

Supplementary Materials

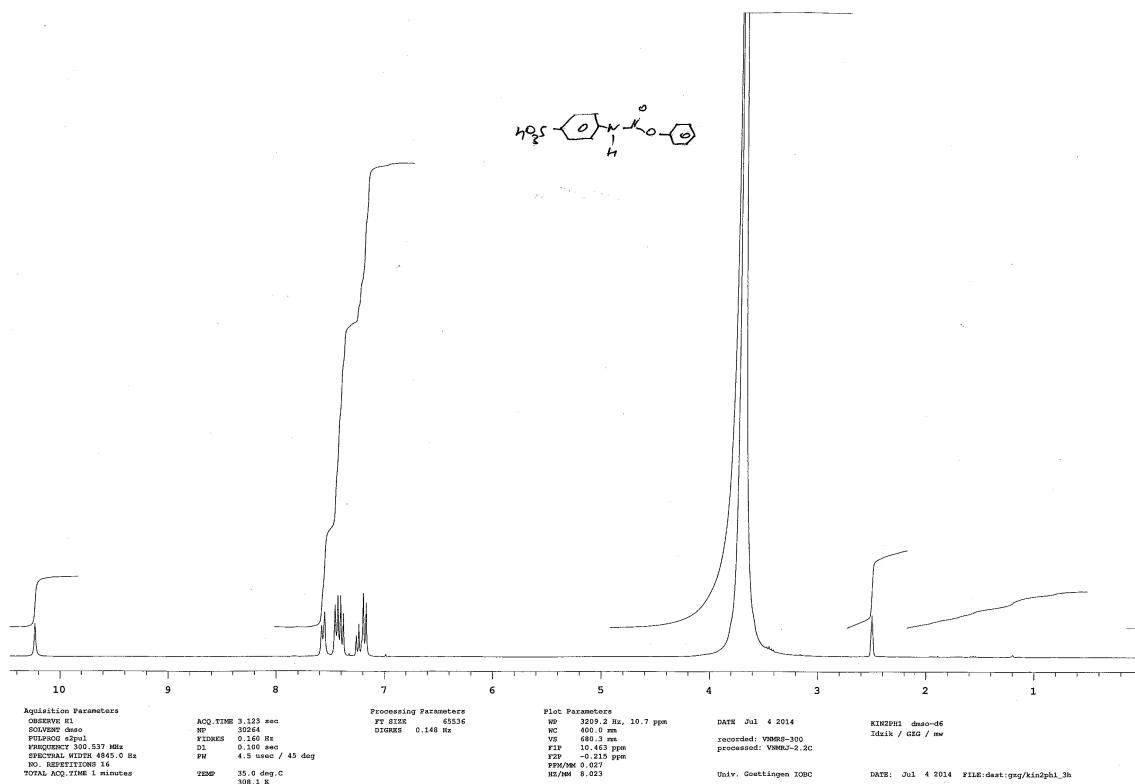


Figure S1. $^1\text{H-NMR}$ spectrum of 4-[(phenoxy carbonyl)amino]benzenesulfonic (**1**). $^1\text{H-NMR}$ (300 MHz, DMSO- d_6) δ , ppm, 10.23 (s, 1H), 7.57 (d, J = 8.1 Hz, 2H), 7.44 (d, J = 7.8 Hz, 2H), 7.39 (d, J = 7.8 Hz, 2H), 7.24 (t, J = 7.4 Hz, 1H), 7.18 (d, J = 7.8 Hz, 2H).

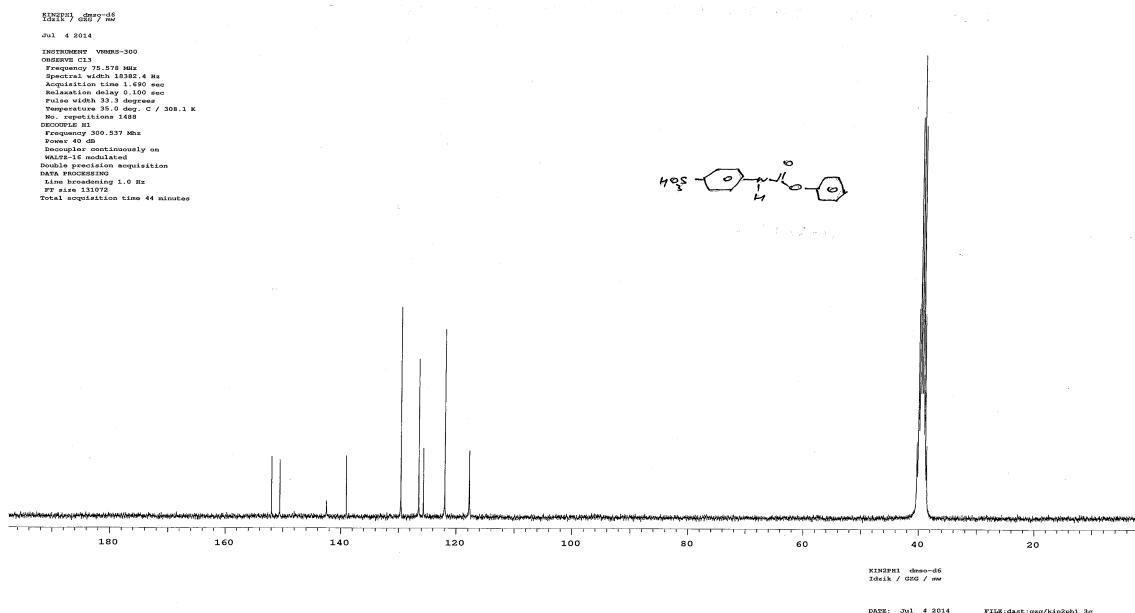


Figure S2. ^{13}C -NMR spectrum of 4-[(phenoxy carbonyl)amino]benzenesulfonic (**1**). ^{13}C -NMR (300 MHz, DMSO- d_6) δ , ppm, 151.93, 150.52, 142.48, 139.05, 129.58, 126.48, 125.65, 121.96, 117.76.

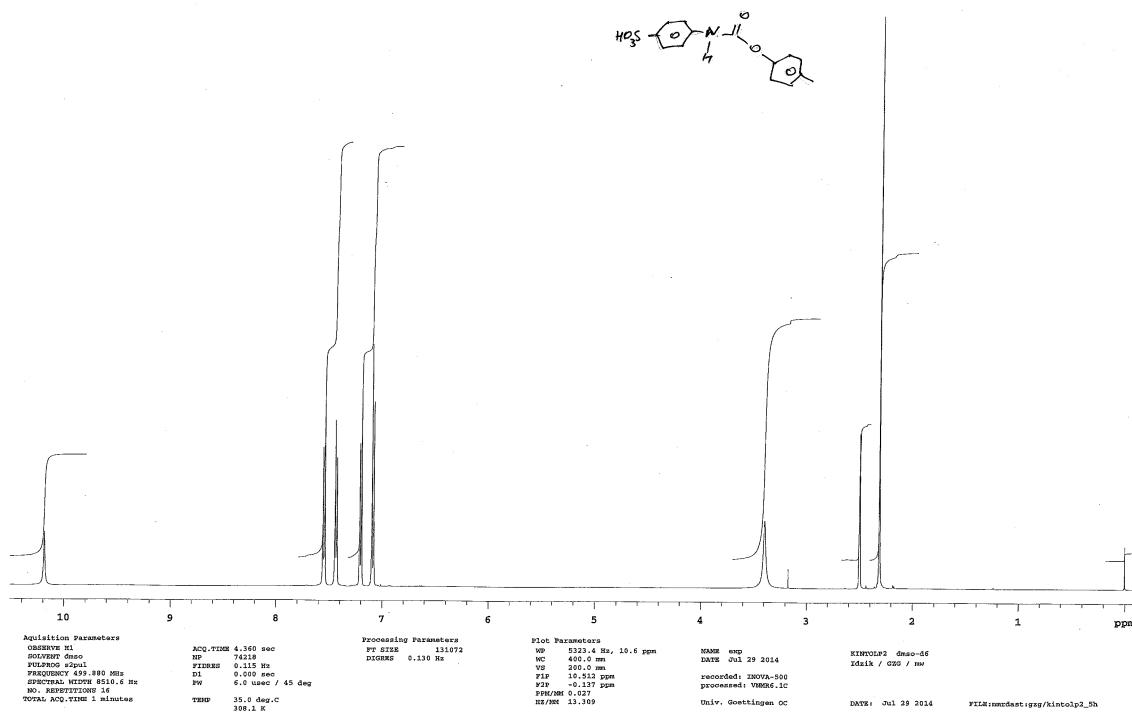


Figure S3. ¹H-NMR spectrum of 4-{[(4-methylphenoxy)carbonyl]amino}benzenesulfonic acid (**2**). ¹H-NMR (300 MHz, DMSO-*d*₆) δ , ppm, 10.19 (s, 1H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 2.31 (s, 3H).

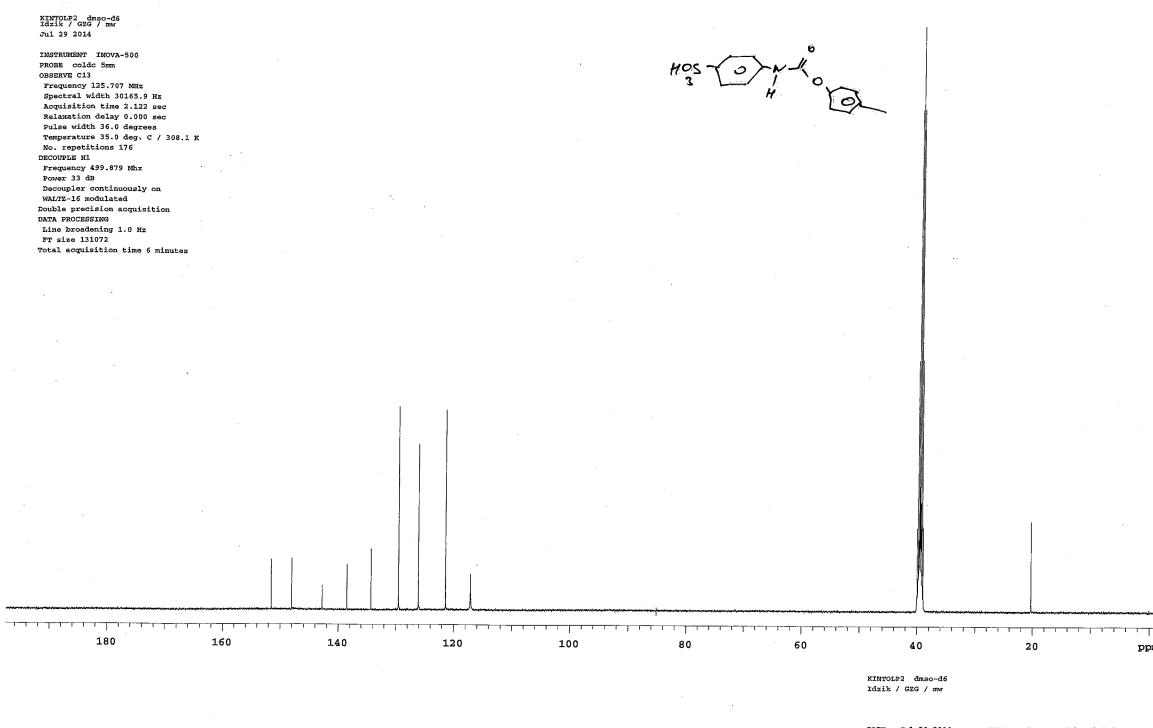


Figure S4. ¹³C-NMR spectrum of 4-{[(4-methylphenoxy)carbonyl]amino}benzenesulfonic acid (**2**). ¹³C-NMR (300 MHz, DMSO-*d*₆) δ , ppm, 151.54, 148.02, 142.79, 138.49, 134.29, 129.49, 126.07, 121.38, 117.15, 20.30.

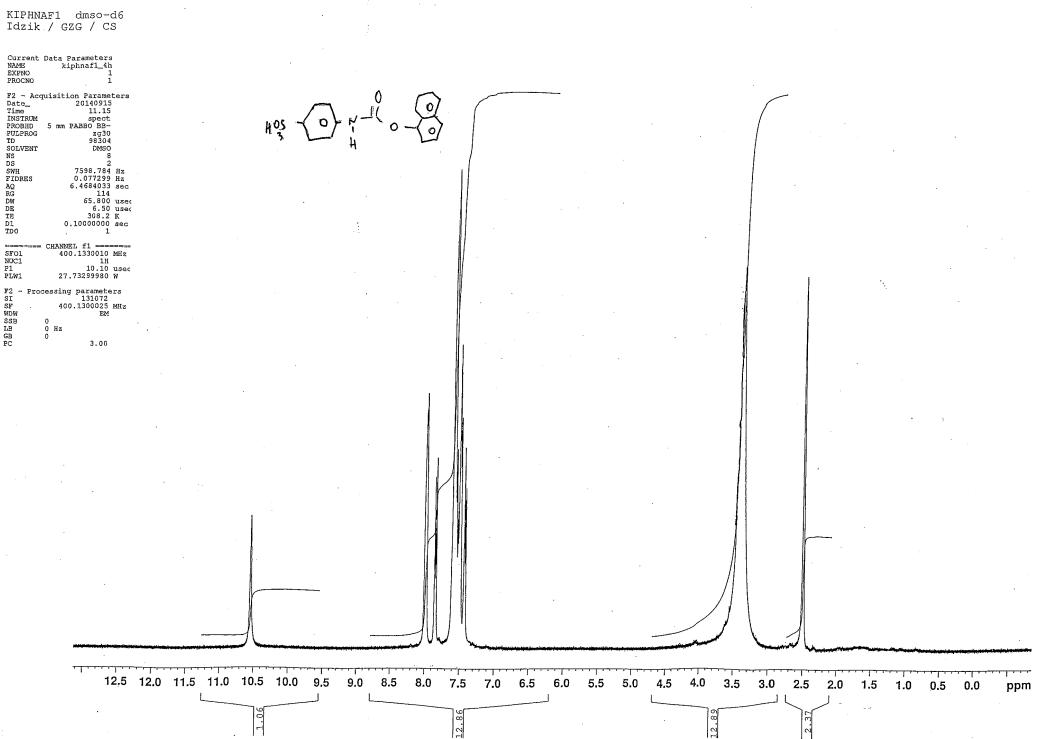


Figure S5. ^1H -NMR spectrum of 4-[(naphthalen-1-yloxy)carbonyl]amino}benzenesulfonic acid (**3**). ^1H -NMR (300 MHz, DMSO-*d*₆) δ , ppm, 10.53 (s, 1H), 8.08–7.96 (m, 2H), 7.86 (d, J = 8.0 Hz, 2H), 7.69–7.49 (m, 5H), 7.43 (d, J = 7.6 Hz, 2H).

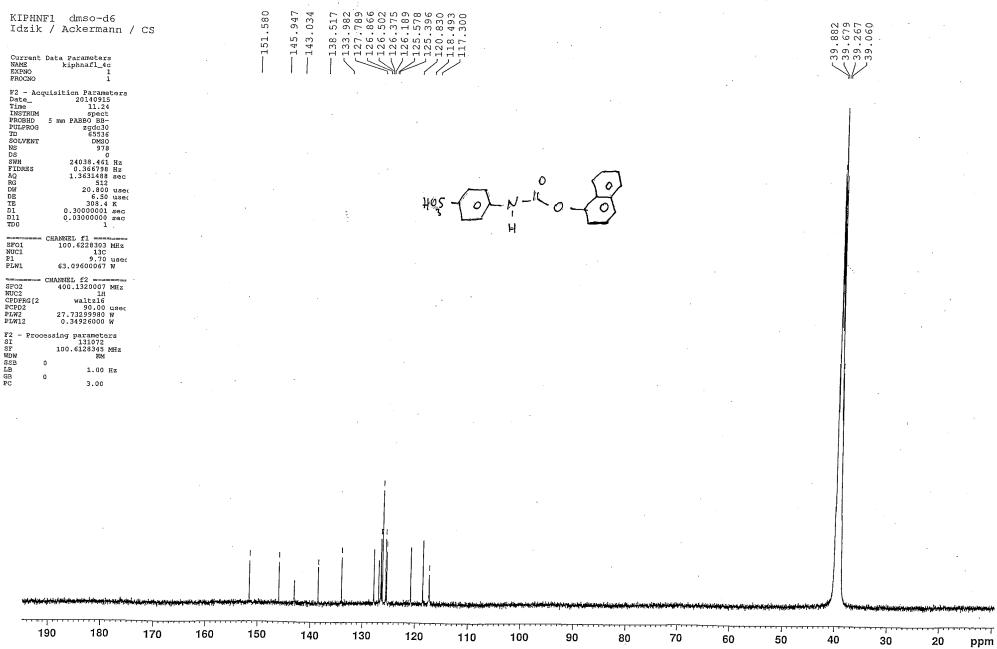


Figure S6. ^{13}C -NMR Spectrum of 4-[(naphthalen-1-yloxy)carbonyl]amino}benzenesulfonic acid (**3**). ^{13}C -NMR (300 MHz, DMSO-*d*₆) δ , ppm, 151.59, 145.96, 143.05, 138.53, 133.99, 127.80, 126.88, 126.51, 126.39, 126.20, 125.59, 125.41, 120.84, 118.51, 117.31.

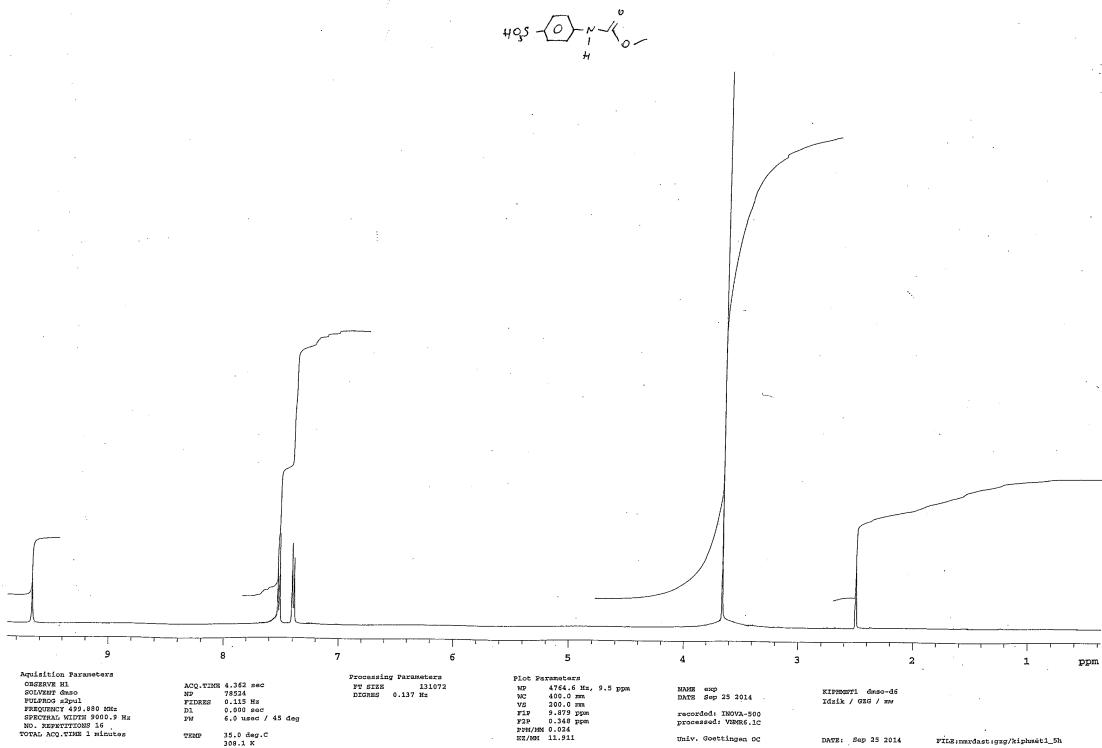


Figure S7. ^1H -NMR spectrum of 4-[(methoxycarbonyl)amino]benzenesulfonic acid (**4**). ^1H -NMR (300 MHz, DMSO- d_6) δ , ppm, 9.67 (s, 1H), 7.52 (d, J = 8.5 Hz, 2H), 7.39 (d, J = 8.5 Hz, 2H), 3.66 (s, 3H).

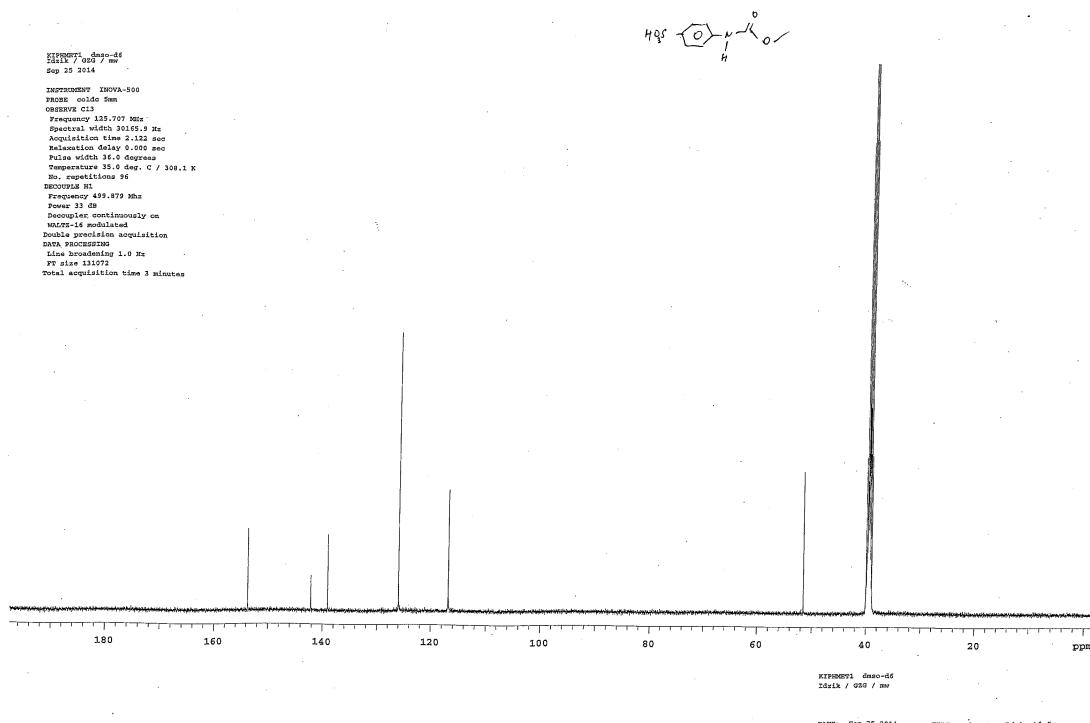


Figure S8. ^{13}C -NMR spectrum of 4-[(methoxycarbonyl)amino]benzenesulfonic acid (**4**). ^{13}C -NMR (300 MHz, DMSO- d_6) δ , ppm, 153.70, 142.13, 139.05, 125.99, 116.84, 51.53.

KIPPRN2 dmso-d₆
Idzik / GZG / CS

Current Data Parameters
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PROCNO 1
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TD0 1

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D1C 1H

P1 10.000 usec

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F2 - Processing parameters

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SF 400.1330016 Hz

NM 1

SSB 0

LB 0 Hz

Gh 0

PC 3.00

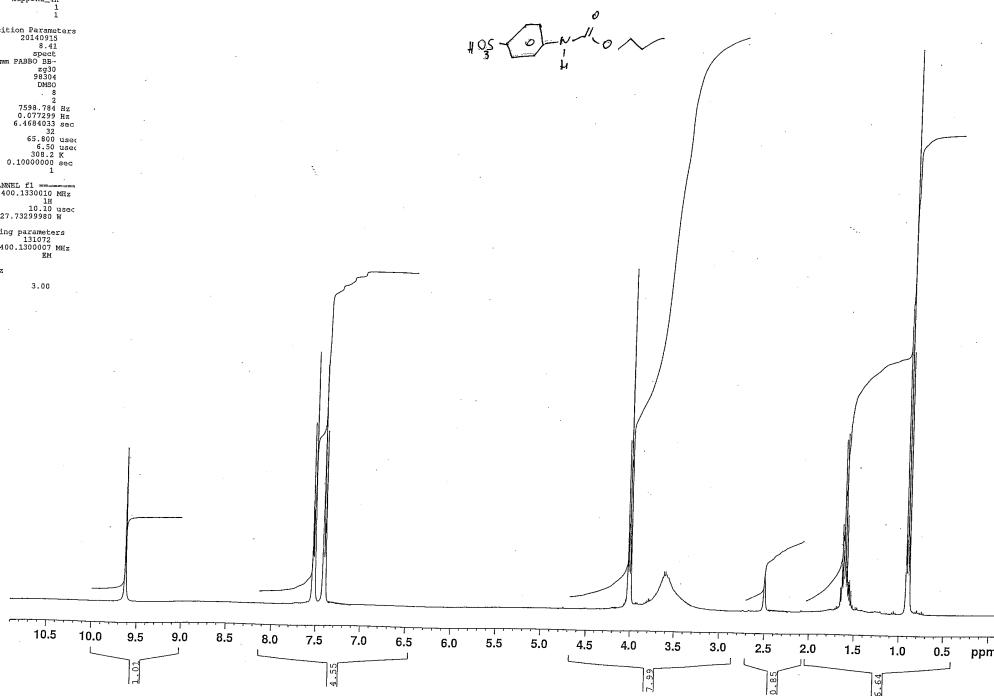


Figure S9. ¹H-NMR spectrum of 4-[(propoxycarbonyl)amino]benzenesulfonic acid (**5**). ¹H-NMR (300 MHz, DMSO-*d*₆) δ, ppm, 9.63 (s, 1H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 4.01 (t, *J* = 6.6 Hz, 2H), 1.65–1.56 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H).

KIPPRN2 dmso-d₆
Idzik / Ackermann / CS

Current Data Parameters
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PROCNO 1
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D1C 1H

P1 9.70 usec

PL1 43.0960000 W

CHANNEL FID

SFO2 130.6238303 MHz

D1C 13C

P1 1.00 usec

PL1 27.7329980 W

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F2 - Processing parameters

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PC 3.00

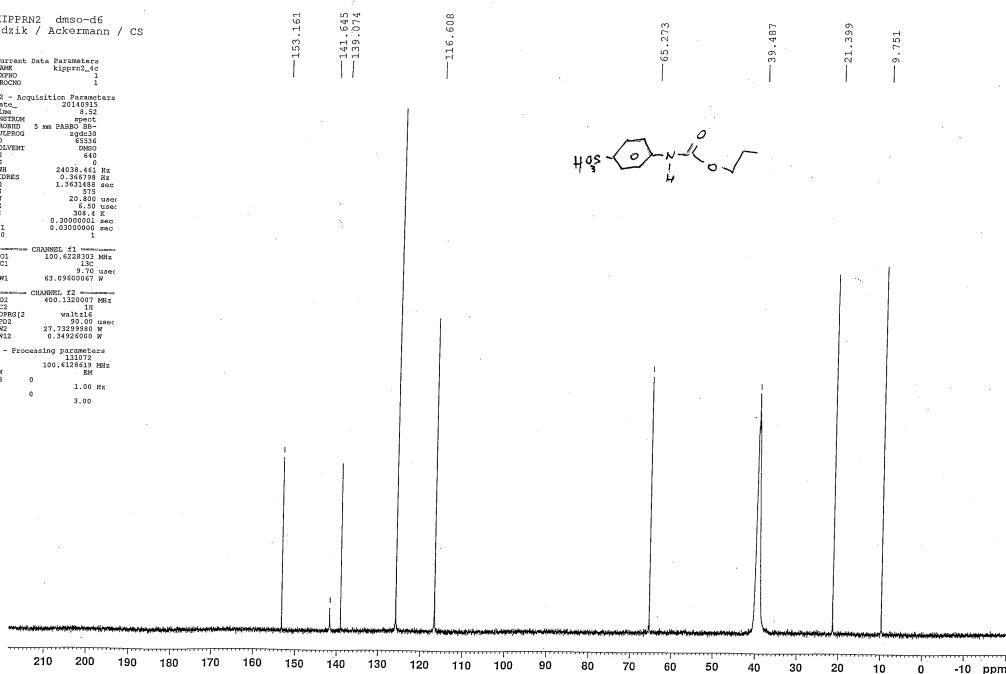


Figure S10. ¹³C-NMR spectrum of 4-[(propoxycarbonyl)amino]benzenesulfonic acid (**5**). ¹³C-NMR (300 MHz, DMSO-*d*₆) δ, ppm, 153.17, 141.66, 139.08, 125.76, 116.62, 65.29, 21.42, 9.77.

KITPNO dmso-d6
Idzik / GZG / CS

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PULPROG zg30
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SOLVENT DMSO
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FIDRES 0.011912 KHz
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TD0 1

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NUC1 1H
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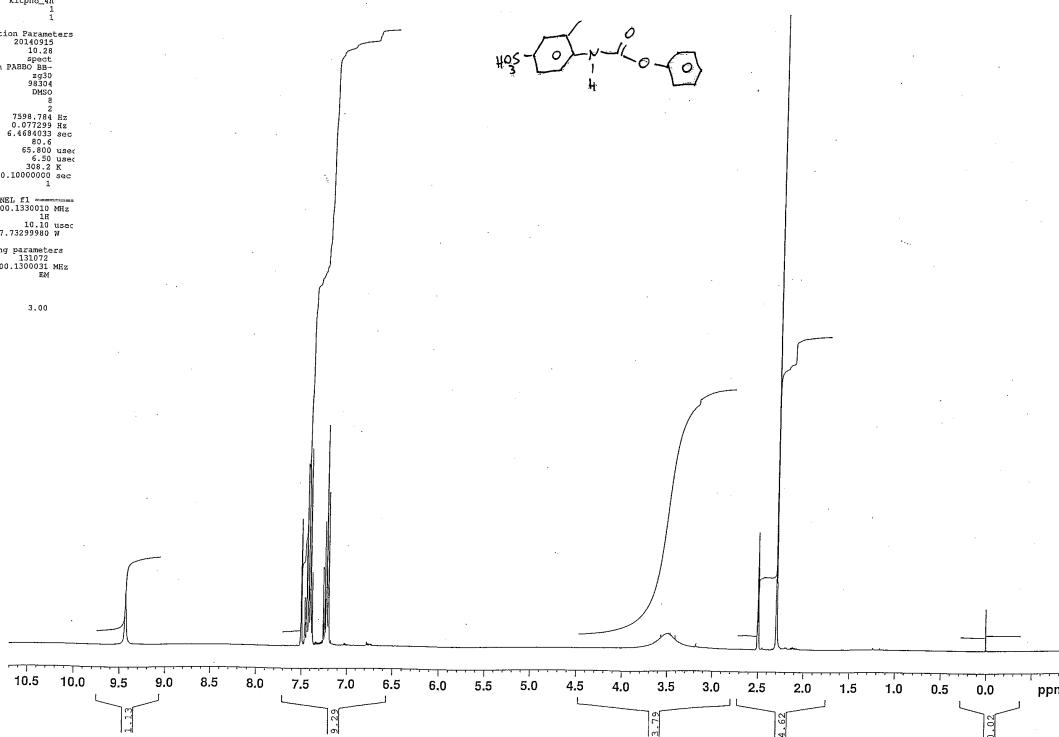


Figure S11. ^1H -NMR spectrum of 3-methyl-4-[(phenoxy carbonyl)amino]benzenesulfonic acid (**6**). ^1H -NMR (300 MHz, DMSO-*d*₆) δ , ppm, 9.41 (s, 1H), 7.47 (s, 1H), 7.42–7.35 (m, 4H), 7.23 (t, J = 6.0 Hz, 1H), 7.20 (d, J = 6.0 Hz, 2H), 2.29 (s, 3H).

KITPNO dmso-d6
Idzik / GZG / CS

Current Data Parameters
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EXPTYP 1
PRCNO 1
F2 - Acquisition Parameters
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Time 10:28
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TD 65536
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RG 20.800
DW 65.0 usec
DE 6.50 usec
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D11 0.3000000 sec
TD0 1

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NUC1 100.6228303 MHz
PC1 9.70 usec
PML1 63.09600067 W

CHANNEL F2
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NUC2 1H
PCP1/2 width 1.0
PCP2/2 90.00 usec
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F2 - Processing parameters
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LB 1.00 Hz
GS 3.00

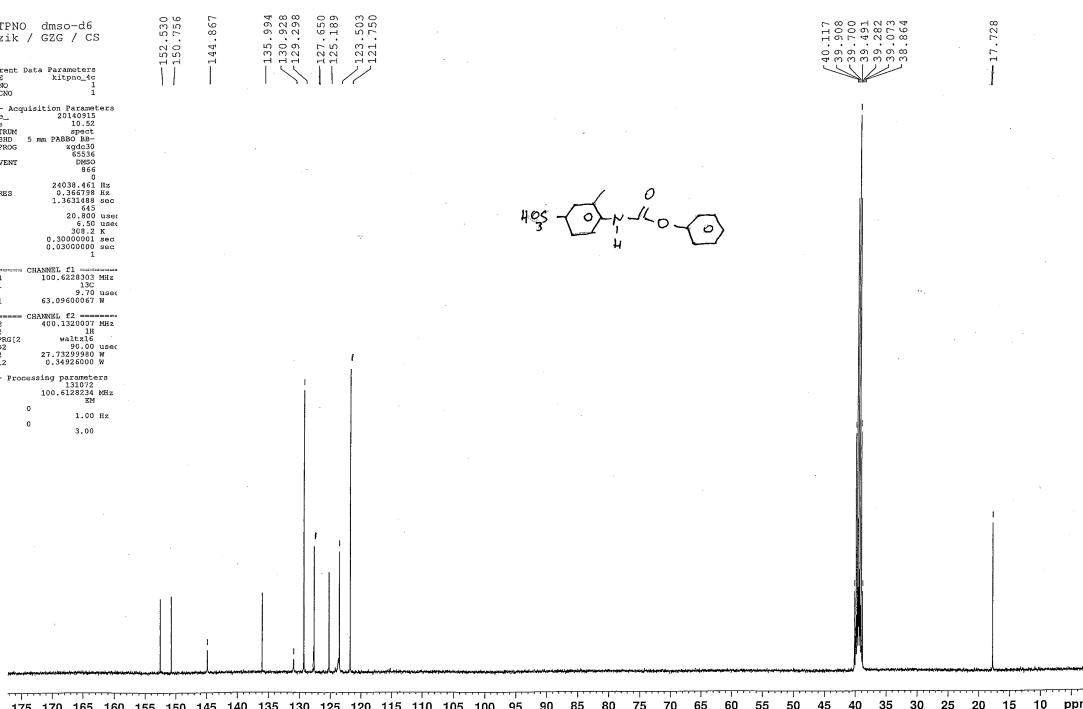


Figure S12. ^{13}C -NMR spectrum of 3-methyl-4-[(phenoxy carbonyl)amino]benzenesulfonic acid (**6**). ^{13}C -NMR (300 MHz, DMSO-*d*₆) δ , ppm, 152.53, 150.76, 144.87, 135.99, 130.93, 129.30, 127.65, 125.19, 124.20, 123.50, 121.75, 17.73.

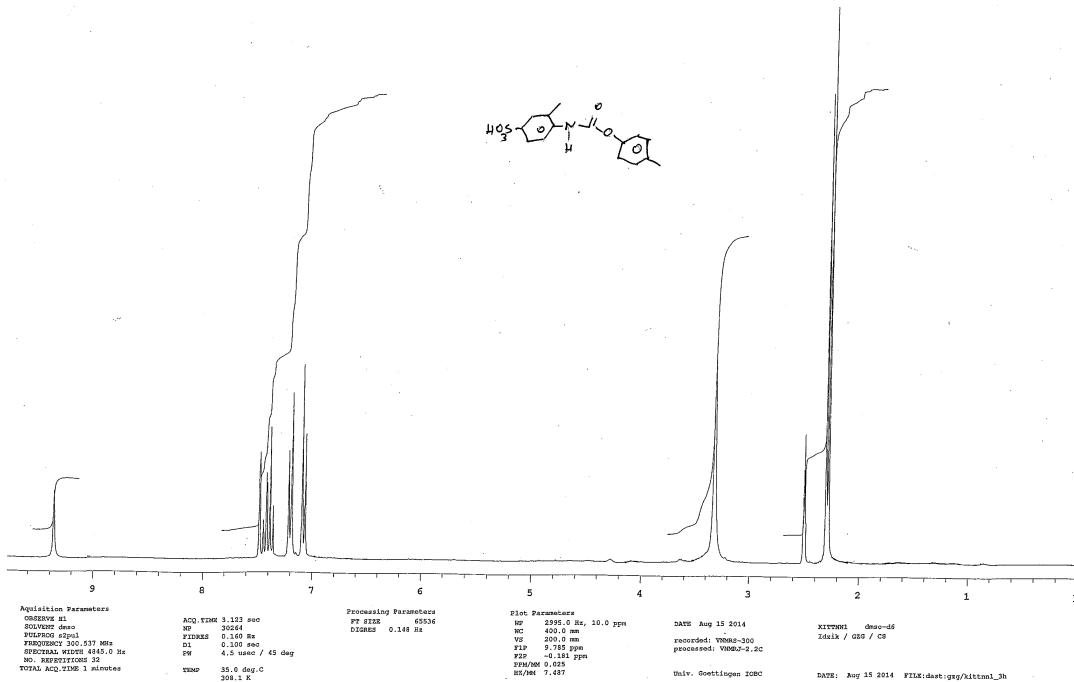


Figure S13. ^1H -NMR spectrum of 3-methyl-4-[(4-methylphenoxy)carbonyl]amino benzenesulfonic acid (**7**). ^1H -NMR (300 MHz, $\text{DMSO}-d_6$) δ , ppm, 9.37 (s, 1H), 7.48 (s, 1H), 7.43 (d, J = 8.4 Hz, 1H), 7.37 (d, J = 8.4 Hz, 1H), 7.21 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 8.4 Hz, 2H), 2.31 (s, 3H), 2.28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

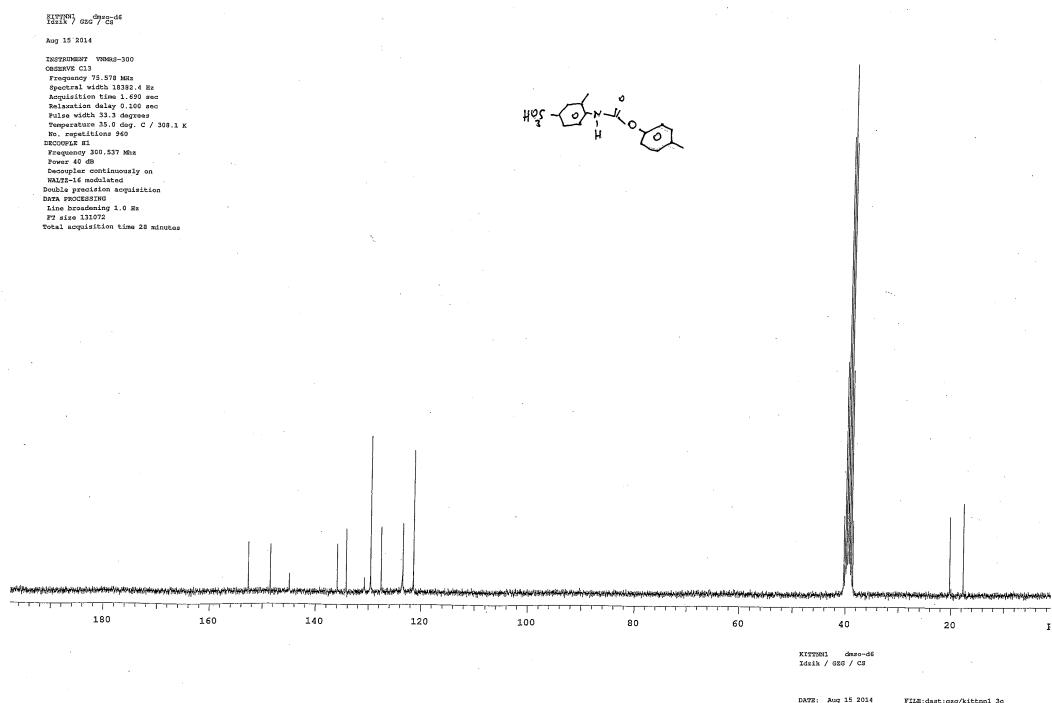
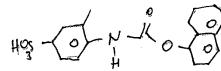


Figure S14. ^{13}C -NMR spectrum of 3-methyl-4-[(4-methylphenoxy)carbonyl]amino benzenesulfonic acid (**7**). ^{13}C -NMR (300 MHz, $\text{DMSO}-d_6$) δ , ppm, 152.62, 148.50, 144.96, 135.92, 134.24, 130.76, 129.58, 127.58, 123.56, 123.43, 121.43, 20.26, 17.69.

KITOLNAL dmso-d₆
Idzik / GZG / CS

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DW: 65.000 usec
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TE: 399.8 K
D1: 0.1000000 sec
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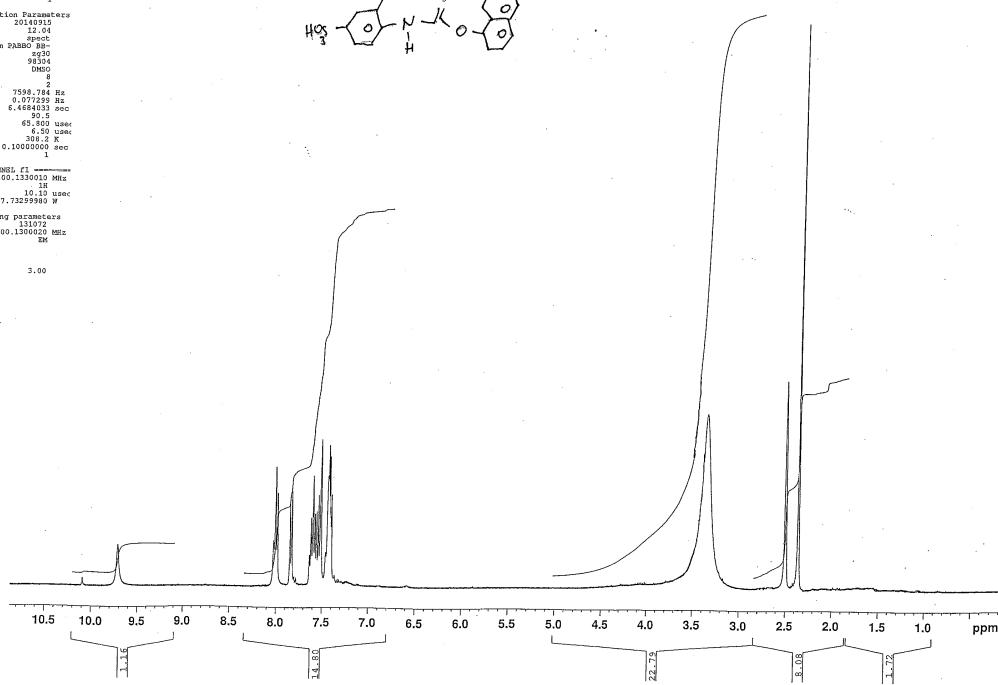
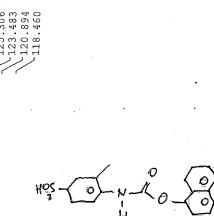


Figure S15. ¹H-NMR spectrum of 3-methyl-4-[(naphthalen-1-yloxy)carbonyl]amino benzenesulfonic acid (**8**). ¹H-NMR (300 MHz, DMSO-*d*₆) δ, ppm, 9.72 (s, 1H), 8.03–7.98 (m, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.64–7.52 (m, 4H), 7.46–7.40 (m, 3H), 2.36 (s, 3H).

KITOLNAL dmso-d₆
Idzik / GZG / CS

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PROCNO: 1
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SWH: 24030.403 Hz
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AQ: 1.000000 sec
RG: 515
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TDR: 1



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SF: 100.6258303 MHz
NUC1: 13C
NUC2: 1H
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PCPQ2: 27.33290000 usec
PLM1: 0.34926000 W
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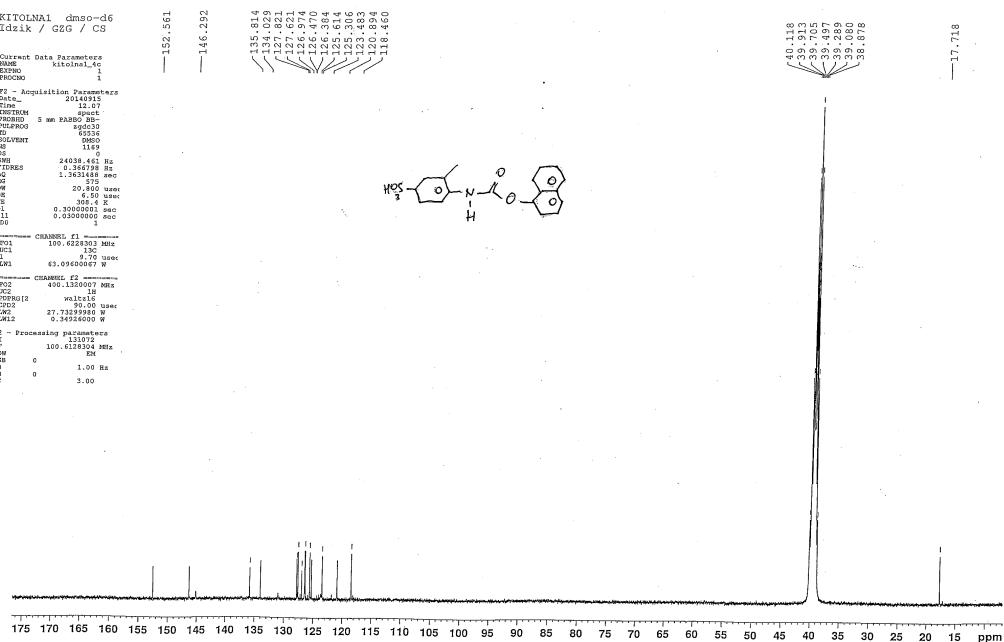


Figure S16. ¹³C-NMR spectrum of 3-methyl-4-[(naphthalen-1-yloxy)carbonyl]amino benzenesulfonic acid (**8**). ¹³C-NMR (300 MHz, DMSO-*d*₆) δ, ppm, 152.57, 146.30, 145.14, 135.83, 134.04, 130.99, 127.83, 127.63, 126.99, 126.48, 126.40, 125.63, 125.32, 124.07, 123.50, 120.91, 118.47, 17.74.

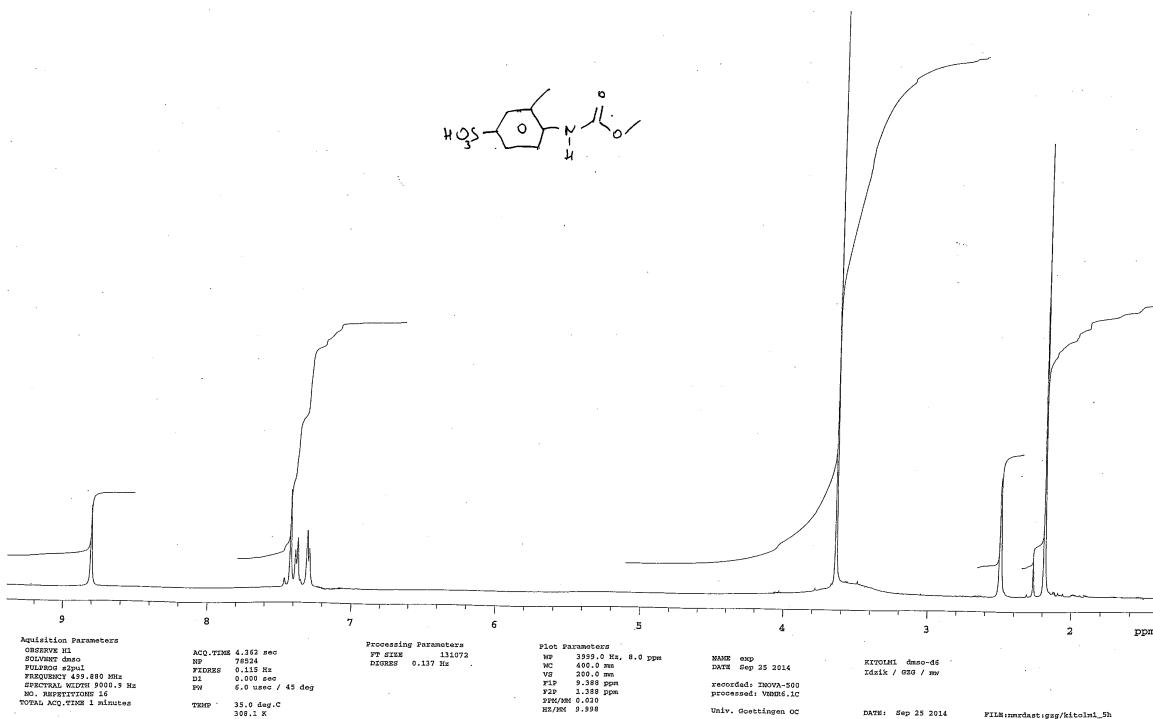


Figure S17. ^1H -NMR spectrum of 4-[(methoxycarbonyl)amino]-3-methylbenzenesulfonic acid (**9**). ^1H -NMR (300 MHz, DMSO- d_6) δ , ppm, 8.80 (s, 1H), 7.42 (s, 1H), 7.38 (d, J = 7.5 Hz, 1H), 7.30 (d, J = 7.5 Hz, 1H), 3.64 (s, 3H), 2.19 (s, 3H).

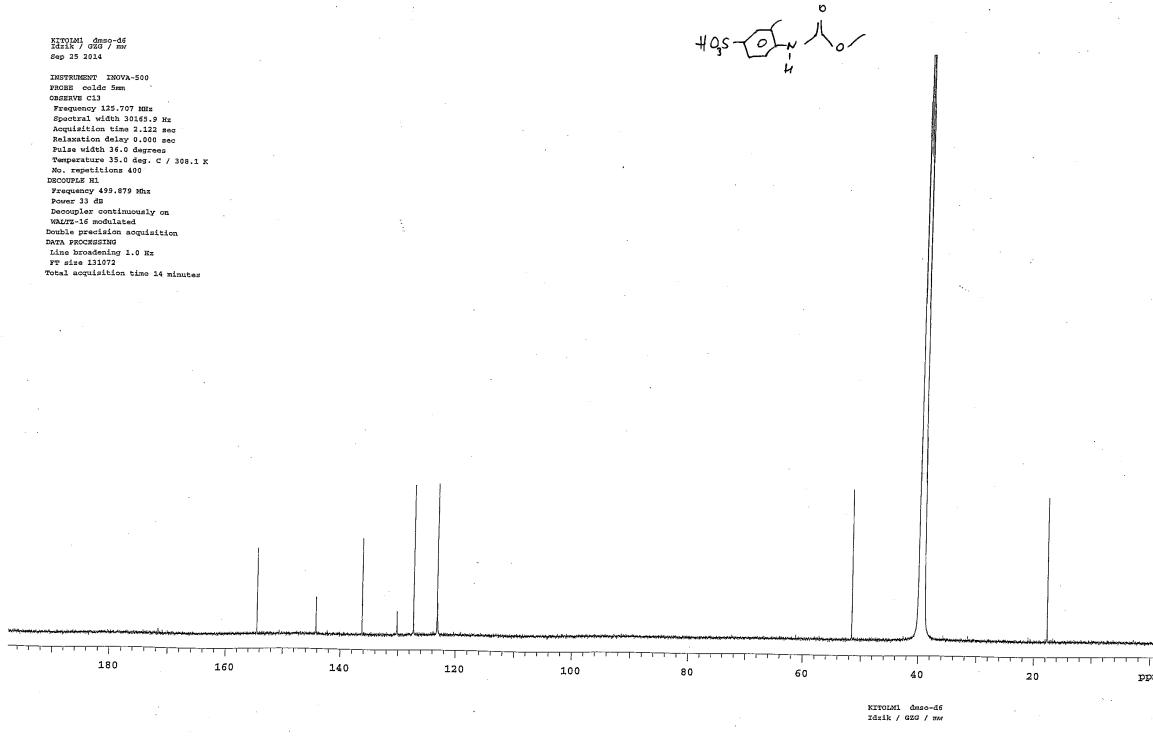


Figure S18. ^{13}C -NMR spectrum of 4-[(methoxycarbonyl)amino]-3-methylbenzenesulfonic acid (**9**). ^{13}C -NMR (300 MHz, DMSO- d_6) δ , ppm, 154.47, 144.23, 136.26, 130.17, 127.31, 123.20, 123.10, 51.56, 17.68.

KITOLPR2 dmso-d6
Idzik / GZG / CS

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RG 1000
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TDC 0.1000000 sec

CHANNEL F1
SF01 400.1330000 MHz
NUC1 1H
P1 10.10 usec
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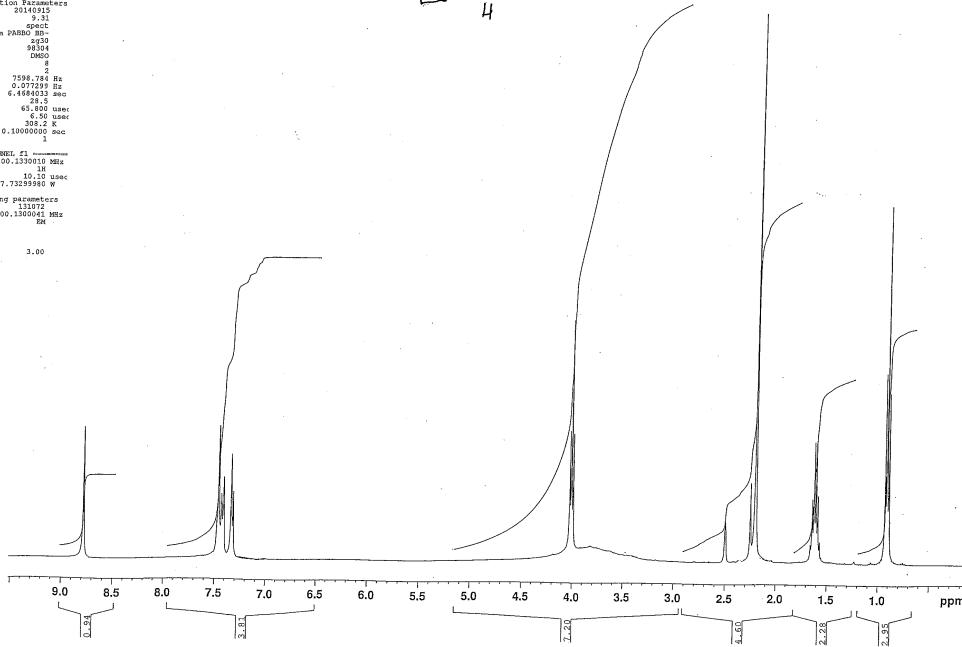
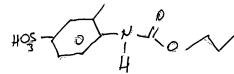


Figure S19. ^1H -NMR spectrum of 3-methyl-4-[(propoxycarbonyl)amino]benzenesulfonic acid (**10**). ^1H -NMR (300 MHz, DMSO-*d*₆) δ , ppm, 8.78 (s, 1H), 7.46 (s, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 4.01 (t, *J* = 6.6 Hz, 2H), 2.20 (s, 3H), 1.66–1.57 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H).

KITOLPR2 dmso-d6
Idzik / GZG / CS

Current Data Parameters
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PROLOG 1

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D11 0.3500000 sec
TDC 0.3500000 sec

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P1 9.70 usec
TML1 63.096300007 W

CHANNEL F2
SF02 400.1320007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCP[2] 90.00 usec
GAMMA 27.332000000 W
TML2 0.34326000 W

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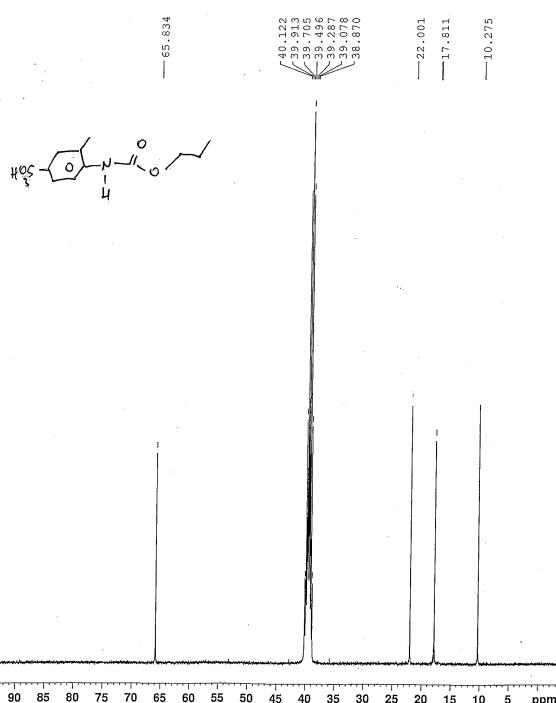


Figure S20. ^{13}C -NMR spectrum of 3-methyl-4-[(propoxycarbonyl)amino]benzenesulfonic acid (**10**). ^{13}C -NMR (300 MHz, DMSO-*d*₆) δ , ppm, 154.52, 143.90, 136.92, 130.63, 127.64, 124.35, 123.51, 65.85, 22.02, 17.83, 10.30.