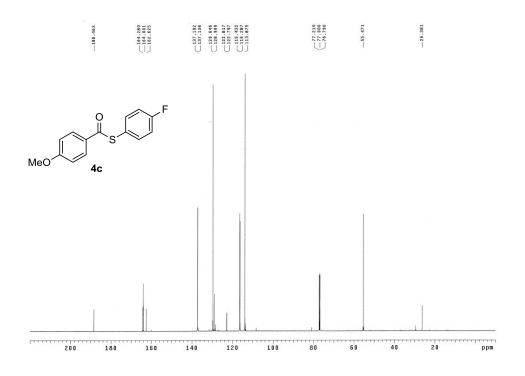


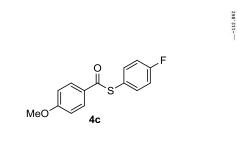


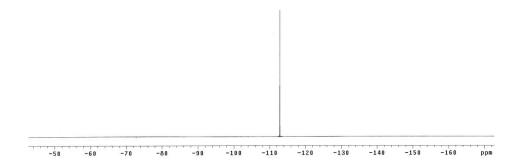


S-(4-Fluorophenyl) 4-methoxybenzothioate (4c)

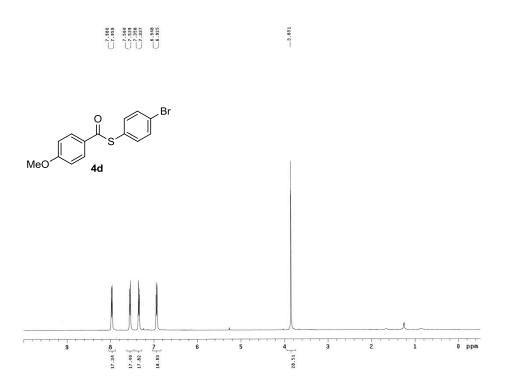


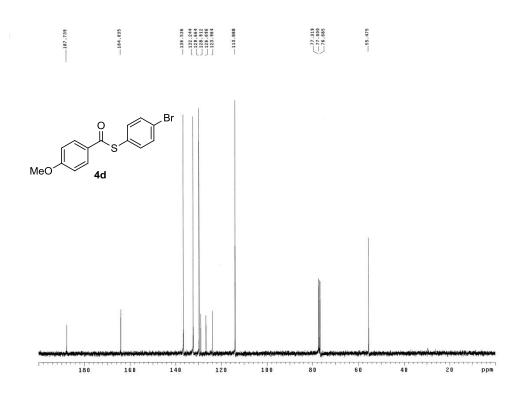




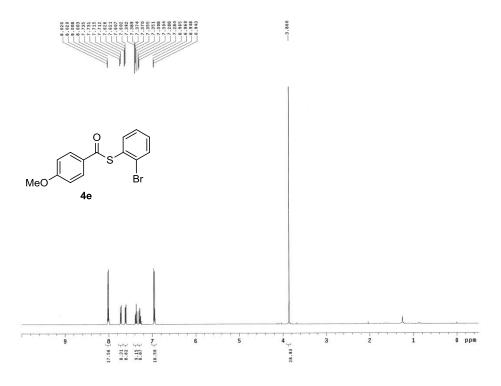


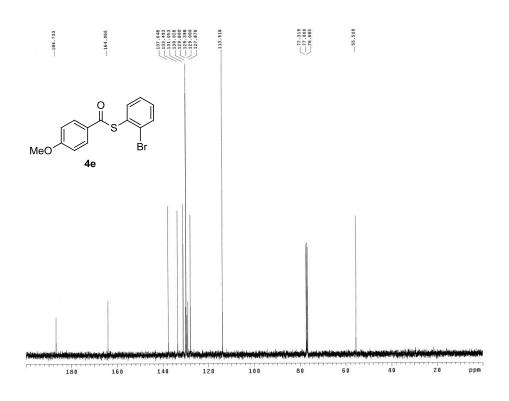
S-(4-Bromophenyl) 4-methoxybenzothioate (4d)



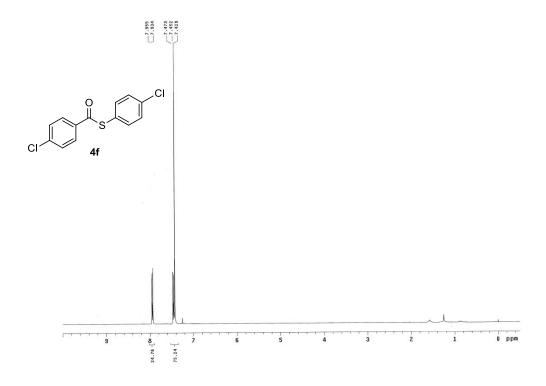


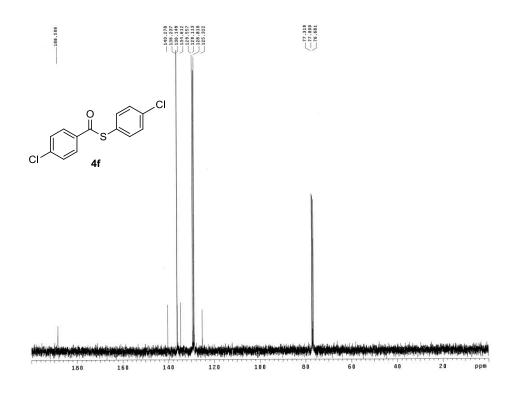
S-(2-Bromophenyl) 4-methoxybenzothioate (4e)



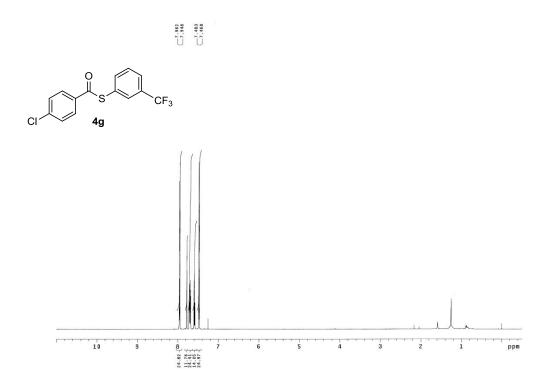


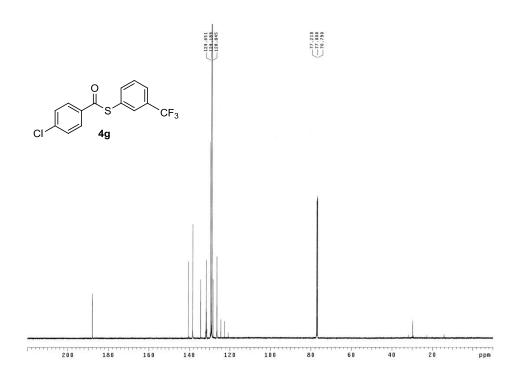
S-(4-Chlorophenyl) 4-chlorobenzothioate (4f)

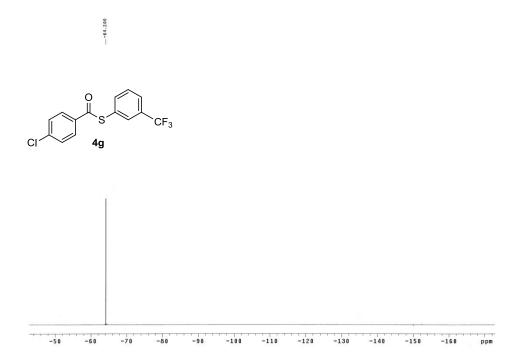




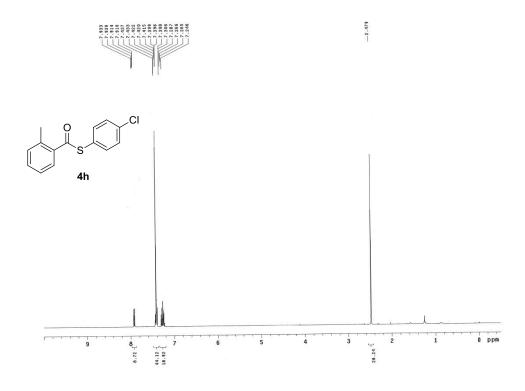
S-(3-(Trifluoromethyl)phenyl) 4-chlorobenzothioate (4g)

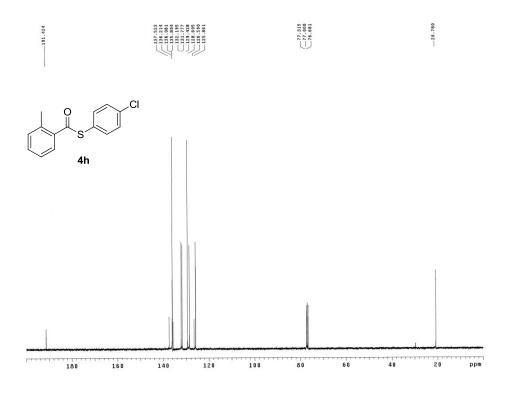




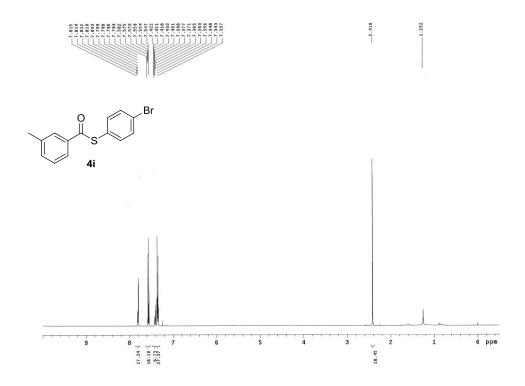


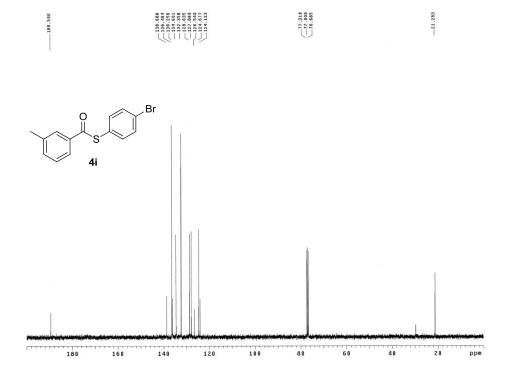
S-(4-Chlorophenyl) 2-methylbenzothioate (4h)



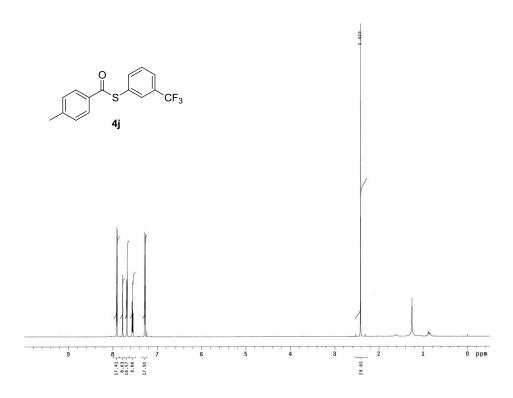


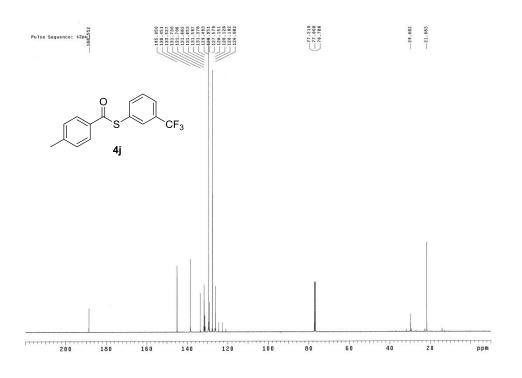
S-(4-Bromophenyl) 3-methylbenzothioate (4i)

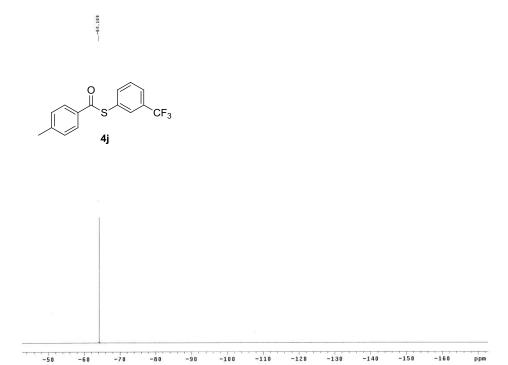




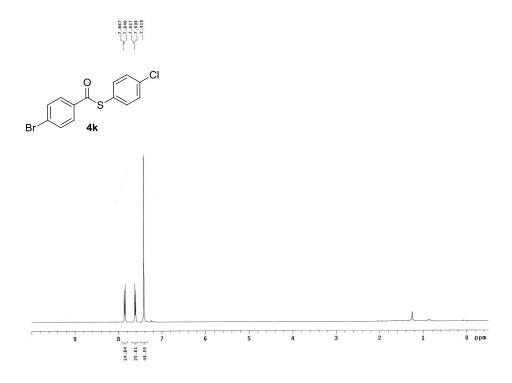
S-(3-(Trifluoromethyl)phenyl) 4-methylbenzothioate (4j)

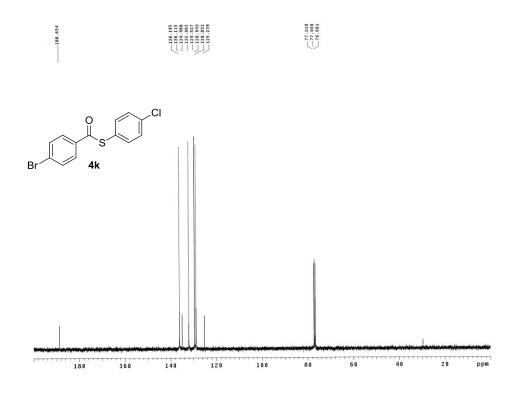




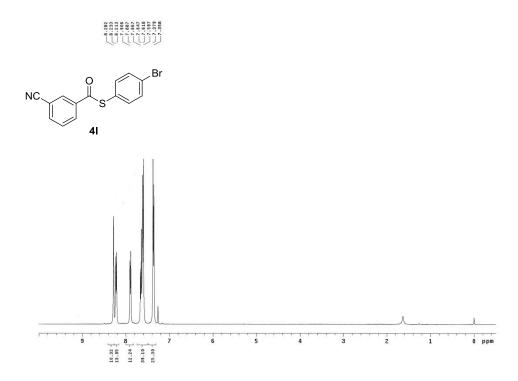


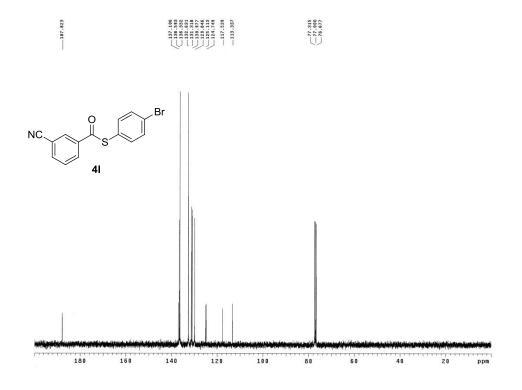
S-(4-Chlorophenyl) 4-bromobenzothioate (4k)



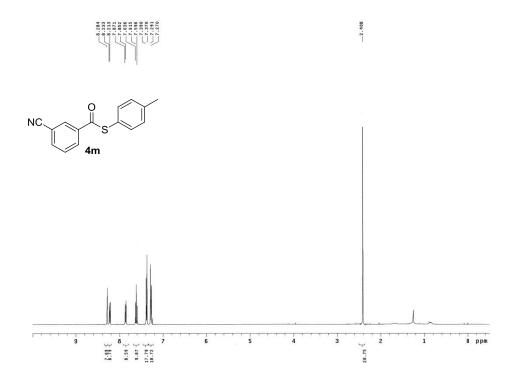


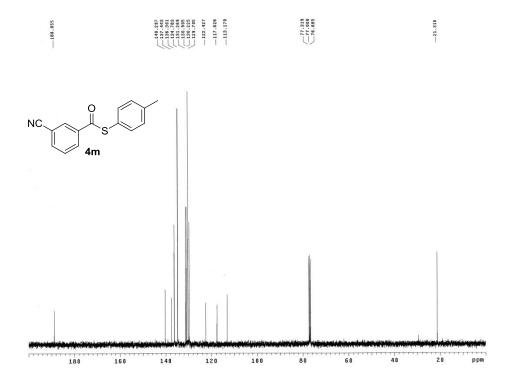
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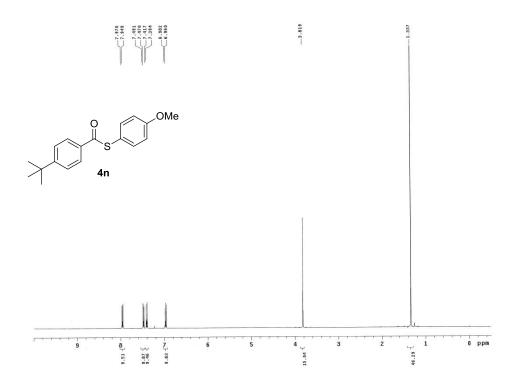


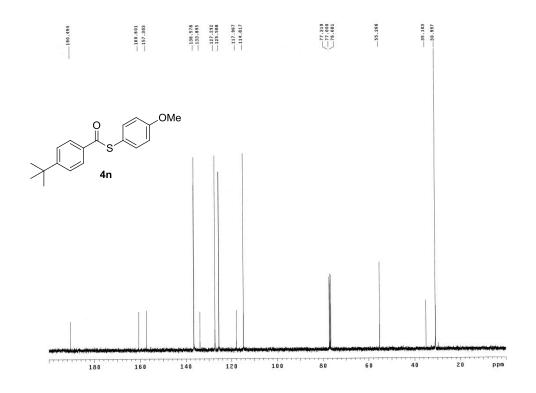
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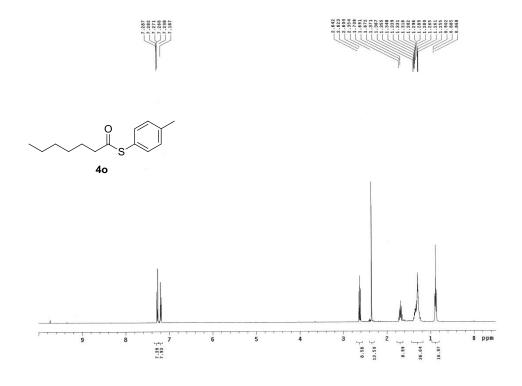


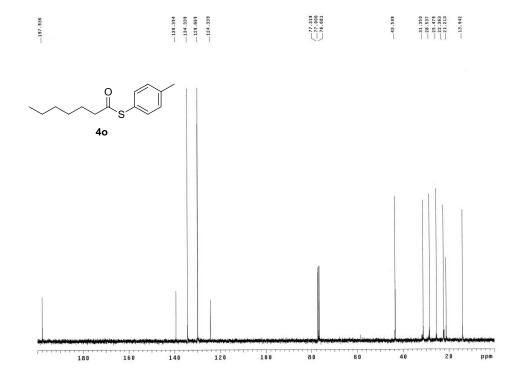
S-(4-Methoxyphenyl) 4-(tert-butyl)benzothioate (4n)



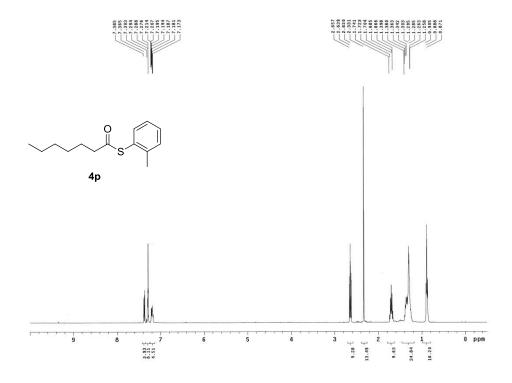


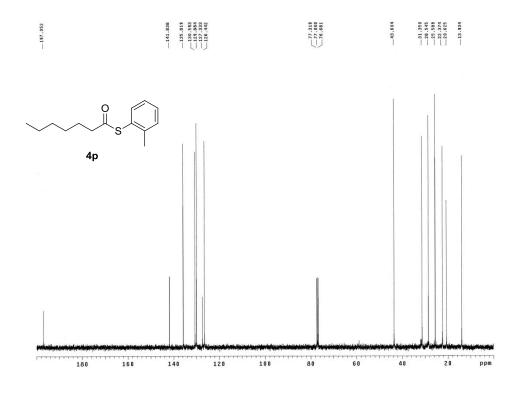
S-p-Tolyl heptanethioate (40)



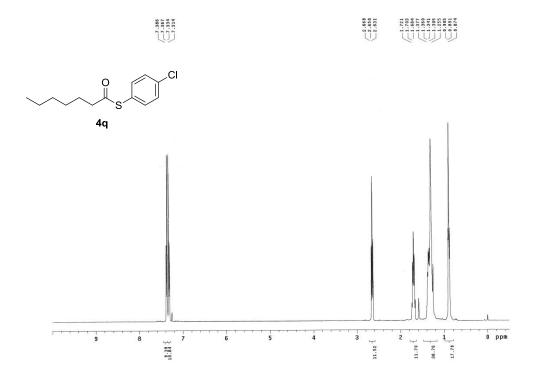


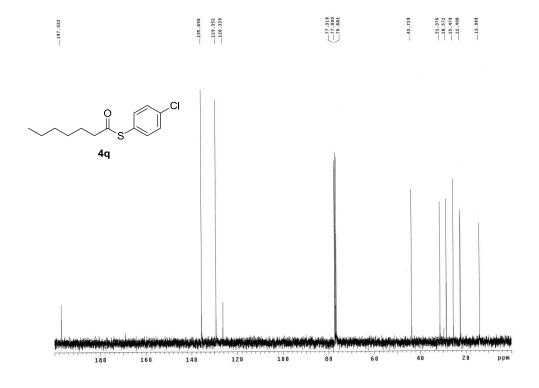
S-o-Tolyl heptanethioate (4p)



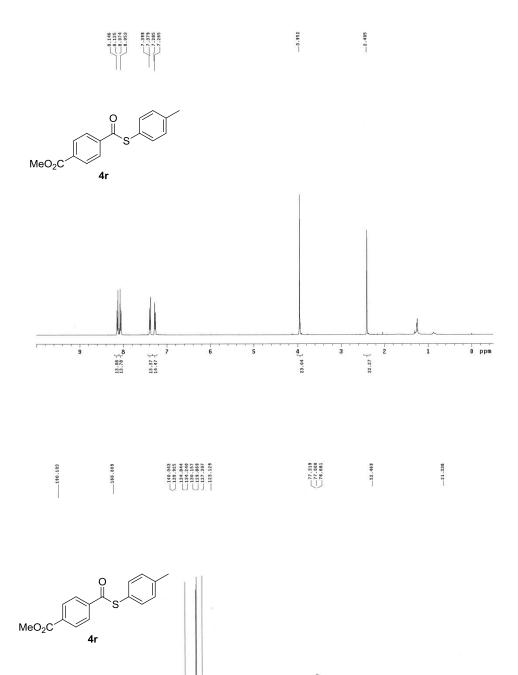


S-(4-Chlorophenyl) heptanethioate (4q)





Methyl 4-((p-tolylthio)carbonyl)benzoate (4r)



S-p-Tolyl thiophene-2-carbothioate (4s)

