

Supplementary Materials

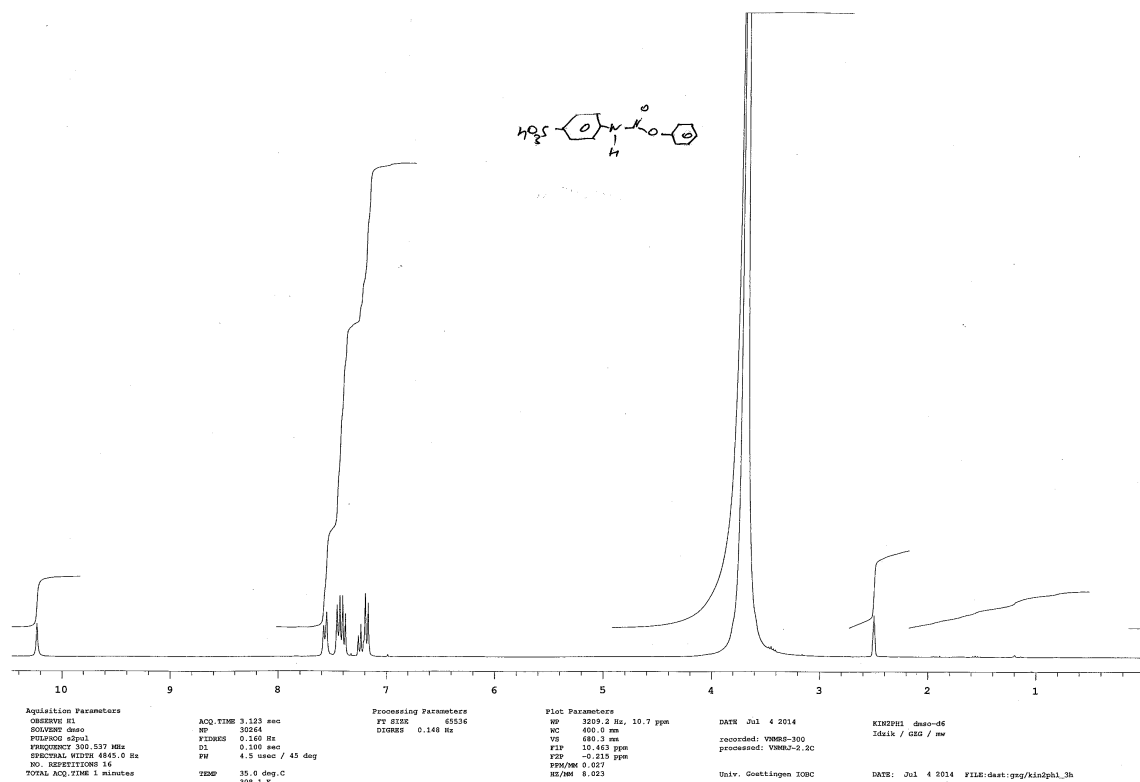


Figure S1. $^1\text{H-NMR}$ spectrum of 4-[(phenoxy carbonyl)amino]benzenesulfonic (**1**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 10.23 (s, 1H), 7.57 (d, $J = 8.1$ Hz, 2H), 7.44 (d, $J = 7.8$ Hz, 2H), 7.39 (d, $J = 7.8$ Hz, 2H), 7.24 (t, $J = 7.4$ Hz, 1H), 7.18 (d, $J = 7.8$ Hz, 2H).

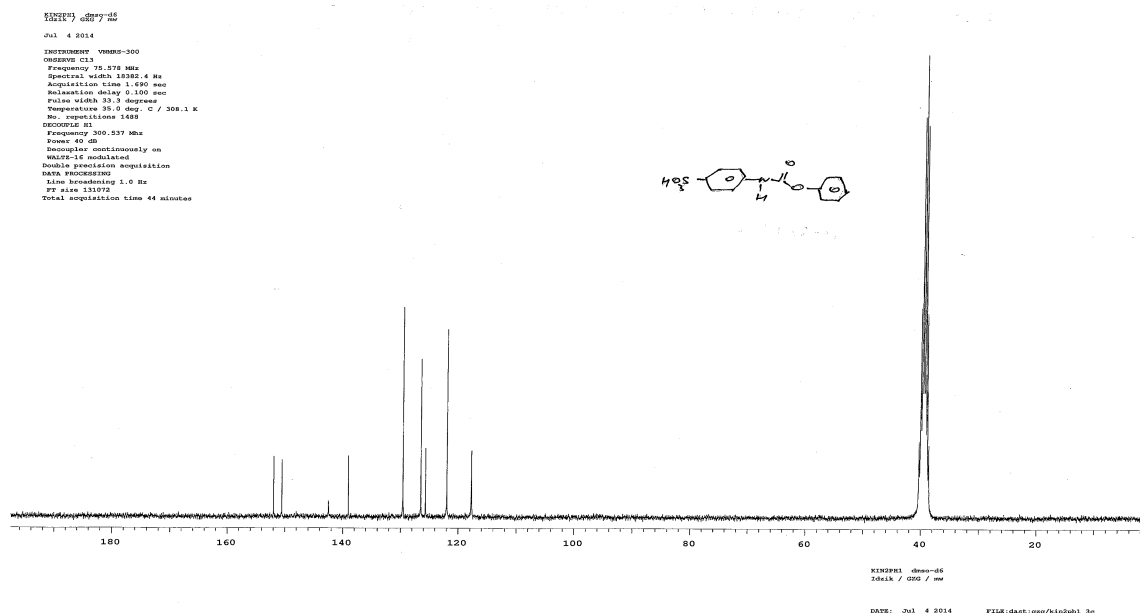


Figure S2. $^{13}\text{C-NMR}$ spectrum of 4-[(phenoxy carbonyl)amino]benzenesulfonic (**1**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 151.93, 150.52, 142.48, 139.05, 129.58, 126.48, 125.65, 121.96, 117.76.

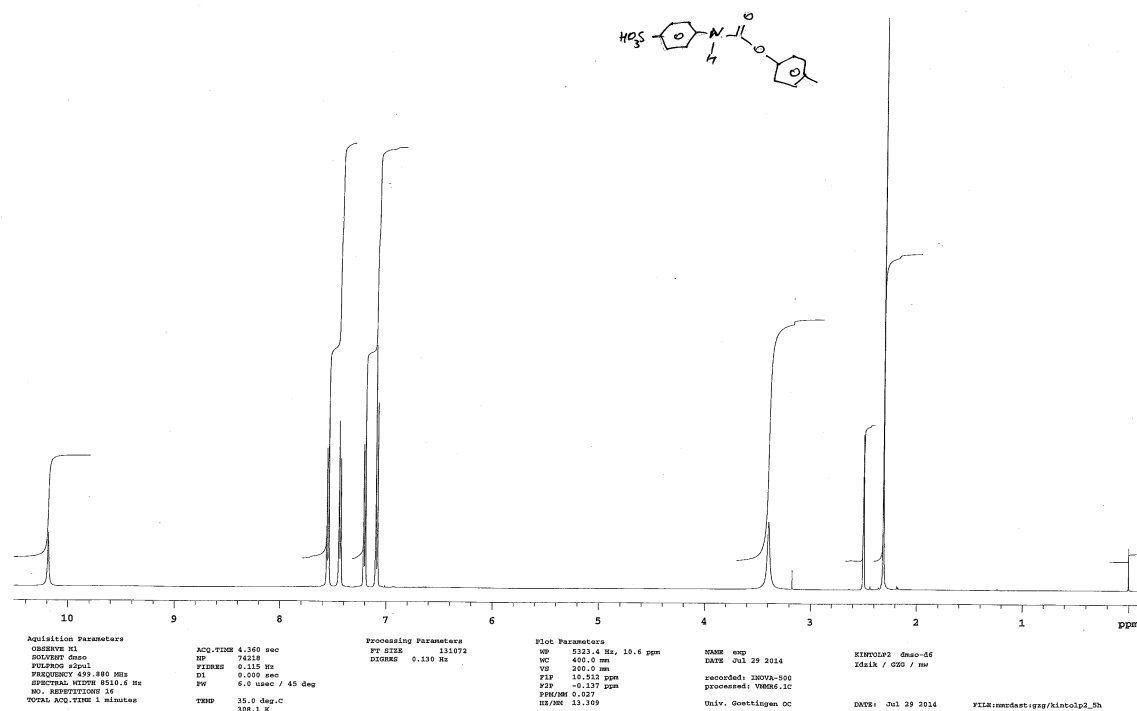


Figure S3. $^1\text{H-NMR}$ spectrum of 4-[[4-(4-methylphenoxy)carbonyl]amino]benzenesulfonic acid (**2**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 10.19 (s, 1H), 7.55 (d, $J = 8.5$ Hz, 2H), 7.44 (d, $J = 8.5$ Hz, 2H), 7.20 (d, $J = 8.5$ Hz, 2H), 7.09 (d, $J = 8.5$ Hz, 2H), 2.31 (s, 3H).

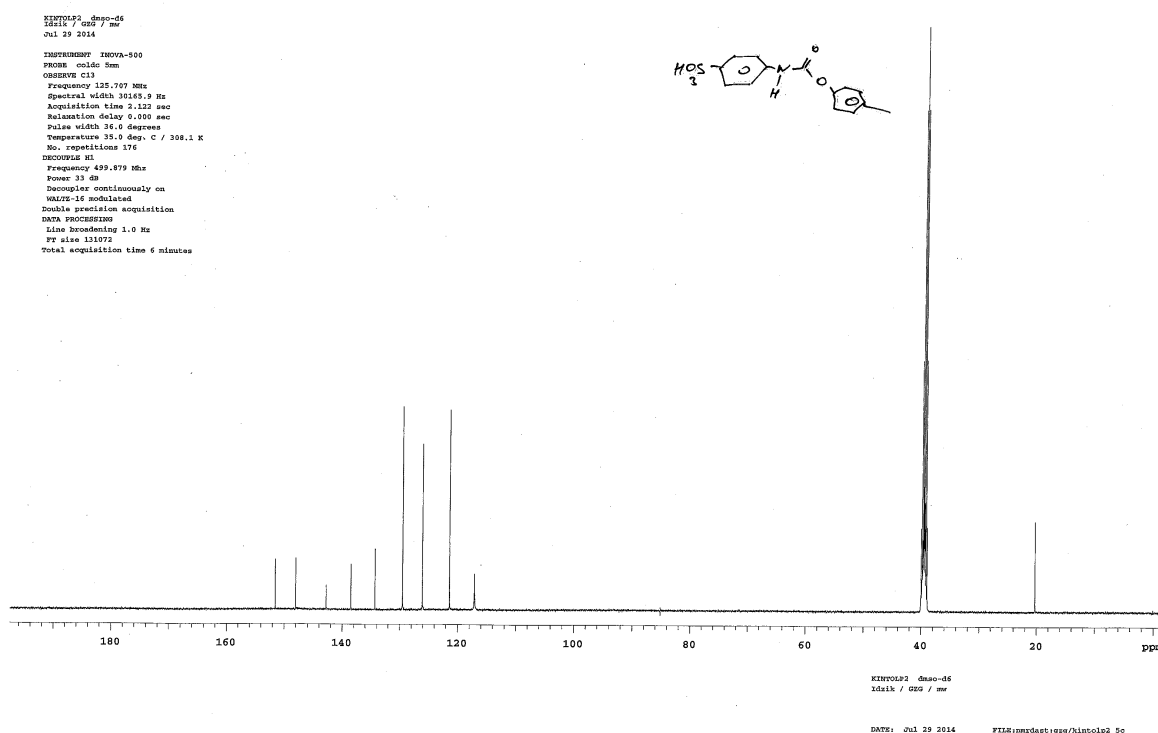


Figure S4. $^{13}\text{C-NMR}$ spectrum of 4-[[4-(4-methylphenoxy)carbonyl]amino]benzenesulfonic acid (**2**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 151.54, 148.02, 142.79, 138.49, 134.29, 129.49, 126.07, 121.38, 117.15, 20.30.

KIPHNAF1 dms0-d6
Idzik / GZG / CS

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PROCNO: 1

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SOLVENT: DMSO
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FIDRES: 0.477250 Hz
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RG: 114
DM: 65.800 usec
DE: 6.50 usec
TE: 308.2 K
D1: 0.1000000 sec
TDO: 1

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P1: 10.10 usec
PL1: 27.7325950 dB
PL2:
PL3:
===== CHANNEL f2 =====
NUC2: 13C
P2: 10.10 usec
PL2: 27.7325950 dB
PL3:

F2 - Processing parameters
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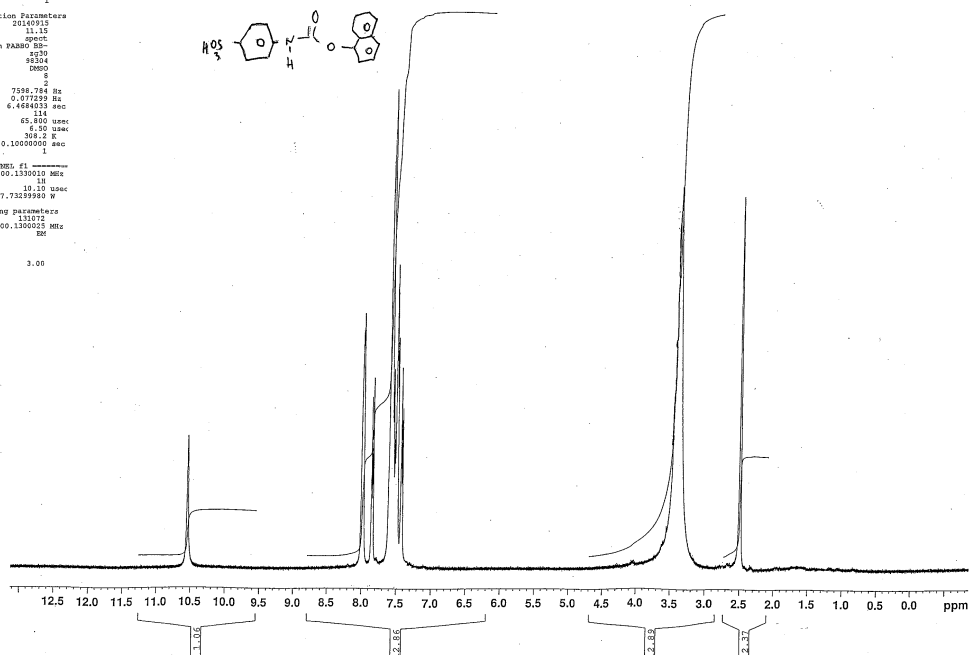


Figure S5. ¹H-NMR spectrum of 4-[[naphthalen-1-yloxy]carbonyl]amino}benzenesulfonic acid (3). ¹H-NMR (300 MHz, DMSO-*d*₆) δ, ppm, 10.53 (s, 1H), 8.08–7.96 (m, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.69–7.49 (m, 5H), 7.43 (d, *J* = 7.6 Hz, 2H).

KIPHNF1 dms0-d6
Idzik / Ackermann / CS

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PROCNO: 1

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FIDRES: 4.0367748 Hz
AQ: 1.7322189 sec
RG: 20
DM: 20.100 usec
DE: 6.50 usec
TE: 308.1 K
D1: 0.5000001 sec
D11: 0.1000000 sec
TDO: 1

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PL1: 63.0960000 dB
PL2:
PL3:

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P2: 8.70 usec
PL2: 63.0960000 dB
PL3:

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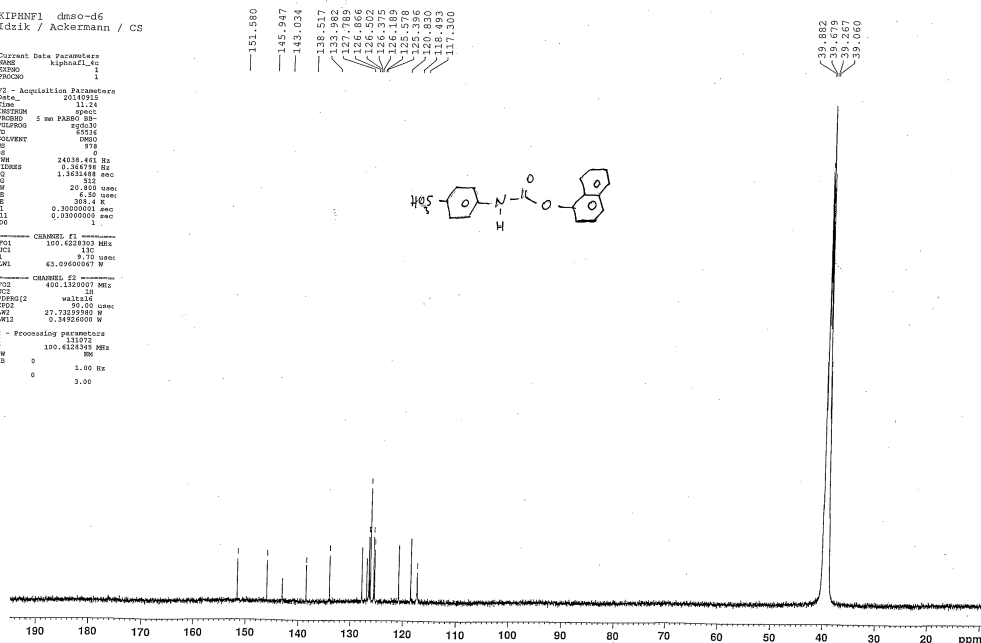


Figure S6. ¹³C-NMR Spectrum of 4-[[naphthalen-1-yloxy]carbonyl]amino}benzenesulfonic acid (3). ¹³C-NMR (300 MHz, DMSO-*d*₆) δ, ppm, 151.59, 145.96, 143.05, 138.53, 133.99, 127.80, 126.88, 126.51, 126.39, 126.20, 125.59, 125.41, 120.84, 118.51, 117.31.

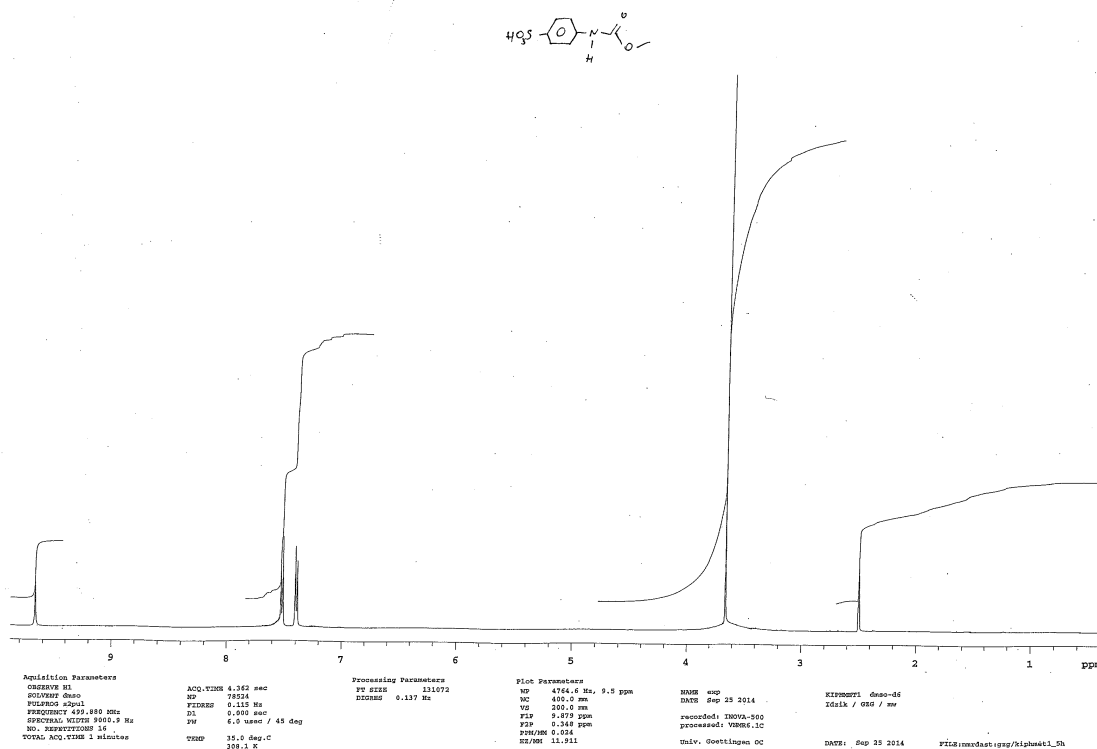


Figure S7. $^1\text{H-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]benzenesulfonic acid (**4**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.67 (s, 1H), 7.52 (d, $J = 8.5$ Hz, 2H), 7.39 (d, $J = 8.5$ Hz, 2H), 3.66 (s, 3H).

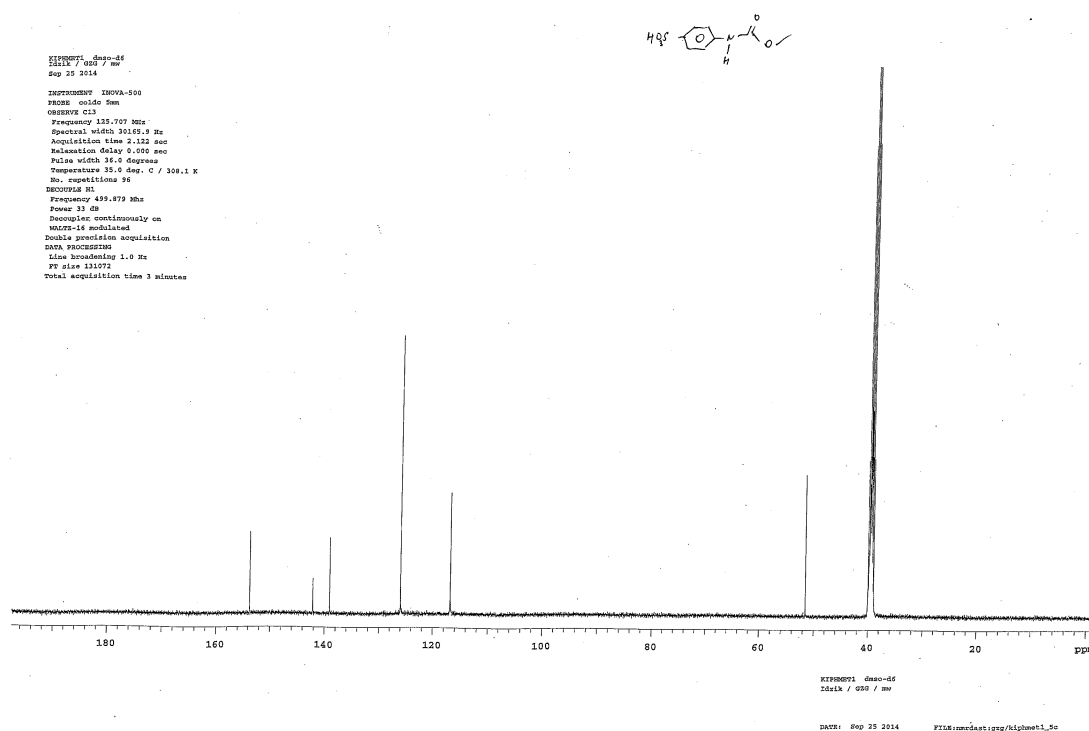


Figure S8. $^{13}\text{C-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]benzenesulfonic acid (**4**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 153.70, 142.13, 139.05, 125.99, 116.84, 51.53.

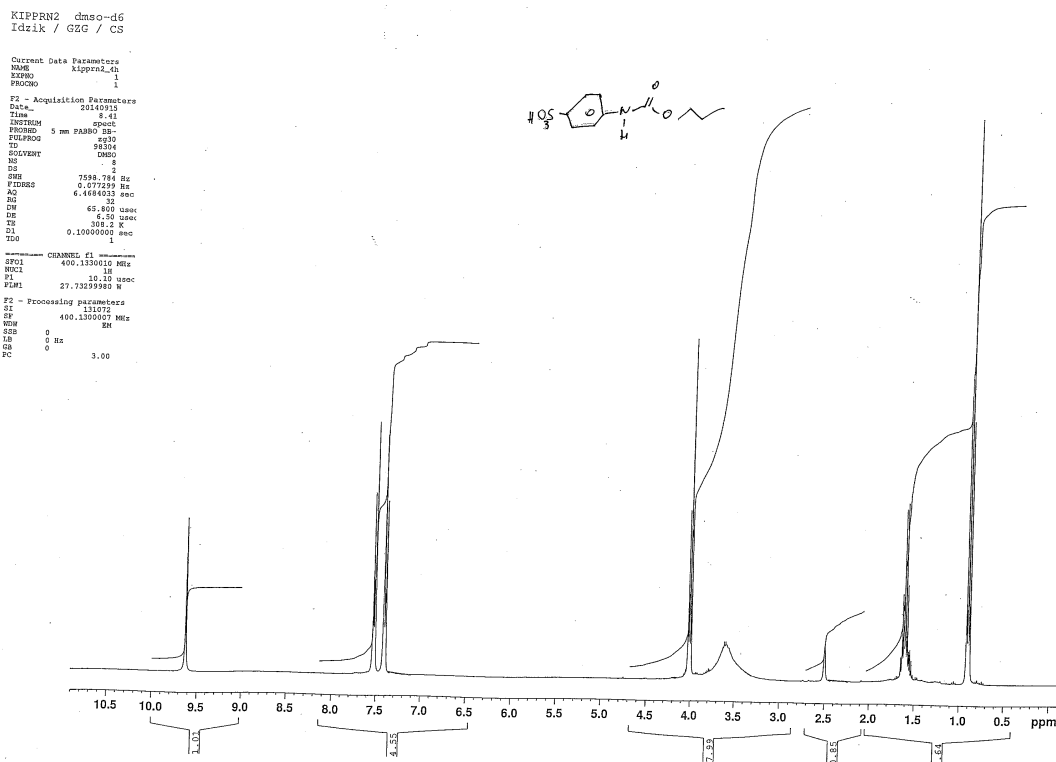


Figure S9. $^1\text{H-NMR}$ spectrum of 4-[(propoxycarbonyl)amino]benzenesulfonic acid (**5**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.63 (s, 1H), 7.52 (d, $J = 8.8$ Hz, 2H), 7.41 (d, $J = 8.4$ Hz, 2H), 4.01 (t, $J = 6.6$ Hz, 2H), 1.65–1.56 (m, 2H), 0.90 (t, $J = 7.4$ Hz, 3H).

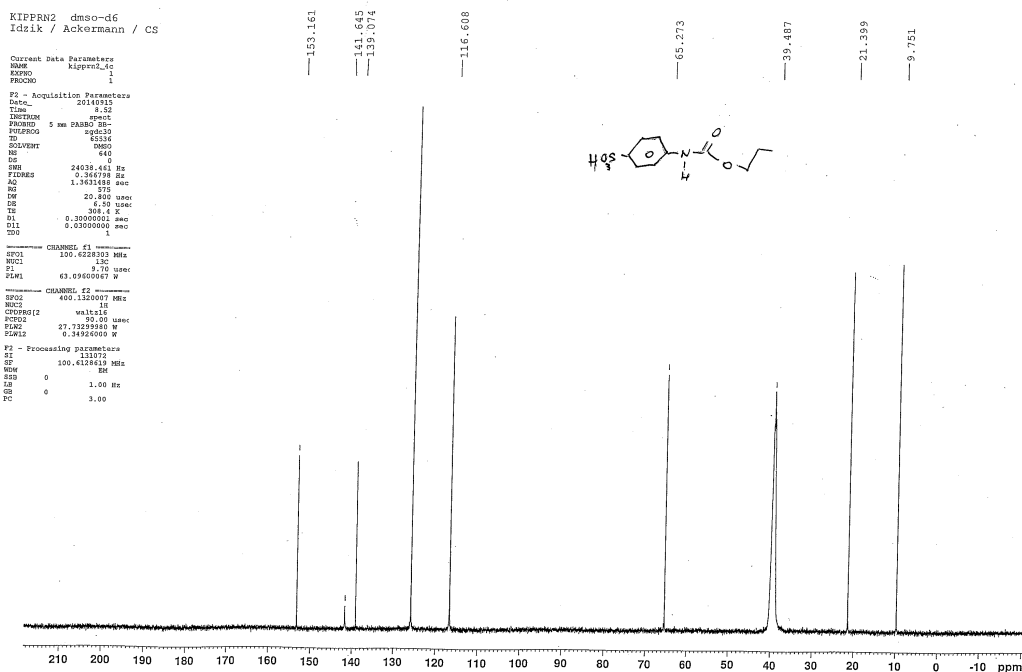


Figure S10. $^{13}\text{C-NMR}$ spectrum of 4-[(propoxycarbonyl)amino]benzenesulfonic acid (**5**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 153.17, 141.66, 139.08, 125.76, 116.62, 65.29, 21.42, 9.77.

KITPNO dms0-d6
Idzik / GZG / CS

```

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PROCNO   1

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DS        2
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RG        60.5
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TE        303.2 K
D1        0.10000000 sec
TDO       1

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NUC1     1H
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PL1      27.73299980 W

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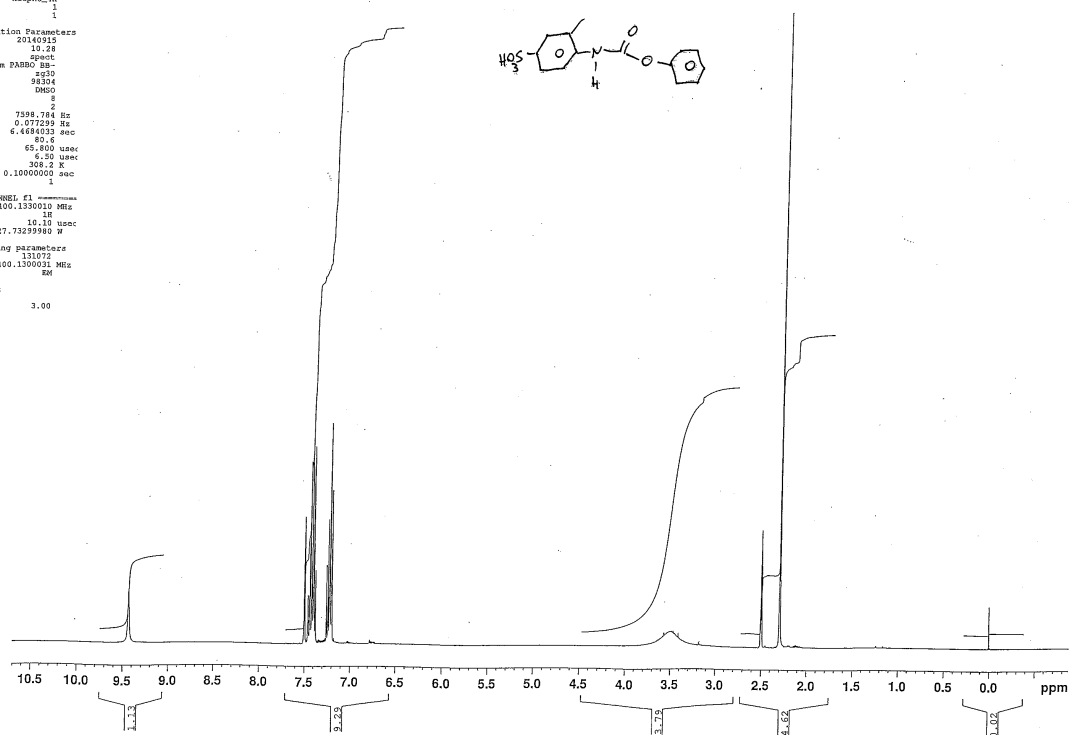


Figure S11. $^1\text{H-NMR}$ spectrum of 3-methyl-4-[(phenoxyacetyl)amino]benzenesulfonic acid (**6**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.41 (s, 1H), 7.47 (s, 1H), 7.42–7.35 (m, 4H), 7.23 (t, $J = 6.0$ Hz, 1H), 7.20 (d, $J = 6.0$ Hz, 2H), 2.29 (s, 3H).

KITPNO dms0-d6
Idzik / GZG / CS

```

Current Data Parameters
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PROCNO   1

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INSTRUM spect
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PULPROG zg30
TD        65536
SOLVENT  DMSO
NS        2
DS        2
SHE       24039.461 Hz
FIDRES   0.360788 Hz
AQ        1.3631988 sec
RG        145
DE        20.800 usec
TE        303.2 K
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D11       0.03000000 sec
TDO       1

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NUC1     13C
P1        9.70 usec
PL1      63.05000000 W

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NUC2     1H
CPDPRG12 waltz16
PCPD12   30.00 usec
PLM2     27.73299980 W
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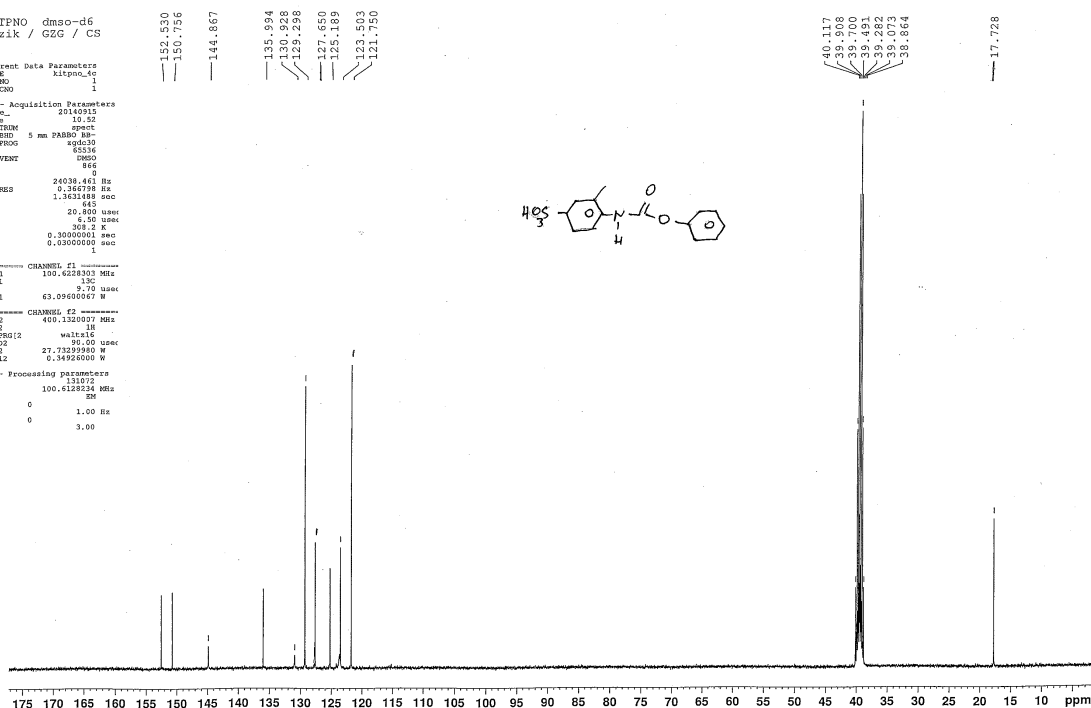


Figure S12. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-[(phenoxyacetyl)amino]benzenesulfonic acid (**6**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 152.53, 150.76, 144.87, 135.99, 130.93, 129.30, 127.65, 125.19, 124.20, 123.50, 121.75, 17.73.

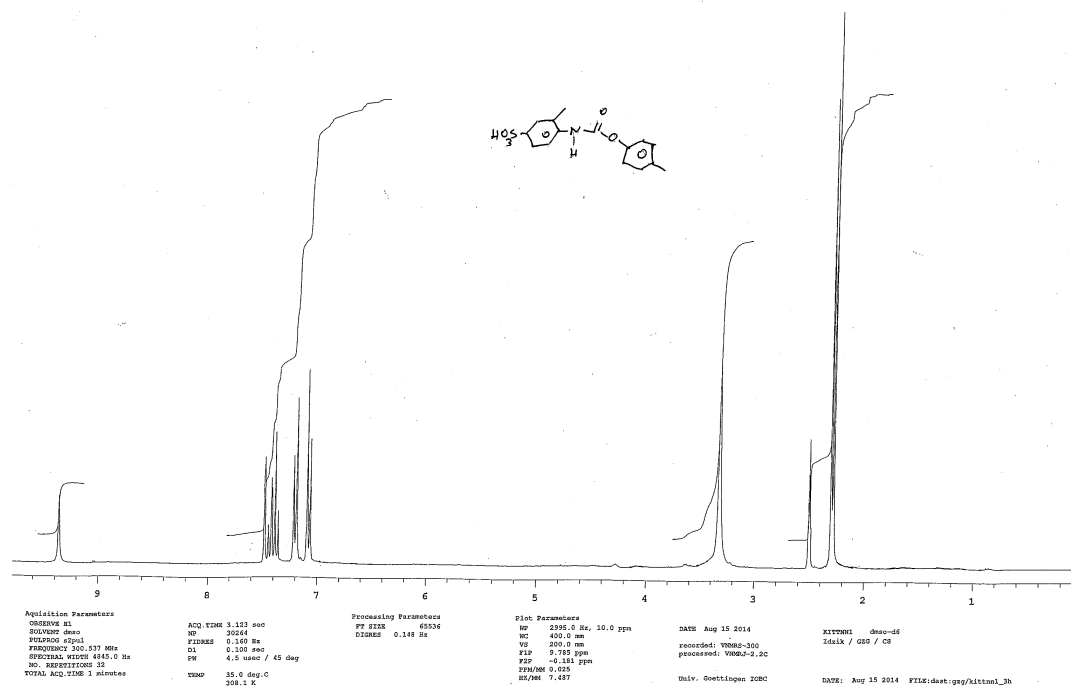


Figure S13. $^1\text{H-NMR}$ spectrum of 3-methyl-4-[[[(4-methylphenoxy)carbonyl]amino] benzenesulfonic acid (**7**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.37 (s, 1H), 7.48 (s, 1H), 7.43 (d, $J = 8.4$ Hz, 1H), 7.37 (d, $J = 8.4$ Hz, 1H), 7.21 (d, $J = 8.4$ Hz, 2H), 7.08 (d, $J = 8.4$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

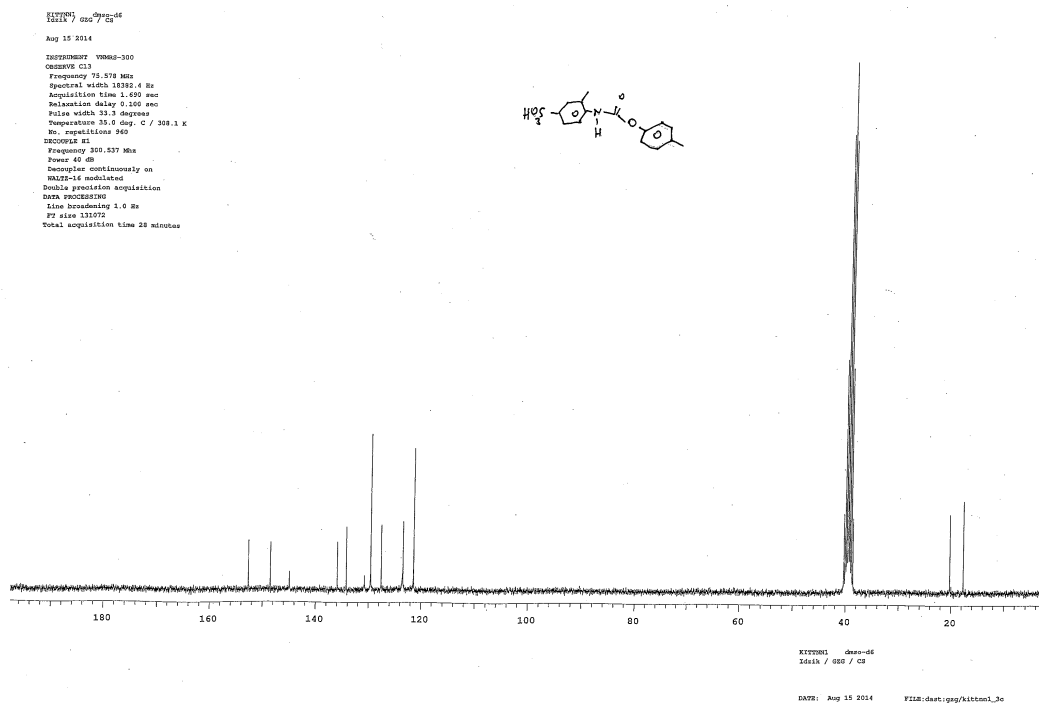


Figure S14. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-[[[(4-methylphenoxy)carbonyl]amino] benzenesulfonic acid (**7**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 152.62, 148.50, 144.96, 135.92, 134.24, 130.76, 129.58, 127.58, 123.56, 123.43, 121.43, 20.26, 17.69.

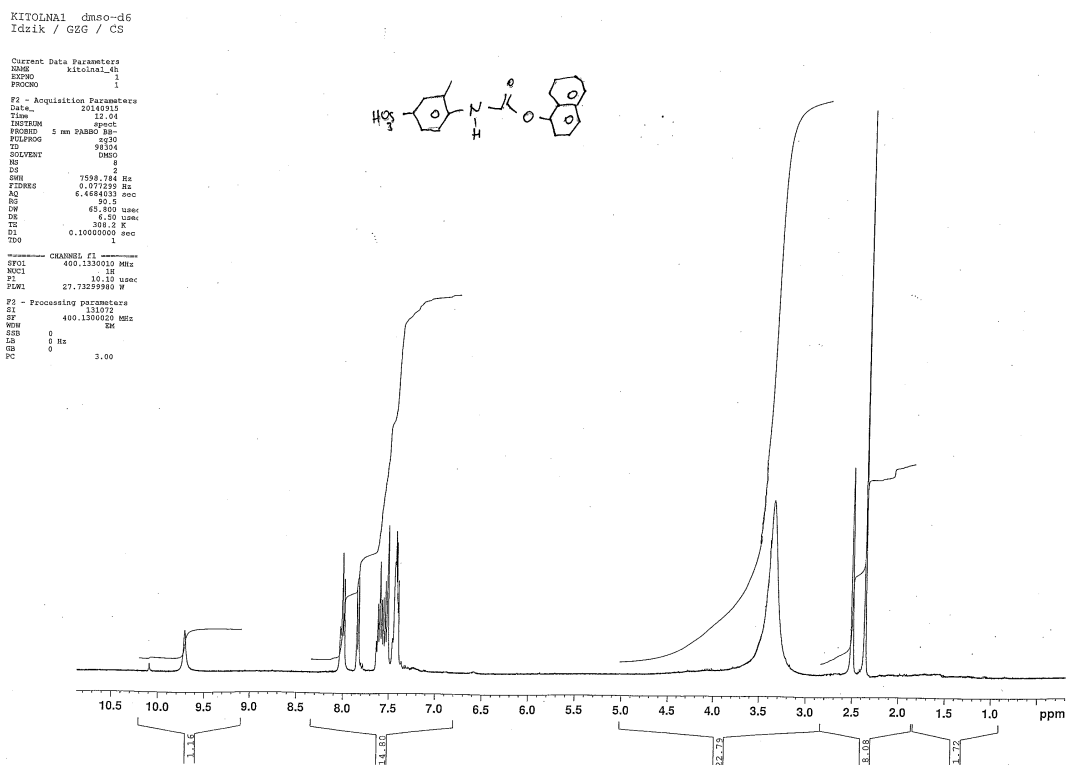


Figure S15. $^1\text{H-NMR}$ spectrum of 3-methyl-4-([(naphthalen-1-yloxy)carbonyl]amino) benzenesulfonic acid (**8**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 9.72 (s, 1H), 8.03–7.98 (m, 2H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.64–7.52 (m, 4H), 7.46–7.40 (m, 3H), 2.36 (s, 3H).

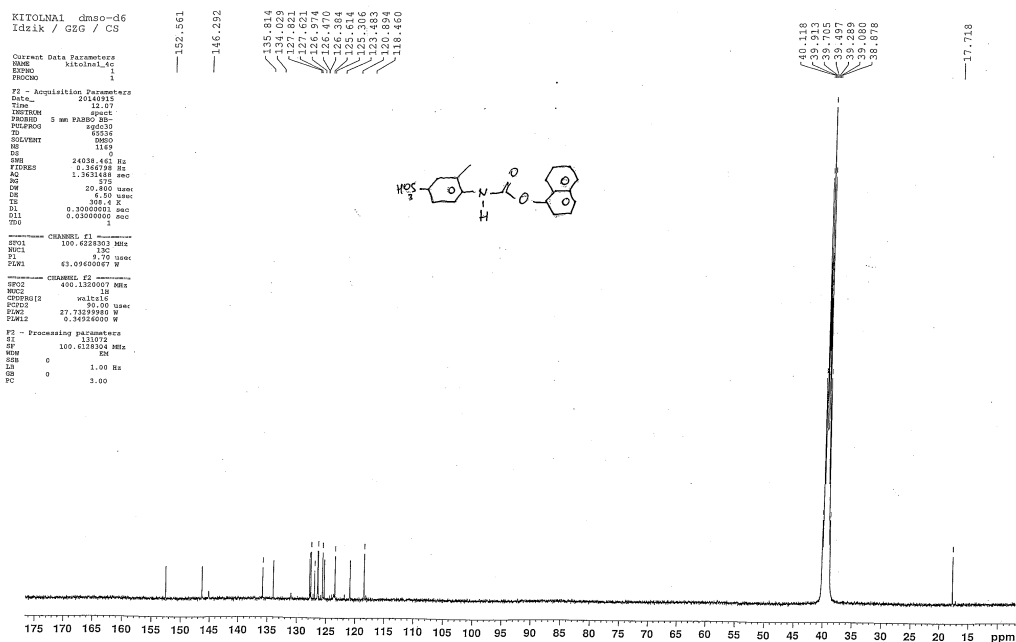


Figure S16. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-([(naphthalen-1-yloxy)carbonyl]amino) benzenesulfonic acid (**8**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 152.57, 146.30, 145.14, 135.83, 134.04, 130.99, 127.83, 127.63, 126.99, 126.48, 126.40, 125.63, 125.32, 124.07, 123.50,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

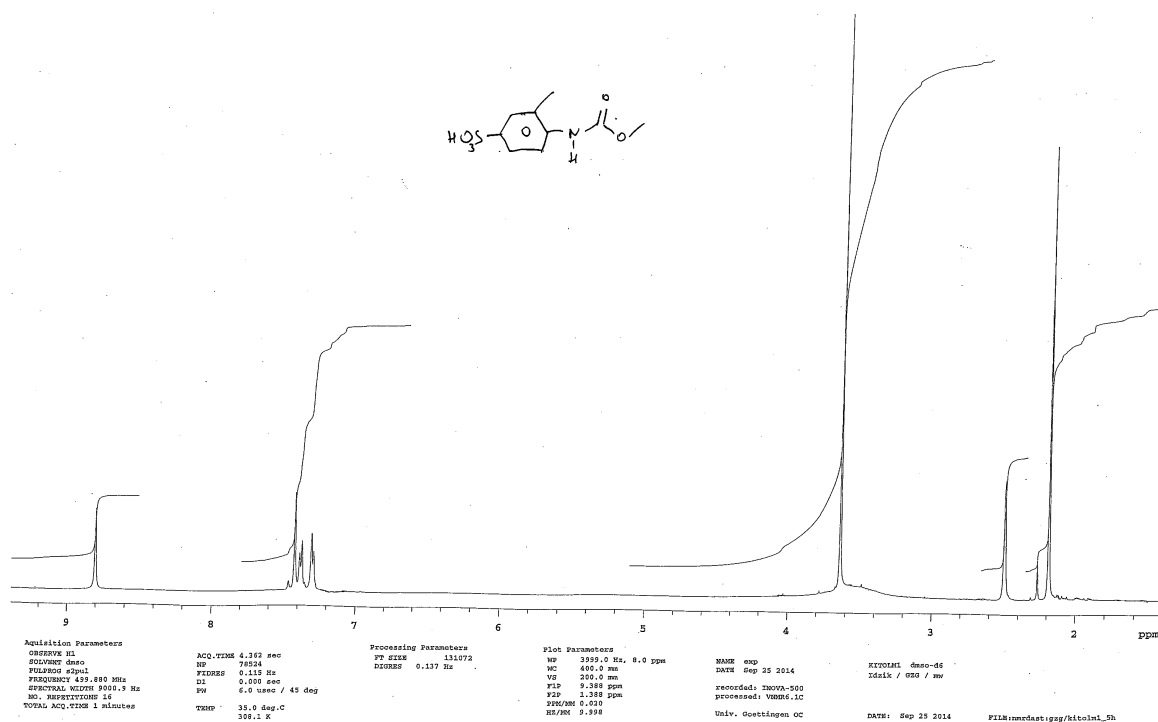


Figure S17. $^1\text{H-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]-3-methylbenzenesulfonic acid (**9**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 8.80 (s, 1H), 7.42 (s, 1H), 7.38 (d, $J = 7.5$ Hz, 1H), 7.30 (d, $J = 7.5$ Hz, 1H), 3.64 (s, 3H), 2.19 (s, 3H).

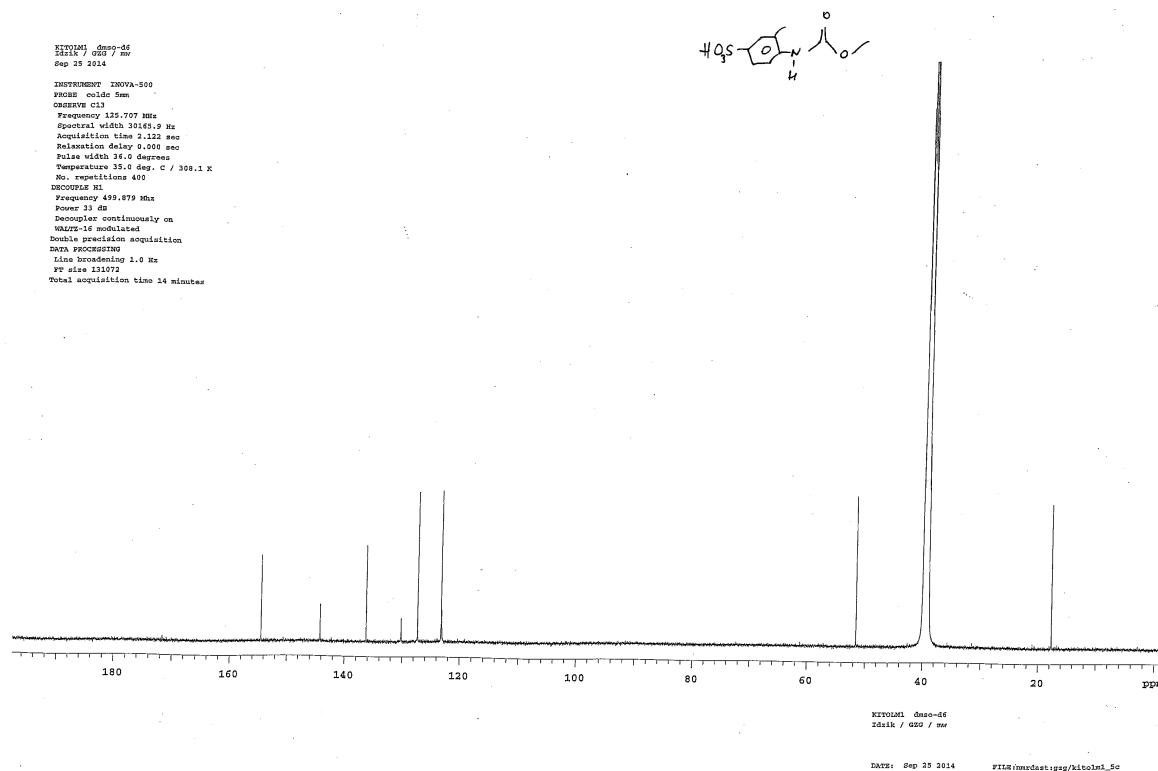


Figure S18. $^{13}\text{C-NMR}$ spectrum of 4-[(methoxycarbonyl)amino]-3-methylbenzenesulfonic acid (**9**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 154.47, 144.23, 136.26, 130.17, 127.31, 123.20, 123.10, 51.56, 17.68.

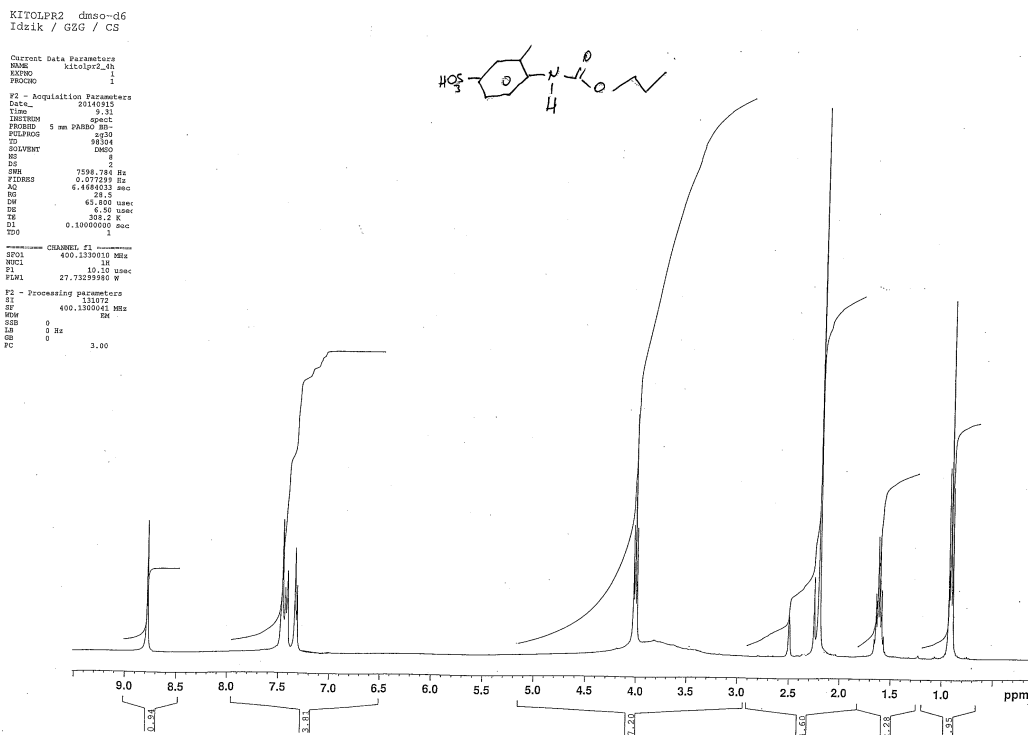


Figure S19. $^1\text{H-NMR}$ spectrum of 3-methyl-4-[(propoxycarbonyl)amino]benzenesulfonic acid (**10**). $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 8.78 (s, 1H), 7.46 (s, 1H), 7.42 (d, $J = 8.4$ Hz, 1H), 7.32 (d, $J = 8.4$ Hz, 1H), 4.01 (t, $J = 6.6$ Hz, 2H), 2.20 (s, 3H), 1.66–1.57 (m,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

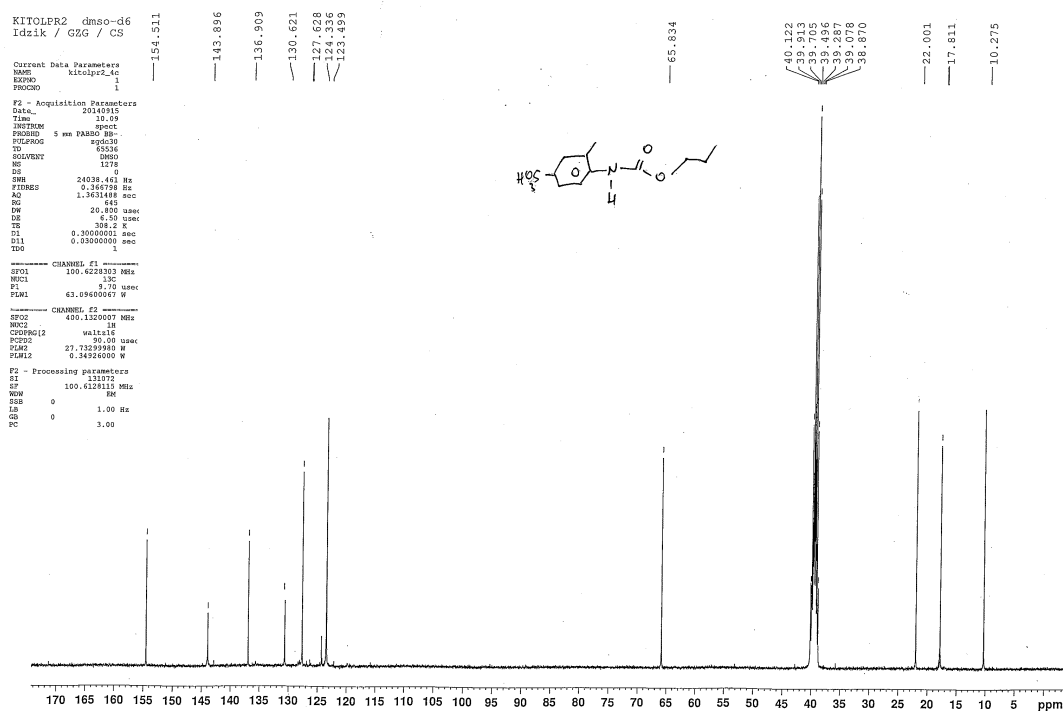


Figure S20. $^{13}\text{C-NMR}$ spectrum of 3-methyl-4-[(propoxycarbonyl)amino]benzenesulfonic acid (**10**). $^{13}\text{C-NMR}$ (300 MHz, $\text{DMSO-}d_6$) δ , ppm, 154.52, 143.90, 136.92, 130.63, 127.64, 124.35, 123.51, 65.85, 22.02, 17.83, 10.30.