

Supplementary Materials

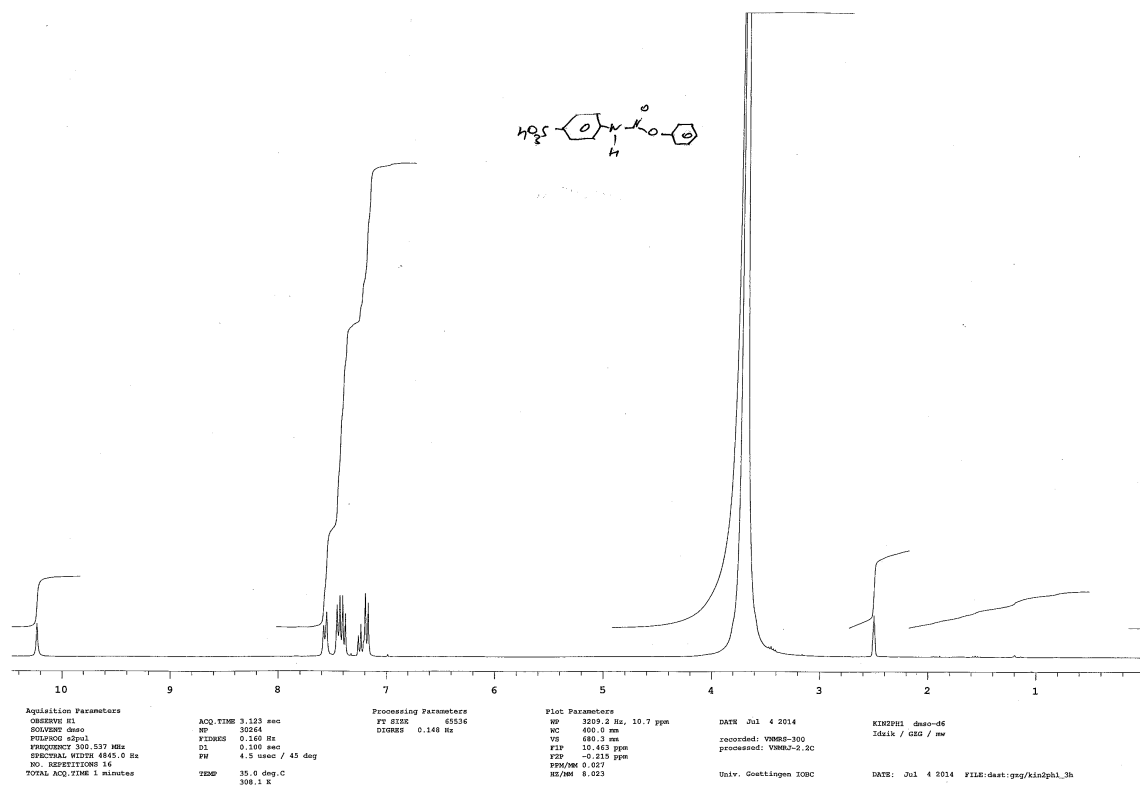


Figure S1. $^1\text{H-NMR}$ spectrum of 4-[(phenoxyacetyl)amino]benzenesulfonic (**1**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 10.23 (s, 1H), 7.57 (d, $J = 8.1$ Hz, 2H), 7.44 (d, $J = 7.8$ Hz, 2H), 7.39 (d, $J = 7.8$ Hz, 2H), 7.24 (t, $J = 7.4$ Hz, 1H), 7.18 (d, $J = 7.8$ Hz, 2H).

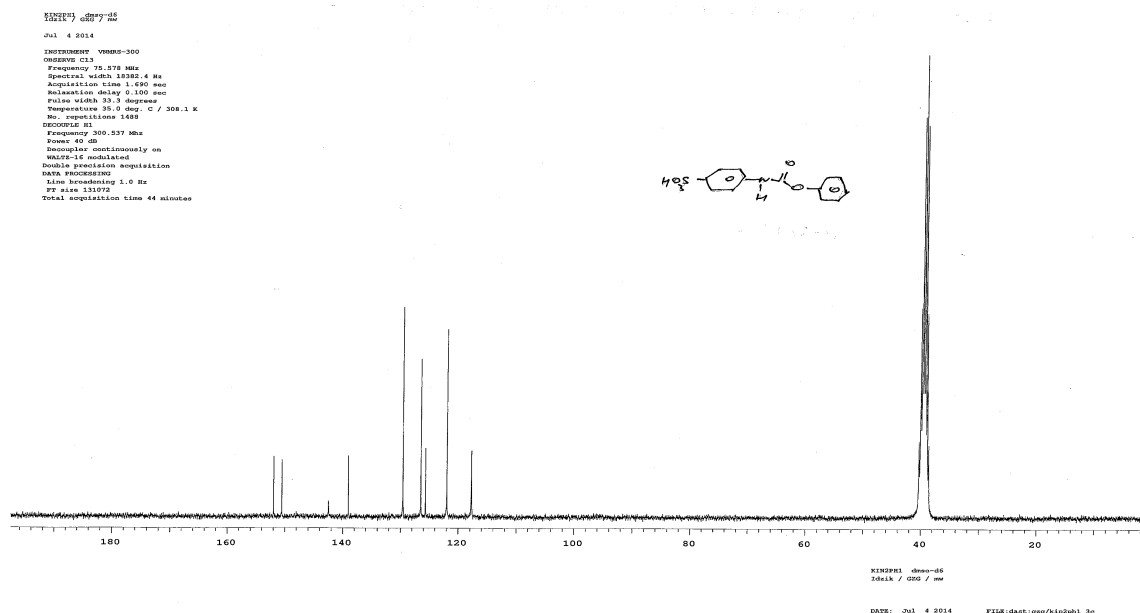


Figure S2. $^{13}\text{C-NMR}$ spectrum of 4-[(phenoxyacetyl)amino]benzenesulfonic (**1**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 151.93, 150.52, 142.48, 139.05, 129.58, 126.48, 125.65, 121.96, 117.76.

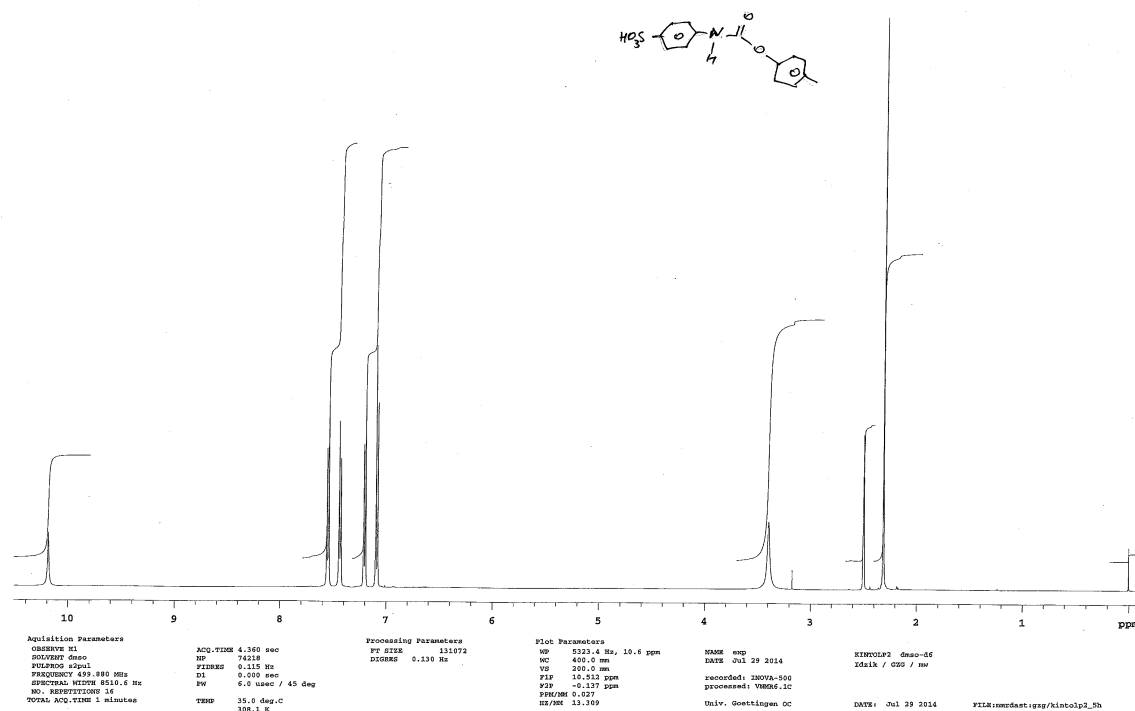


Figure S3. $^1\text{H-NMR}$ spectrum of 4-[[4-(4-methylphenoxy)carbonyl]amino]benzenesulfonic acid (**2**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 10.19 (s, 1H), 7.55 (d, $J = 8.5$ Hz, 2H), 7.44 (d, $J = 8.5$ Hz, 2H), 7.20 (d, $J = 8.5$ Hz, 2H), 7.09 (d, $J = 8.5$ Hz, 2H), 2.31 (s, 3H).

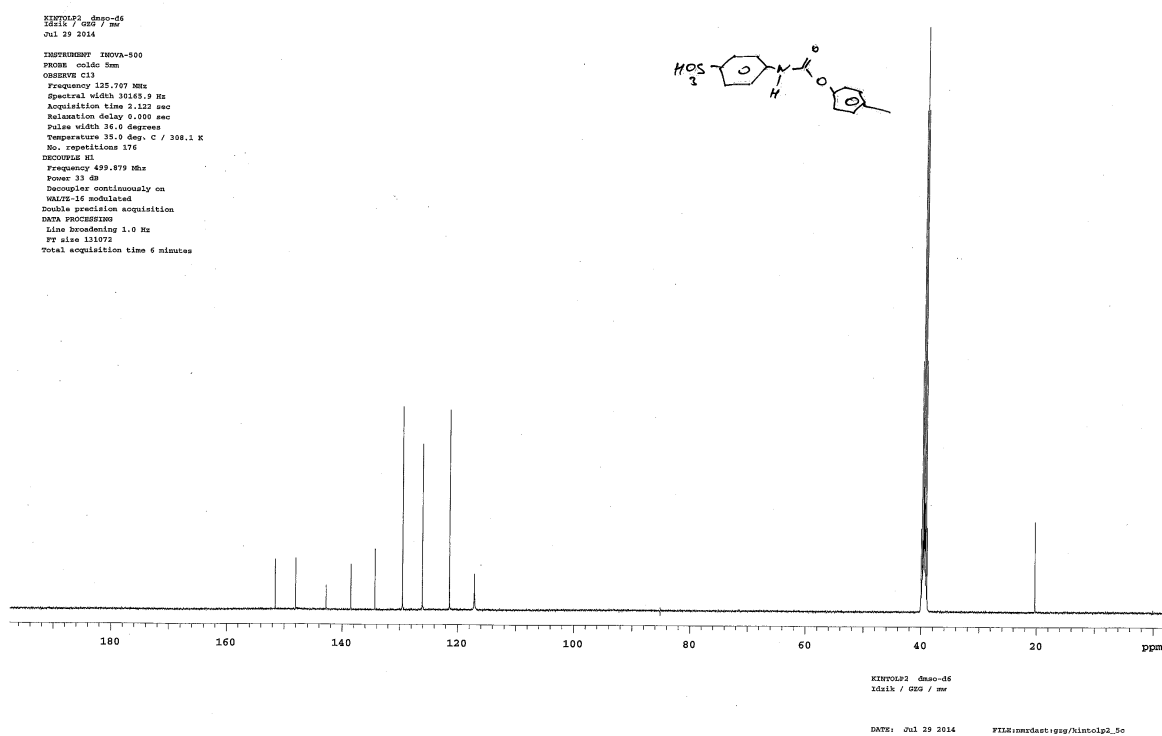


Figure S4. $^{13}\text{C-NMR}$ spectrum of 4-[[4-(4-methylphenoxy)carbonyl]amino]benzenesulfonic acid (**2**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 151.54, 148.02, 142.79, 138.49, 134.29, 129.49, 126.07, 121.38, 117.15, 20.30.

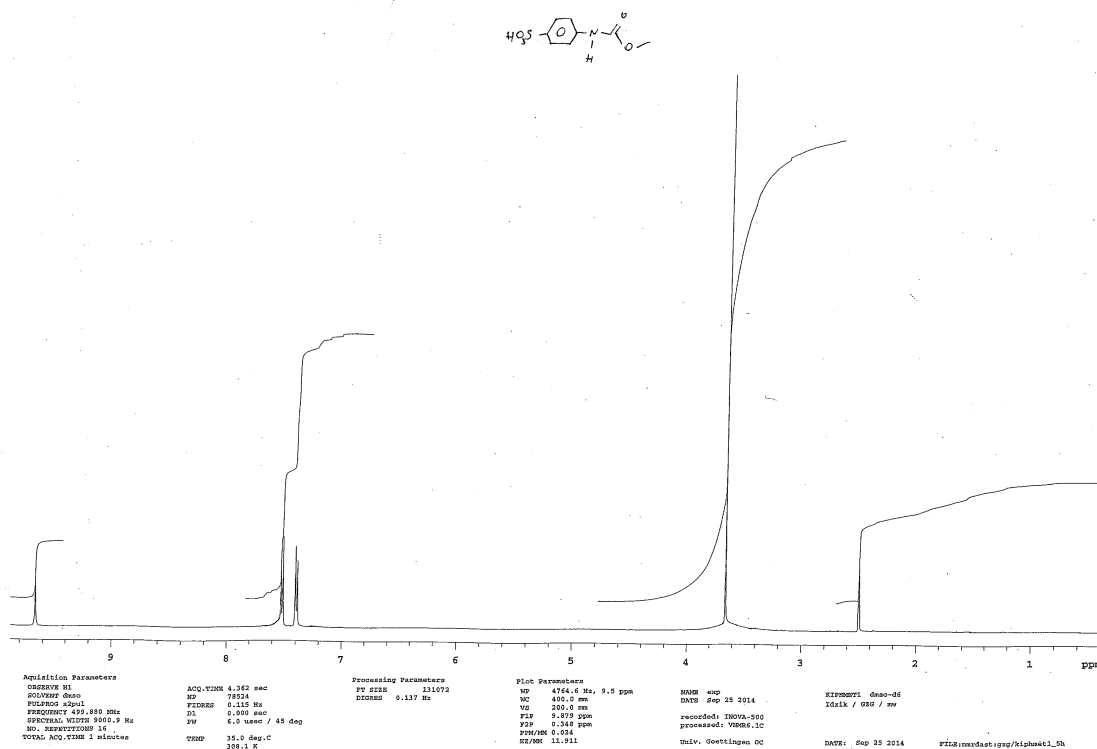


Figure S7. $^1\text{H-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]benzenesulfonic acid (**4**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.67 (s, 1H), 7.52 (d, $J = 8.5$ Hz, 2H), 7.39 (d, $J = 8.5$ Hz, 2H), 3.66 (s, 3H).

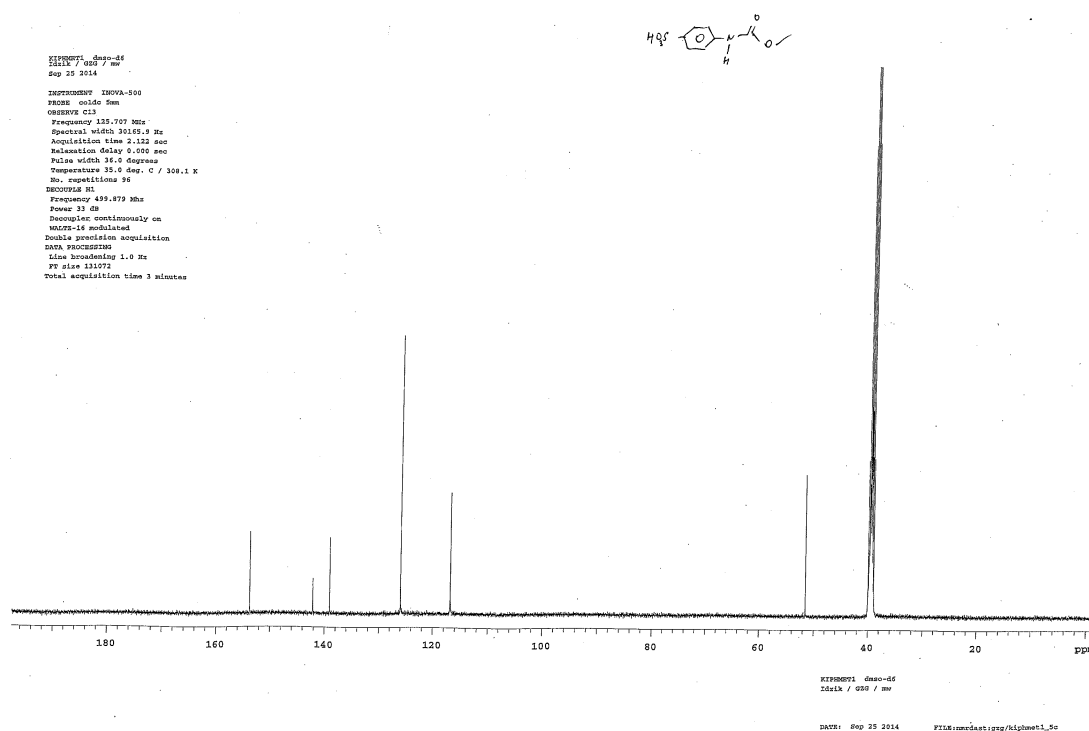


Figure S8. $^{13}\text{C-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]benzenesulfonic acid (**4**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 153.70, 142.13, 139.05, 125.99, 116.84, 51.53.

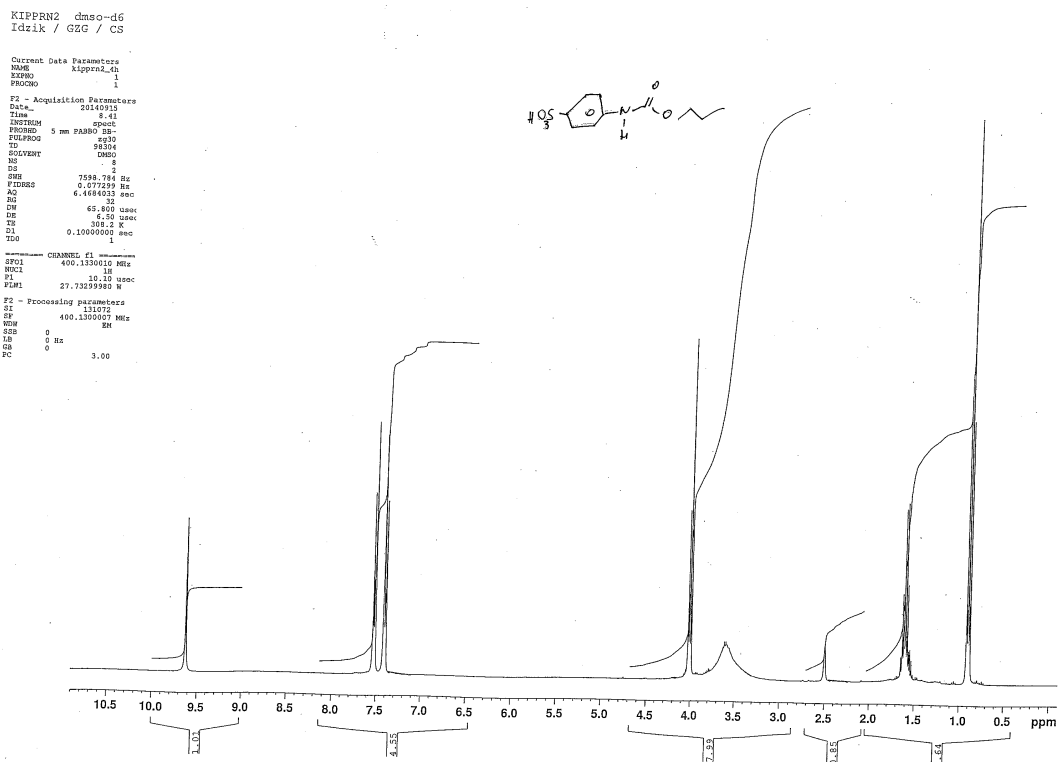


Figure S9. $^1\text{H-NMR}$ spectrum of 4-[(propoxycarbonyl)amino]benzenesulfonic acid (**5**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.63 (s, 1H), 7.52 (d, $J = 8.8$ Hz, 2H), 7.41 (d, $J = 8.4$ Hz, 2H), 4.01 (t, $J = 6.6$ Hz, 2H), 1.65–1.56 (m, 2H), 0.90 (t, $J = 7.4$ Hz, 3H).

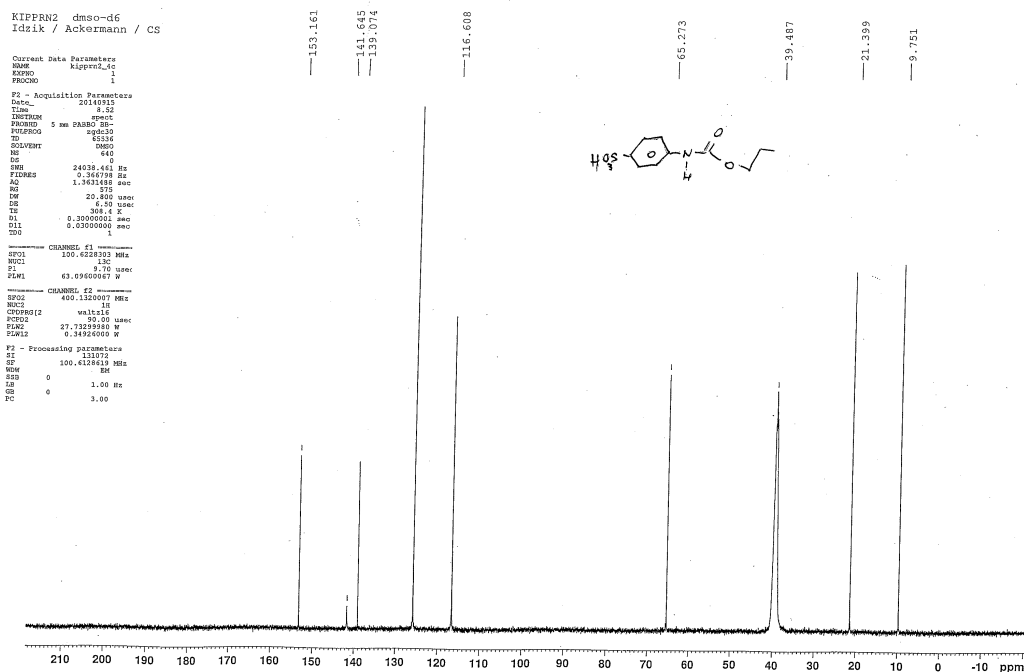


Figure S10. $^{13}\text{C-NMR}$ spectrum of 4-[(propoxycarbonyl)amino]benzenesulfonic acid (**5**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 153.17, 141.66, 139.08, 125.76, 116.62, 65.29, 21.42, 9.77.

KITPNO dmsc-d6
Idzik / GZG / CS

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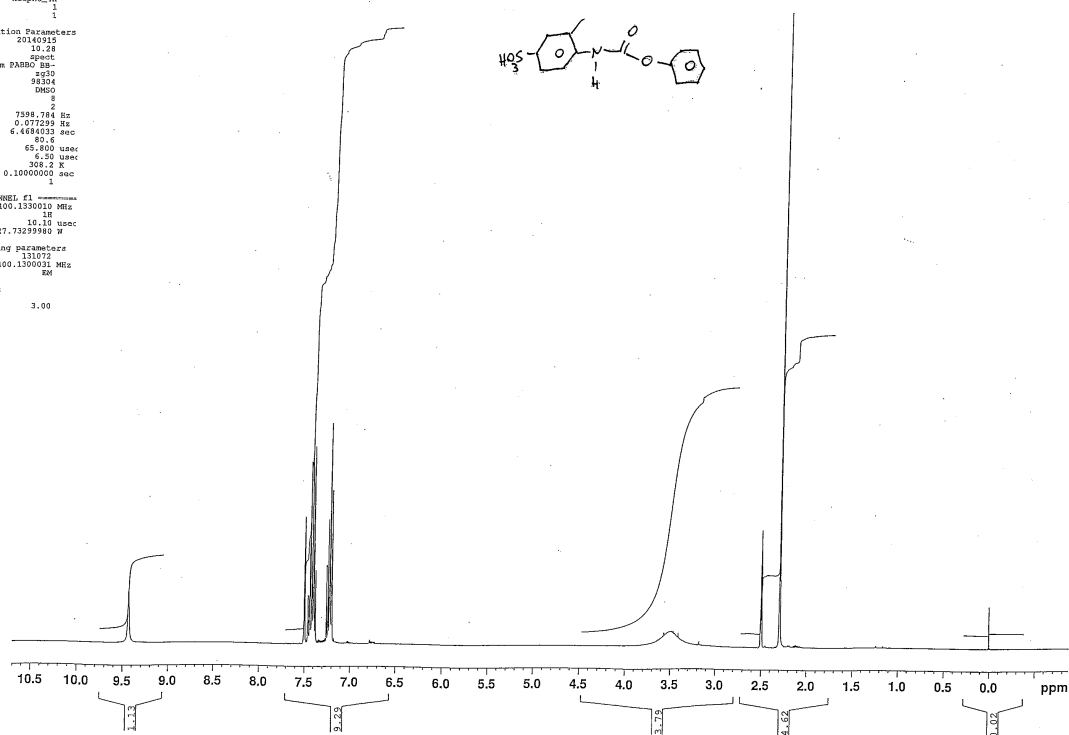


Figure S11. $^1\text{H-NMR}$ spectrum of 3-methyl-4-[(phenoxyacetyl)amino]benzenesulfonic acid (**6**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.41 (s, 1H), 7.47 (s, 1H), 7.42–7.35 (m, 4H), 7.23 (t, $J = 6.0$ Hz, 1H), 7.20 (d, $J = 6.0$ Hz, 2H), 2.29 (s, 3H).

KITPNO dmsc-d6
Idzik / GZG / CS

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Current Data Parameters
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PROCNO   1

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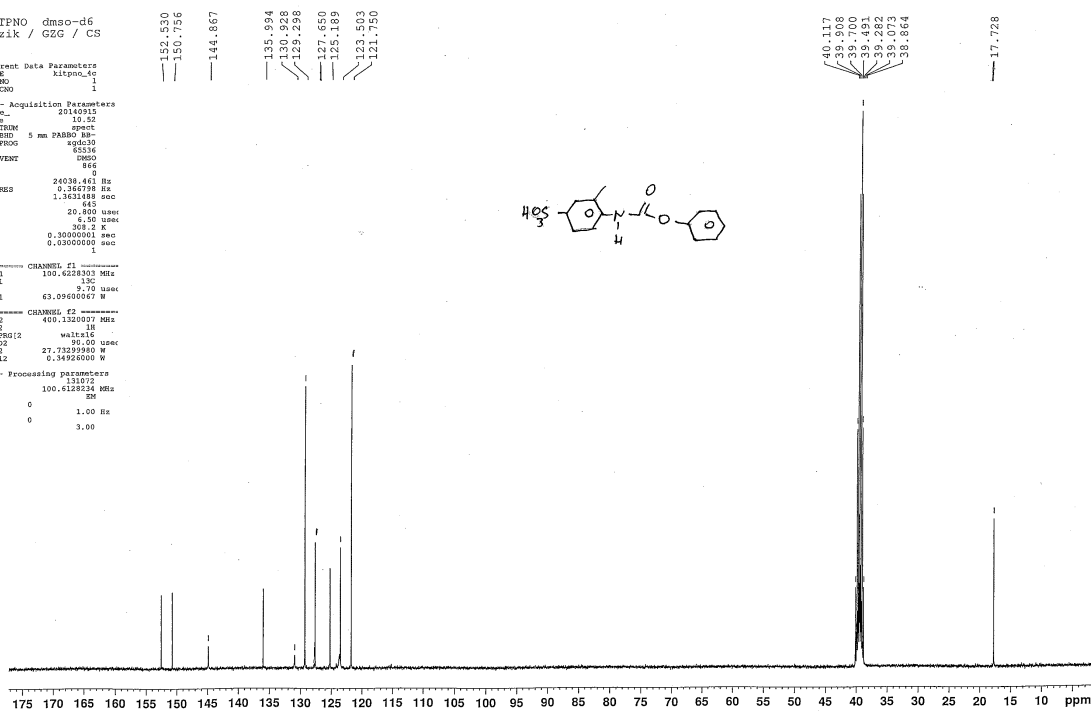


Figure S12. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-[(phenoxyacetyl)amino]benzenesulfonic acid (**6**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 152.53, 150.76, 144.87, 135.99, 130.93, 129.30, 127.65, 125.19, 124.20, 123.50, 121.75, 17.73.

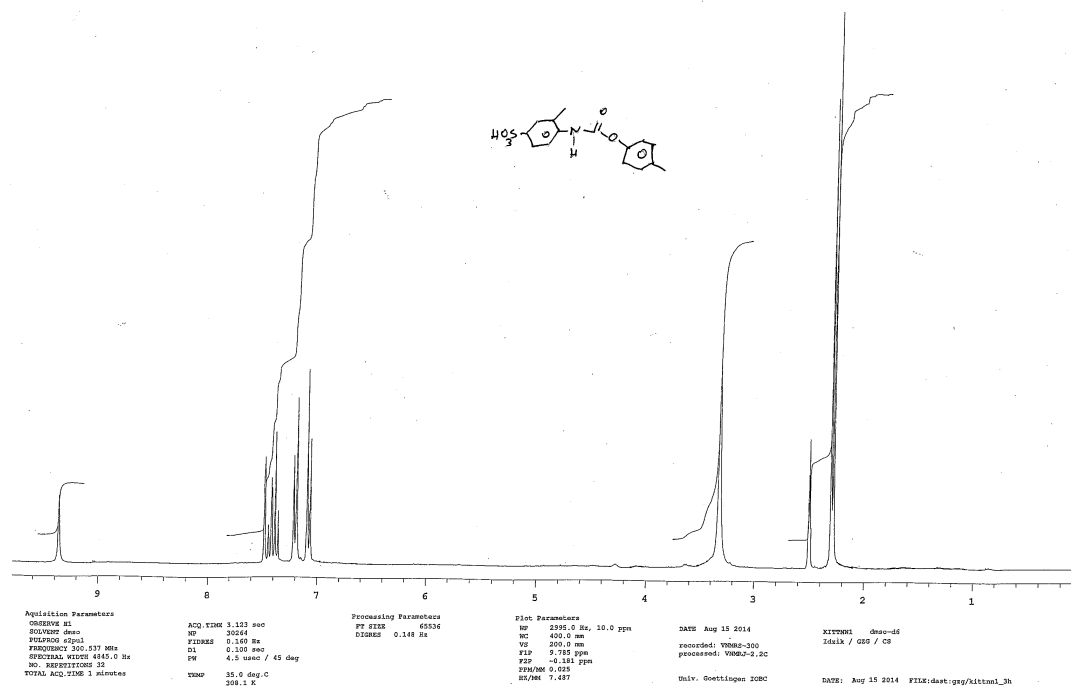


Figure S13. $^1\text{H-NMR}$ spectrum of 3-methyl-4-[[[(4-methylphenoxy)carbonyl]amino] benzenesulfonic acid (**7**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.37 (s, 1H), 7.48 (s, 1H), 7.43 (d, $J = 8.4$ Hz, 1H), 7.37 (d, $J = 8.4$ Hz, 1H), 7.21 (d, $J = 8.4$ Hz, 2H), 7.08 (d, $J = 8.4$ Hz, 2H), 2.31 (s, 3H), 2.28 (s, 3H).

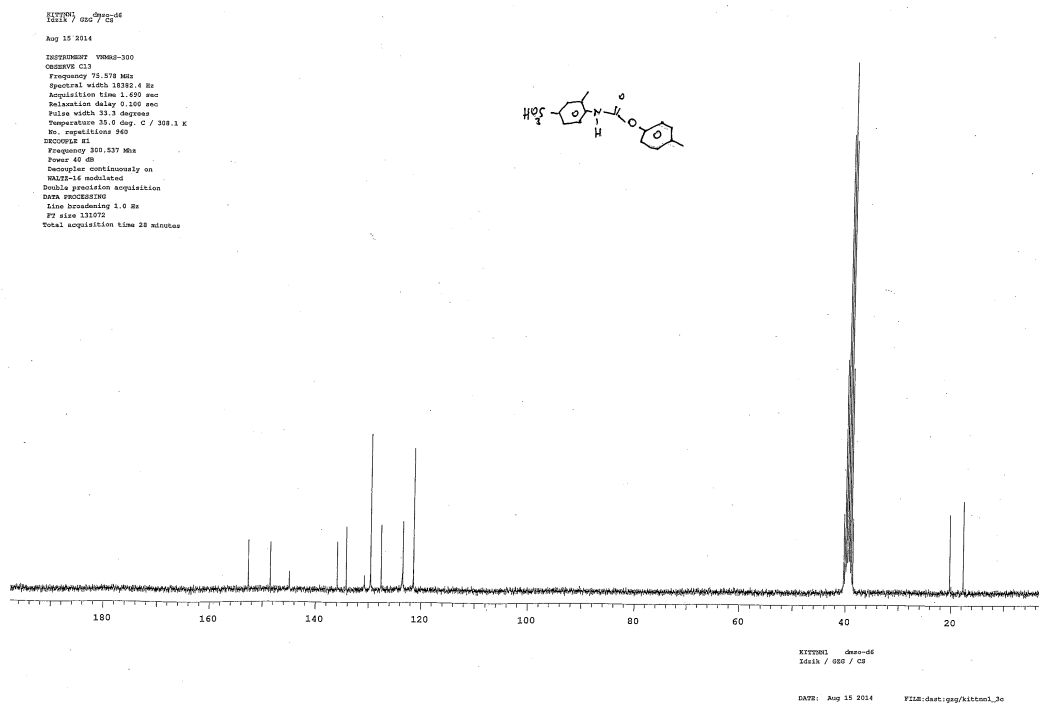


Figure S14. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-[[[(4-methylphenoxy)carbonyl]amino] benzenesulfonic acid (**7**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 152.62, 148.50, 144.96, 135.92, 134.24, 130.76, 129.58, 127.58, 123.56, 123.43, 121.43, 20.26, 17.69.

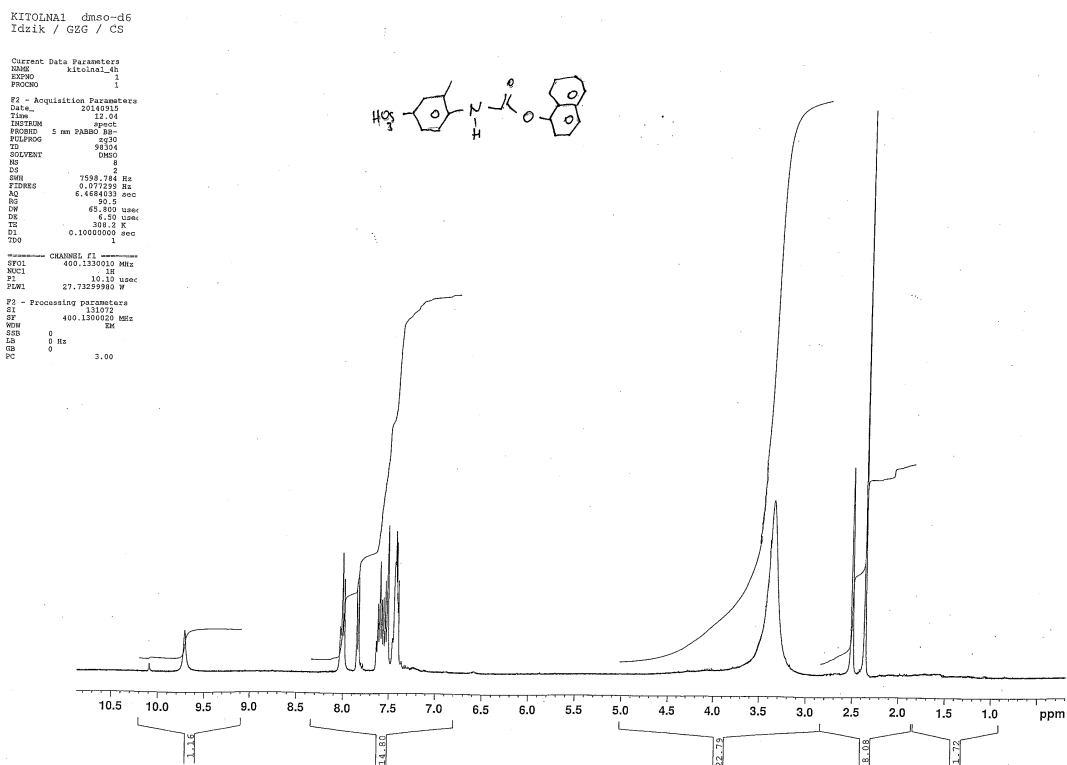


Figure S15. $^1\text{H-NMR}$ spectrum of 3-methyl-4-([(naphthalen-1-yloxy)carbonyl]amino) benzenesulfonic acid (**8**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.72 (s, 1H), 8.03–7.98 (m, 2H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.64–7.52 (m, 4H), 7.46–7.40 (m, 3H), 2.36 (s, 3H).

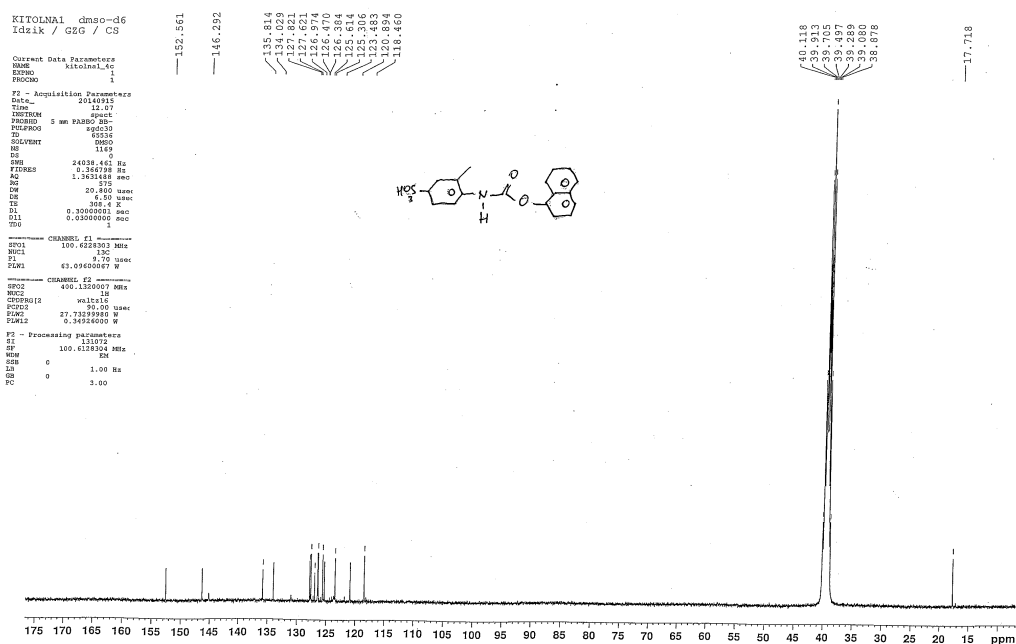


Figure S16. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-([(naphthalen-1-yloxy)carbonyl]amino) benzenesulfonic acid (**8**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 152.57, 146.30, 145.14, 135.83, 134.04, 130.99, 127.83, 127.63, 126.99, 126.48, 126.40, 125.63, 125.32, 124.07, 123.50, 120.91, 118.47, 17.74.

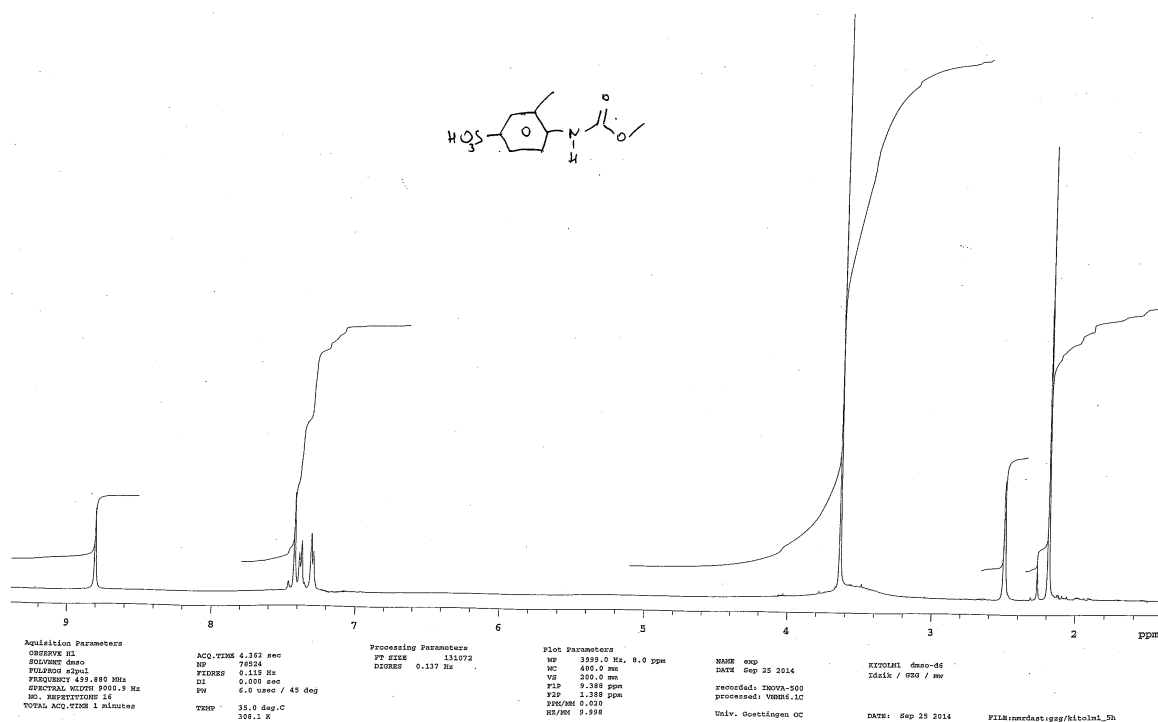


Figure S17. $^1\text{H-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]-3-methylbenzenesulfonic acid (**9**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 8.80 (s, 1H), 7.42 (s, 1H), 7.38 (d, $J = 7.5$ Hz, 1H), 7.30 (d, $J = 7.5$ Hz, 1H), 3.64 (s, 3H), 2.19 (s, 3H).

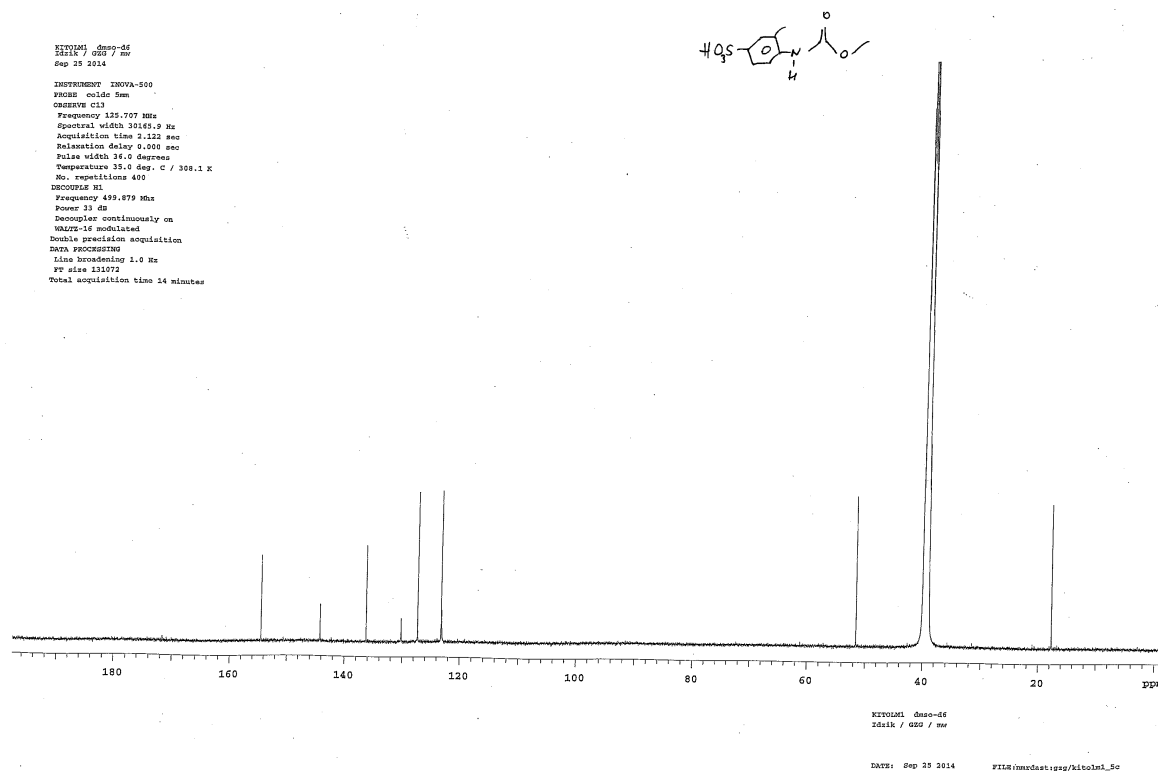


Figure S18. $^{13}\text{C-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]-3-methylbenzenesulfonic acid (**9**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 154.47, 144.23, 136.26, 130.17, 127.31, 123.20, 123.10, 51.56, 17.68.

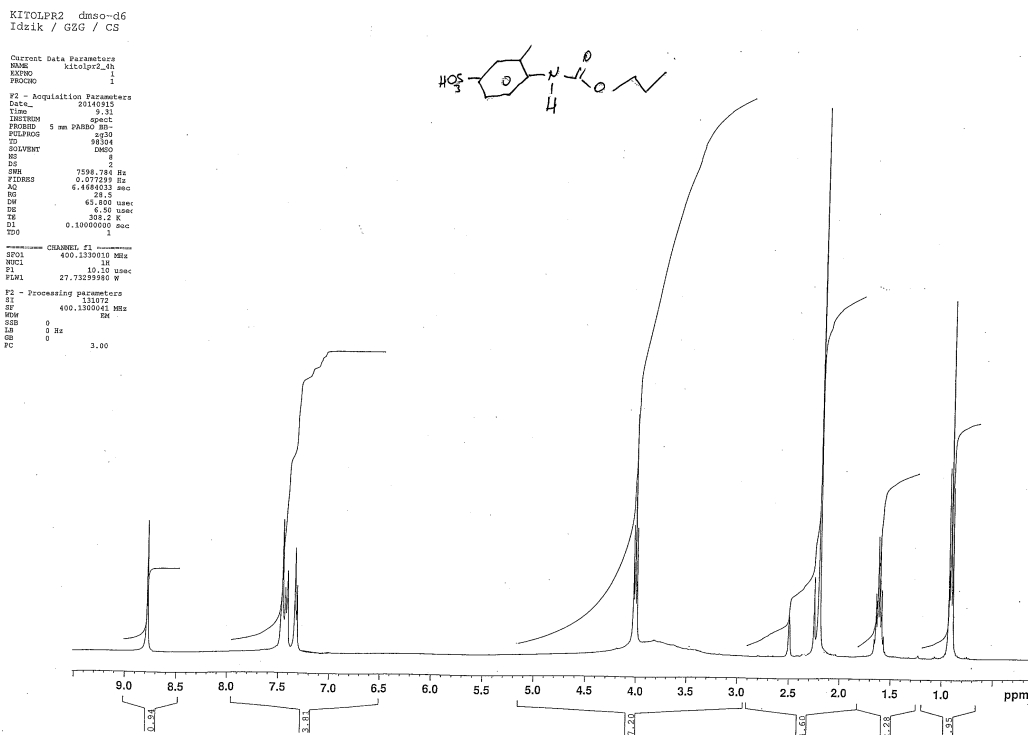


Figure S19. $^1\text{H-NMR}$ spectrum of 3-methyl-4-[(propoxycarbonyl)amino]benzenesulfonic acid (**10**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 8.78 (s, 1H), 7.46 (s, 1H), 7.42 (d, $J = 8.4$ Hz, 1H), 7.32 (d, $J = 8.4$ Hz, 1H), 4.01 (t, $J = 6.6$ Hz, 2H), 2.20 (s, 3H), 1.66–1.57 (m, 2H), 0.91 (t, $J = 7.4$ Hz, 3H).

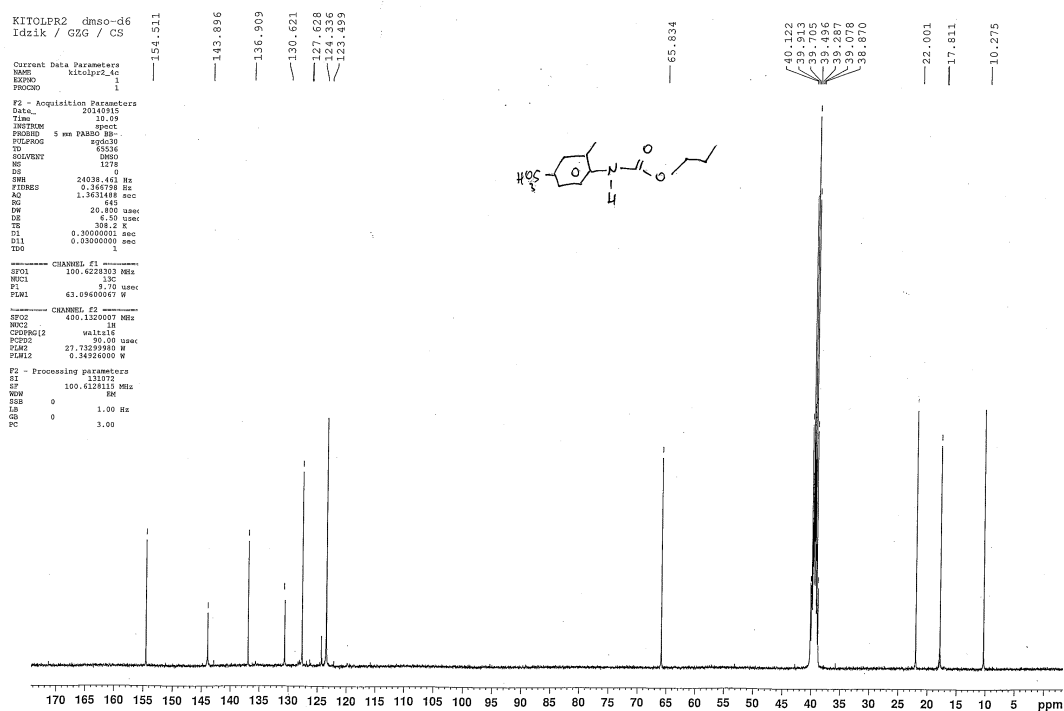


Figure S20. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-[(propoxycarbonyl)amino]benzenesulfonic acid (**10**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 154.52, 143.90, 136.92, 130.63, 127.64, 124.35, 123.51, 65.85, 22.02, 17.83, 10.30.