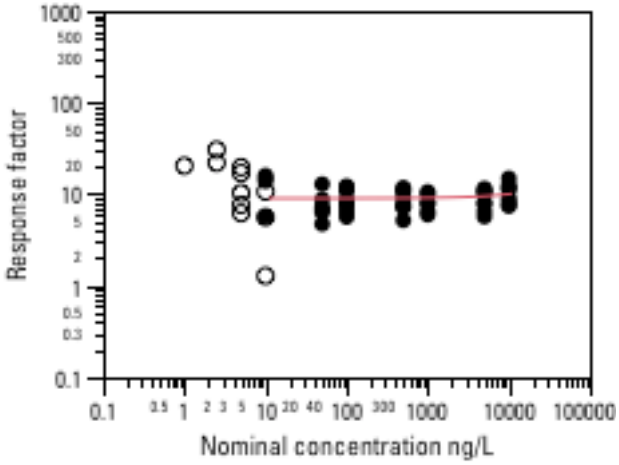
Support Figure S4. Response Factors as a Function of Concentration

Graphs of response factor (peak area/nominal concentration) and parameters of linear fit of response factor by nominal concentration for direct aqueous-injection liquid chromatography-tandem mass spectrometry (LC-MS/MS) method negative electrospray ionization (ESI-) mode analytes. The response factors (peak area divided by nominal concentration) were measured as a function of concentration to evaluate any significant change in response as a function of concentration. In addition, the response factors provide an indication of the magnitude of the signal in electrospray ionization that reflects detection levels, with higher response factors leading to lower detection levels. Response factors were calculated from 10 calibration standards (1, 2.5, 5, 10, 50, 100, 500, 1,000, 5,000, and 10,000 nanograms per liter [ng/L]) analyzed in eight batches. A liner fit (red line) was applied to the response factors as a function of concentration. Response factors were excluded from the linear fit and summaries if the calibration standard was excluded from the calibration curve because qualifier ion response did not meet identification criteria (shown as open circles in the figures).

Bivariate Fit of Response Factor by Nominal Concentration (ng/L)—Negative ESI Analytes

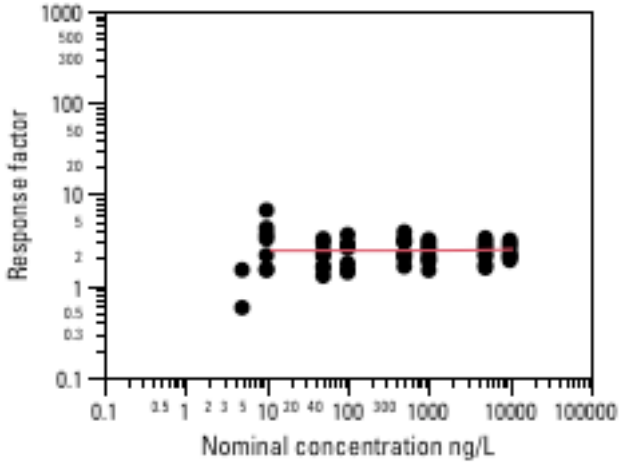
Acetanilide and Amide

Parent=Acetochlor, Compound Name=Acetochlor OA



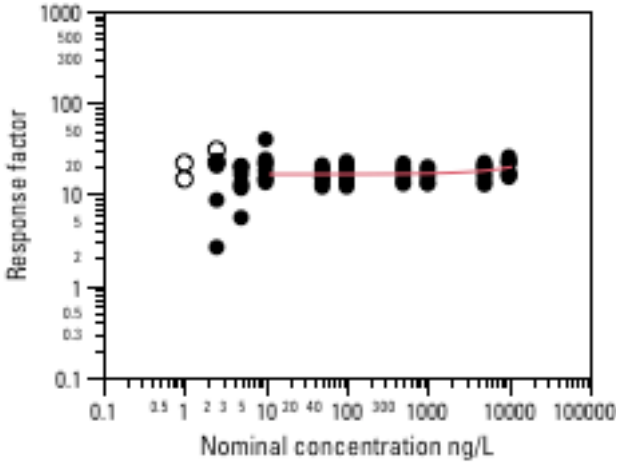
Linear fit: Response factor = 9.0180289 + 0.0001012*Nominal concentration ng/L

Parent=Acetochlor, Compound Name=Acetochlor SAA



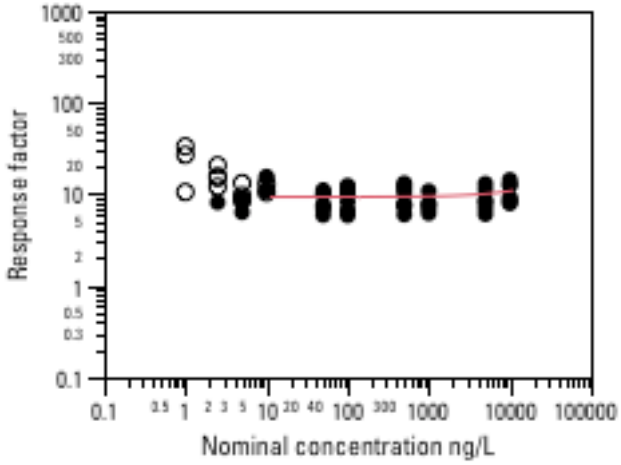
Linear fit: Response factor = 2.4167991 + 8.0477e-6*Nominal concentration ng/L

Parent=Acetochlor, Compound Name=Acetochlor SA



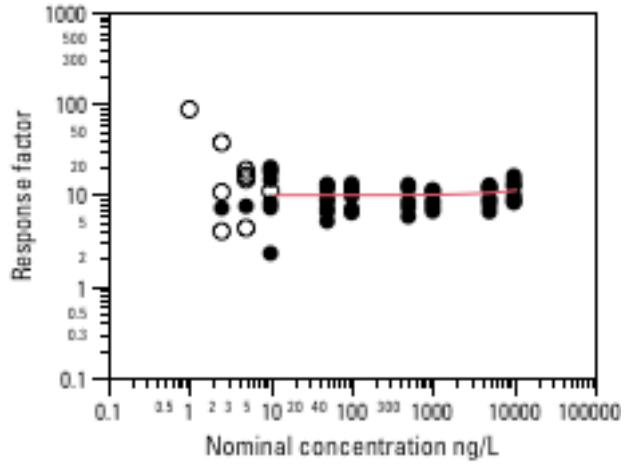
Linear fit: Response factor = 16.509112 + 0.0003067*Nominal concentration ng/L

Parent=Acetochlor/Metolachlor, Compound Name=sec-Acetochlor-OA



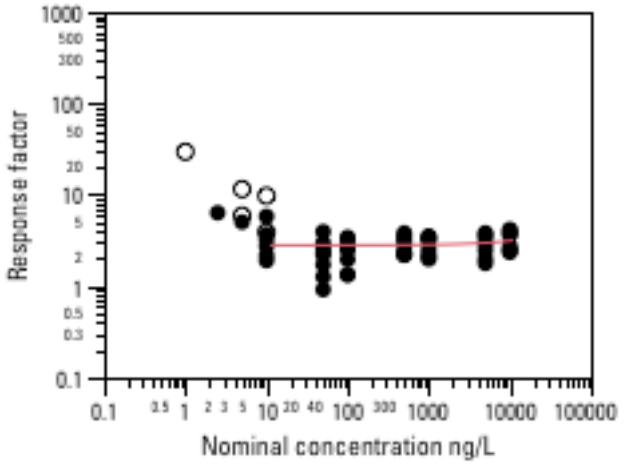
Linear fit: Response factor = 9.3276576 + 0.0001502*Nominal concentration ng/L

Parent=Alachlor, Compound Name=Alachlor OA



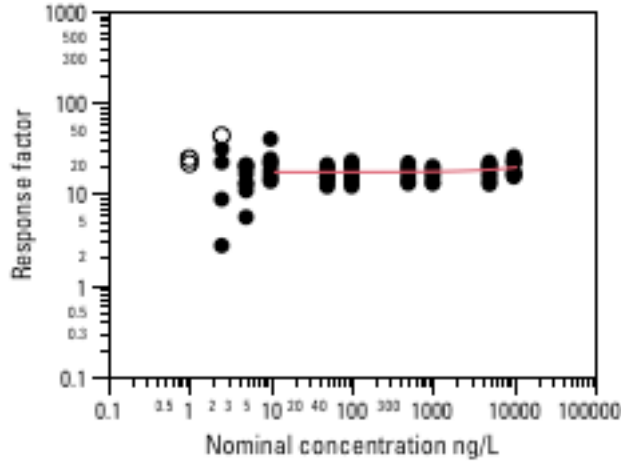
Linear fit: Response factor = 9.8778787 + 0.0001242*Nominal concentration ng/L

Parent=Alachlor, Compound Name=Alachlor SAA



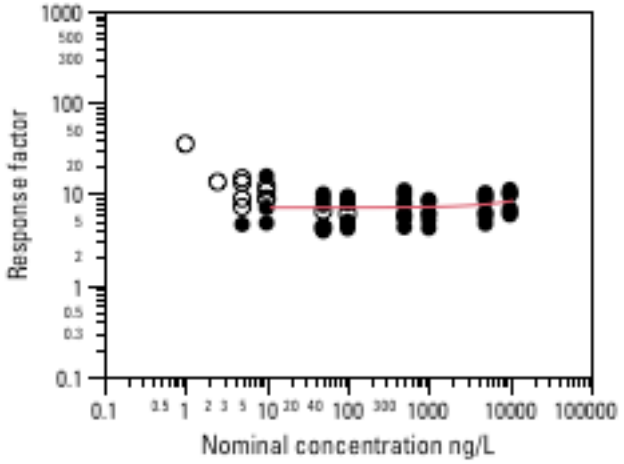
Linear fit: Response factor = 2.811491 + 3.3216e-5*Nominal concentration ng/L

Parent=Alachlor, Compound Name=Alachlor SA



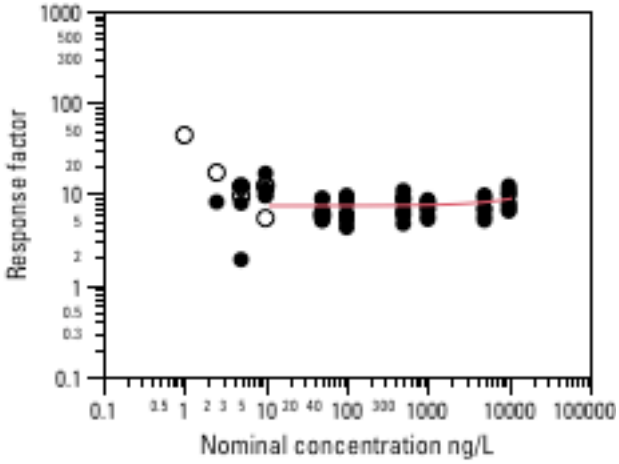
Linear fit: Response factor = 17.274964 + 0.0002057*Nominal concentration ng/L

Parent=Alachlor, Compound Name=sec-Alachlor-OA



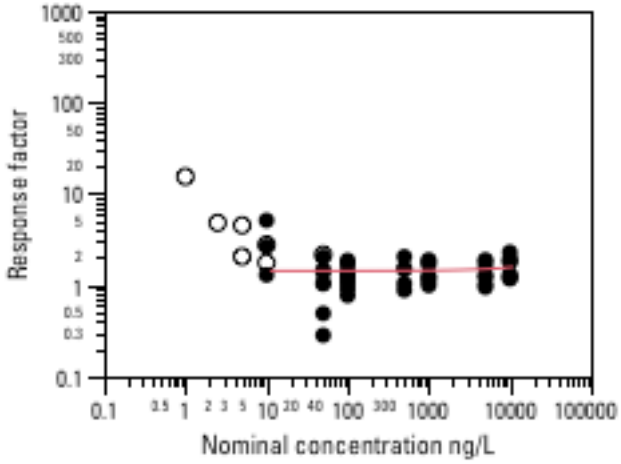
Linear fit: Response factor = 7.0586355 + 0.0001197*Nominal concentration ng/L

Parent=Dimethenamid, Compound Name=Dimethenamid OA



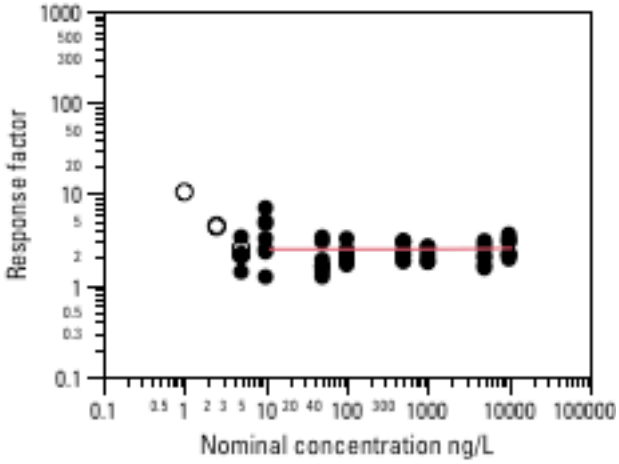
Linear fit: Response factor = 7.3965566 + 0.0001381*Nominal concentration ng/L

Parent=Dimethenamid, Compound Name=Dimethenamid SAA



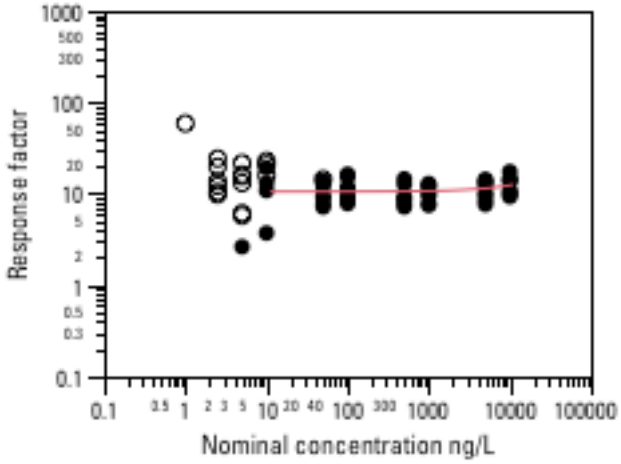
Linear fit: Response factor = 1.4345268 + 1.3388e-5*Nominal concentration ng/L

Parent=Dimethenamid, Compound Name=Dimethenamid SA



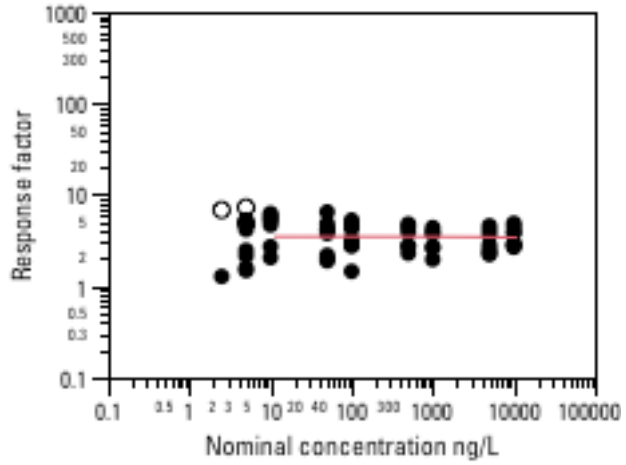
Linear fit: Response factor = 2.4733514 + 6.4868e-6*Nominal concentration ng/L

Parent=Metolachlor, Compound Name=Metolachlor OA



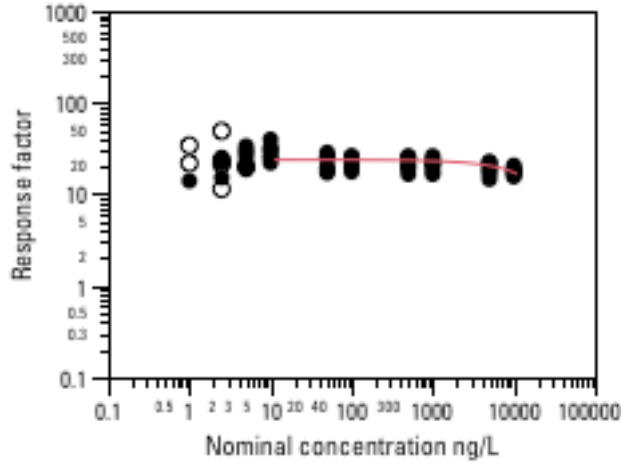
Linear fit: Response factor = 10.552749 + 0.0001852*Nominal concentration ng/L

Parent=Metolachlor, Compound Name=Metolachlor SA



Linear fit: Response factor = 3.4880535 - 8.112e-6*Nominal concentration ng/L

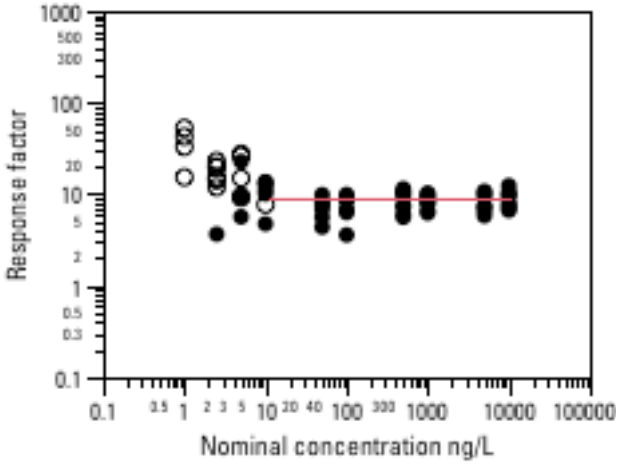
Parent=Propanil, Compound Name=Propanil



Linear fit: Response factor = 23.684095 - 0.0006421*Nominal concentration ng/L

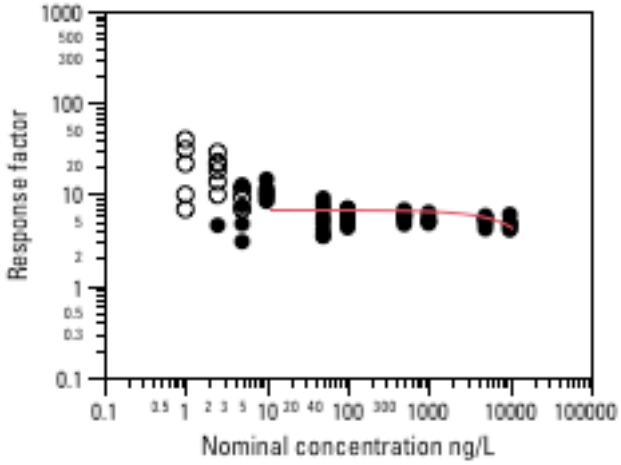
Acid

Parent=2,4-D, Compound Name=2,4-D



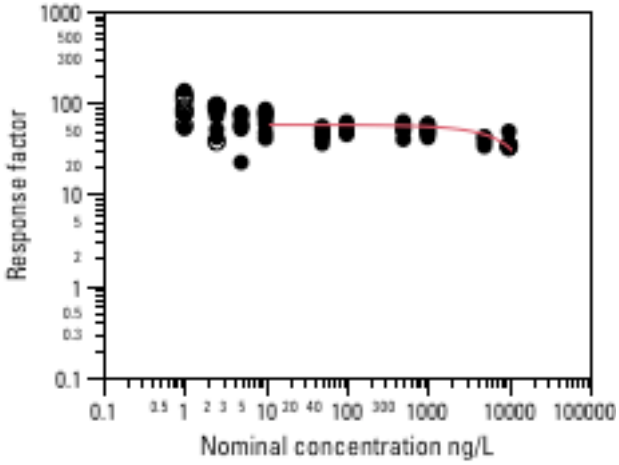
Linear fit: Response factor = 8.7776397 - 6.5279e-6*Nominal concentration ng/L

Parent=Bromoxynil, Compound Name=Bromoxynil



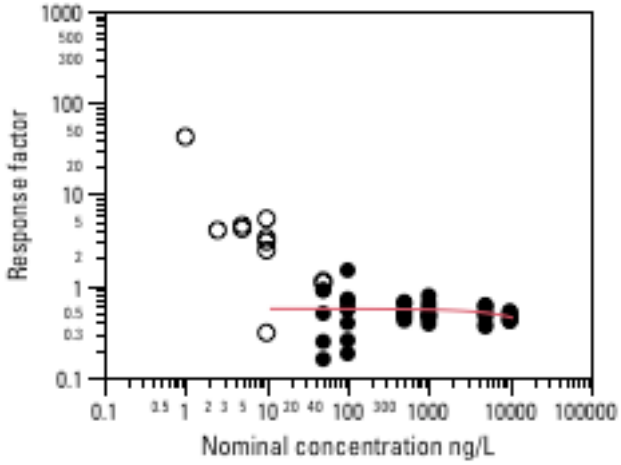
Linear fit: Response factor = 6.6815492 - 0.0002248*Nominal concentration ng/L

Parent=Bentazone, Compound Name=Bentazon



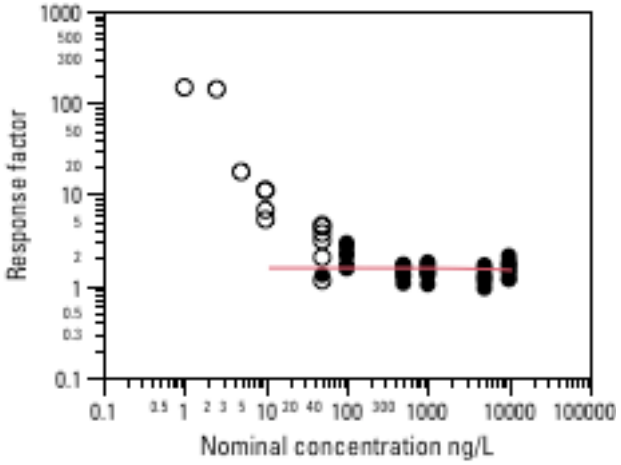
Linear fit: Response factor = 57.12062 - 0.0024534*Nominal concentration ng/L

Parent=Dacthal, Compound Name=Dacthal monoacid



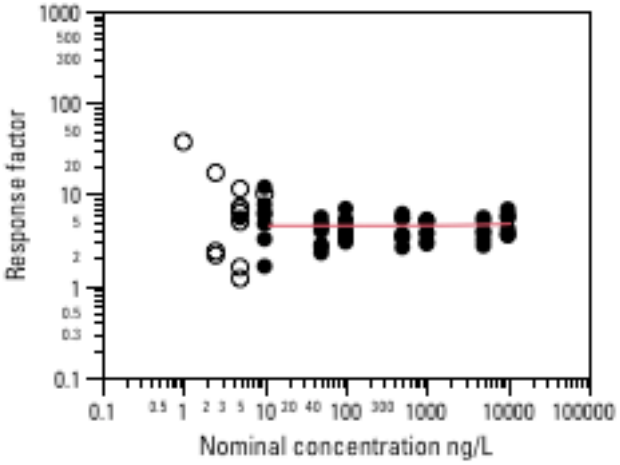
Linear fit: Response factor = 0.5596356 - 1.036e-5*Nominal concentration ng/L

Parent=Dicamba, Compound Name=Dicamba



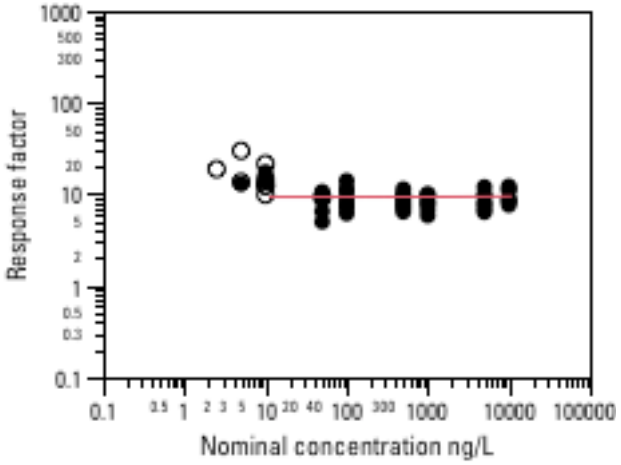
Linear fit: Response factor = 1.5630733 - 7.5905e-6*Nominal concentration ng/L

Parent=Triclopyr, Compound Name=Triclopyr



Linear fit: Response factor = 4.5288961 + 1.9814e-5*Nominal concentration ng/L

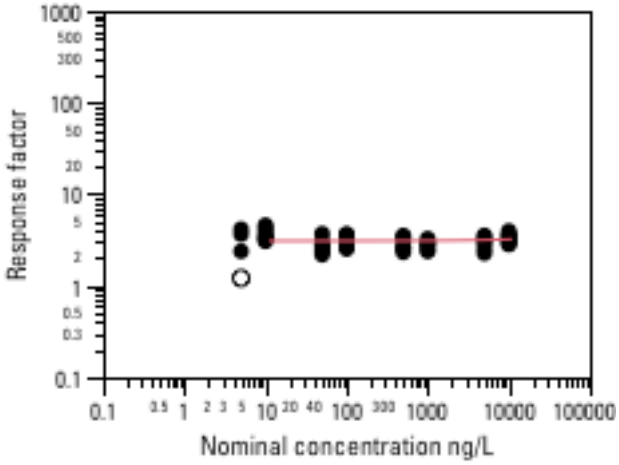
Parent=MCPA, Compound Name=MCPA



Linear fit: Response factor = 9.3300642 + 1.6359e-5*Nominal concentration ng/L

Carbamate and Thiocarbamate

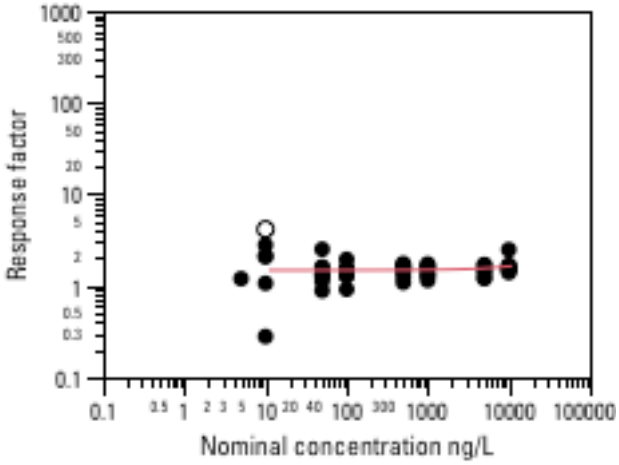
Parent=Triallate, Compound Name=2,3,3-trichloroprop-2-ene-1-SA



Linear fit: Response factor = 3.0895322 + 1.3146e-5*Nominal concentration ng/L

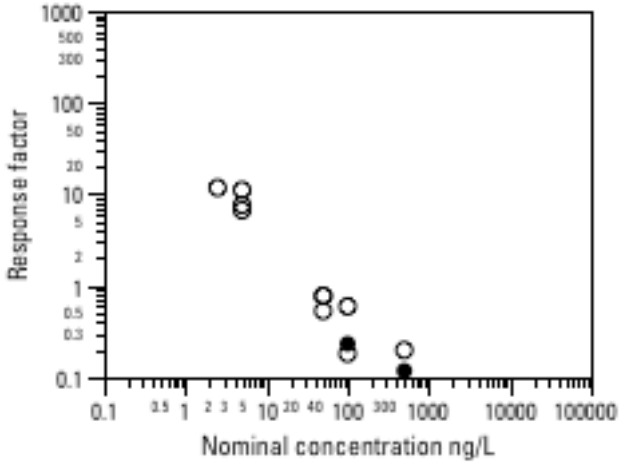
Fungicide

Parent=Chlorothalonil, Compound Name=4-Hydroxychlorothalonil



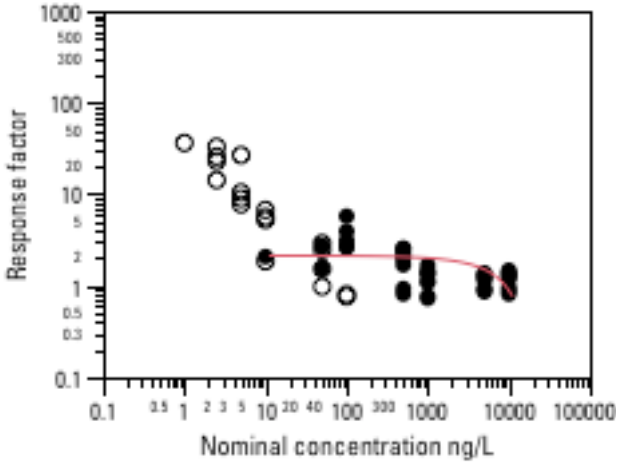
Linear fit: Response factor = 1.4764712 + 1.5613e-5*Nominal concentration ng/L

Parent=Iprodione, Compound Name=Iprodione



Linear fit: Response factor = 0.0727115 - 4.4568e-6*Nominal concentration ng/L

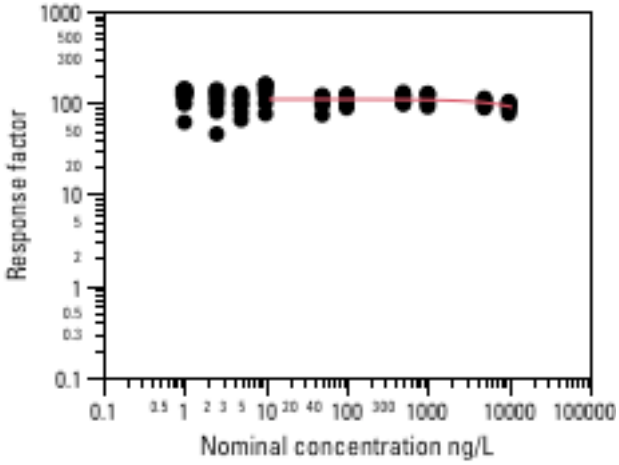
Parent=Iprodione, Compound Name=Deisopropyliprodione



Linear fit: Response factor = 2.1308191 - 0.000124*Nominal concentration ng/L

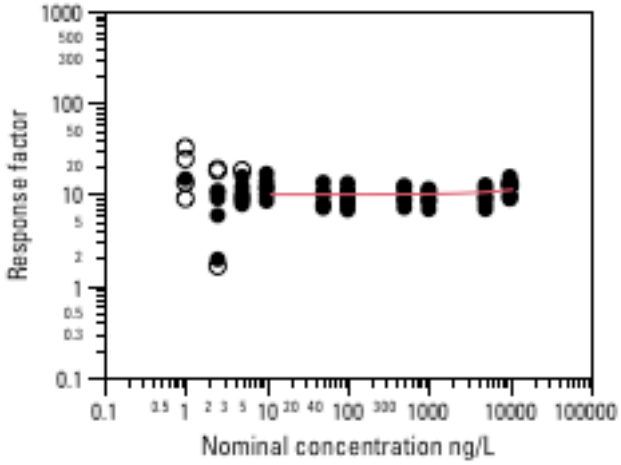
Miscellaneous

Parent=Flubendiamide, Compound Name=Flubendiamide



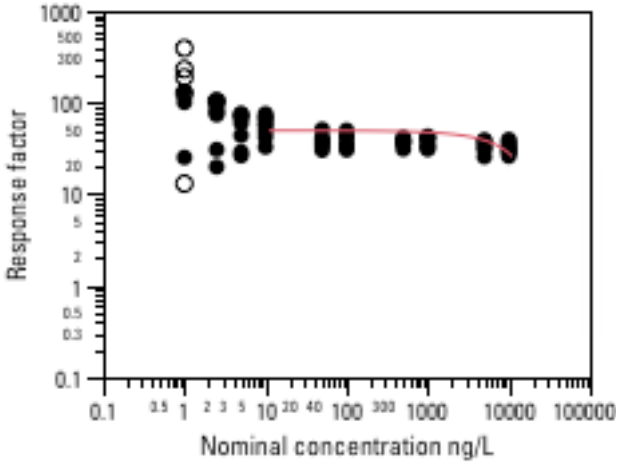
Linear fit: Response factor = 108.80761 - 0.0017728*Nominal concentration ng/L

Parent=Isoxaflutole, Compound Name=Isoxaflutole acid RPA 203328



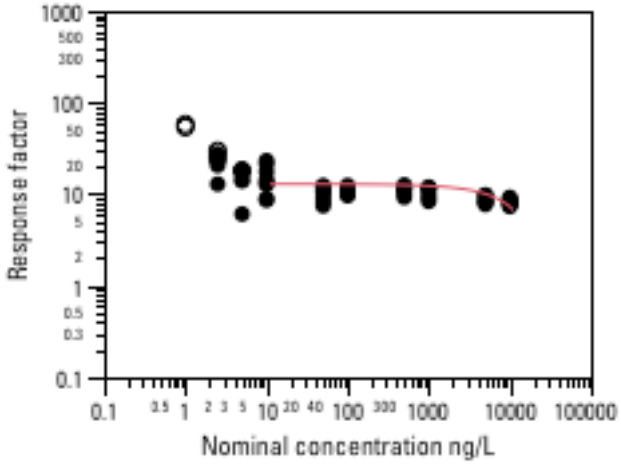
Linear fit: Response factor = 9.9241836 + 0.0001203*Nominal concentration ng/L

Parent=Isoxaflutole, Compound Name=Diketonitrile isoxaflutole



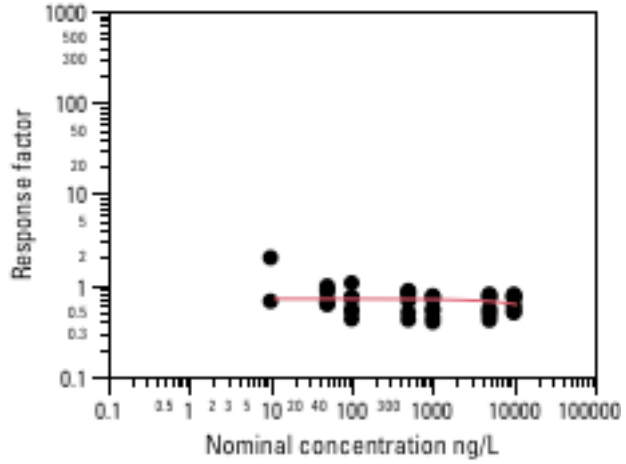
Linear fit: Response factor = 49.514635 - 0.0021375*Nominal concentration ng/L

Parent=Oryzalin, Compound Name=Oryzalin



Linear fit: Response factor = 12.894561 - 0.0005596*Nominal concentration ng/L

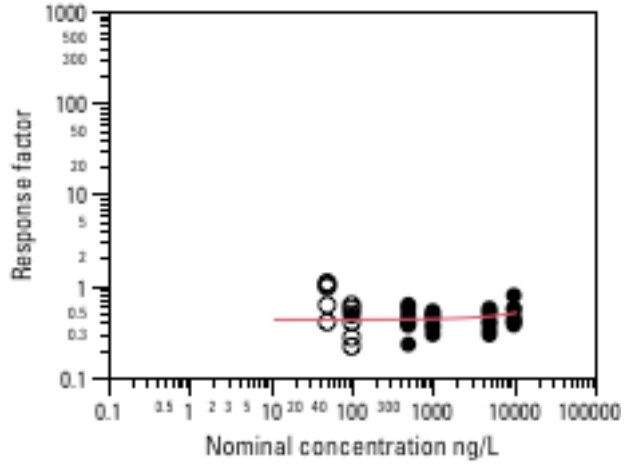
Parent=Pendimethalin, Compound Name=4-(Hydroxymethyl)pendimethalin



Linear fit: Response factor = 0.7080909 - 8.717e-6*Nominal concentration ng/L

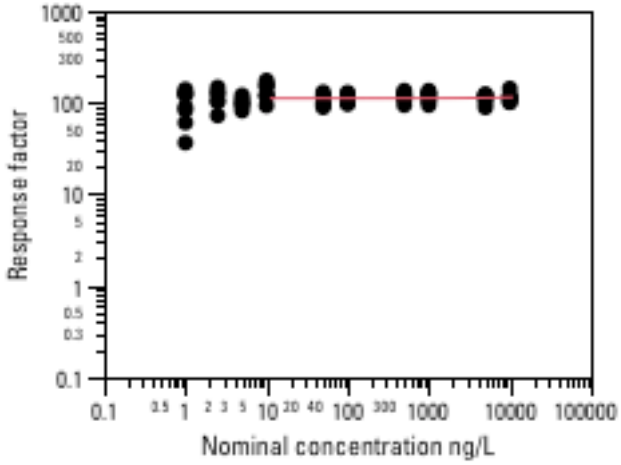
Pyrethroid and Organochlorine and Phenylpyrazine

Parent=Bifenthrin; lambda-cyhalothrin; Tefluthrin, Compound Name=cis-Cyhalothric acid



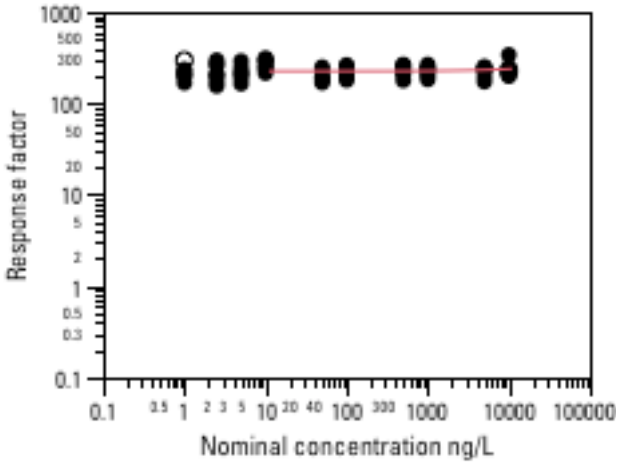
Linear fit: Response factor = 0.426108 + 7.4974e-6*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Dechlorofipronil



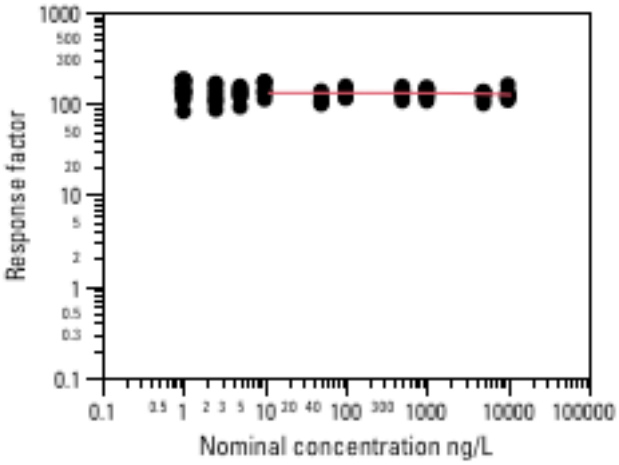
Linear fit: Response factor = 111.30968 + 0.0003189*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Desulfinylfipronil



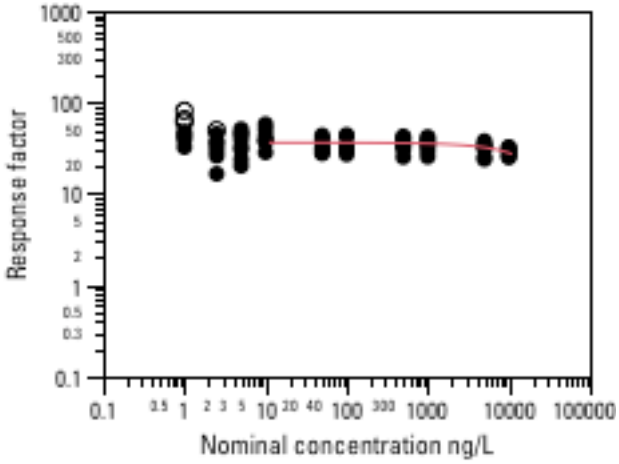
Linear fit: Response factor = 225.48812 + 0.0012926*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Fipronil



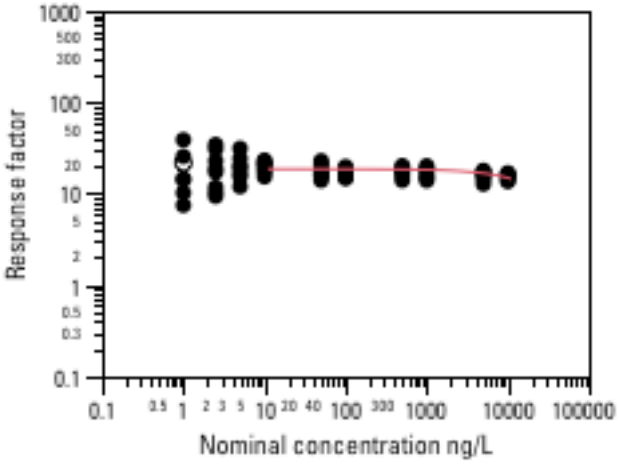
Linear fit: Response factor = 130.01217 - 0.0005658*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Desulfinylfipronil amide



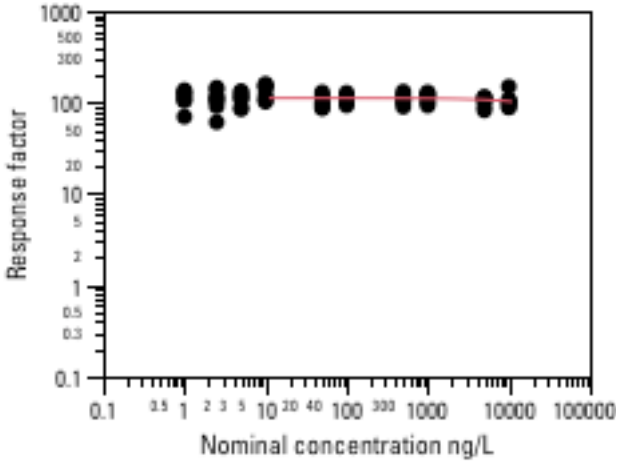
Linear fit: Response factor = 36.29019 - 0.0008237*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Fipronil amide



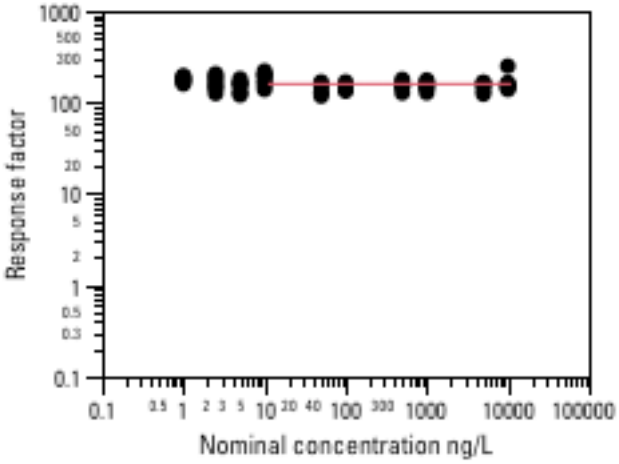
Linear fit: Response factor = 18.663569 - 0.0003745*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Fipronil sulfide



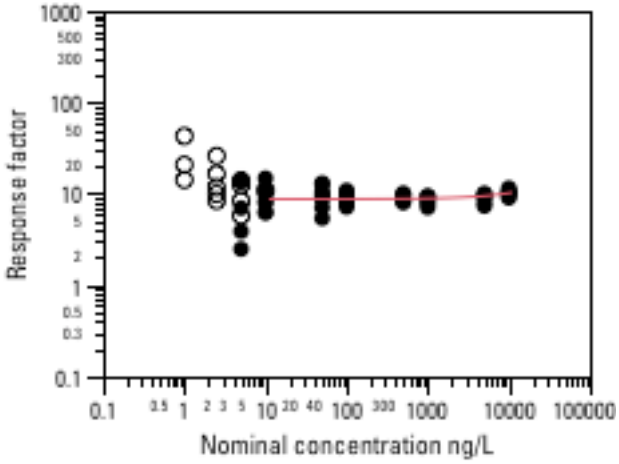
Linear fit: Response factor = 111.2469 - 0.0008492*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Fipronil sulfone



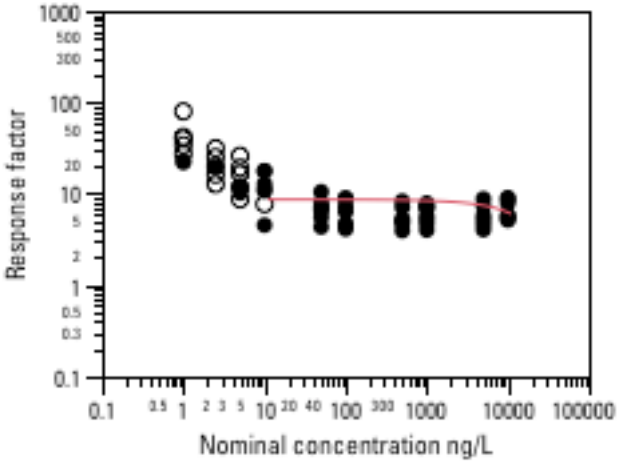
Linear fit: Response factor = 159.19419 + 1.2377e-5*Nominal concentration ng/L

Parent=Fipronil, Compound Name=Fipronil sulfonate



Linear fit: Response factor = 8.7582166 + 0.0001428*Nominal concentration ng/L

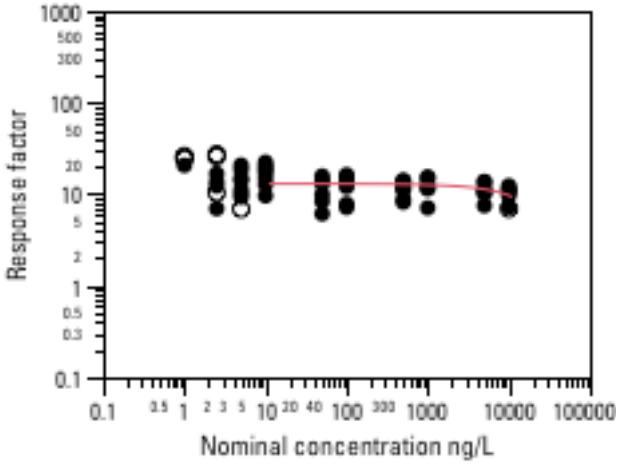
Parent=Permethrin, Compound Name=3-Phenoxybenzoic acid



Linear fit: Response factor = 8.6502638 - 0.0002369*Nominal concentration ng/L

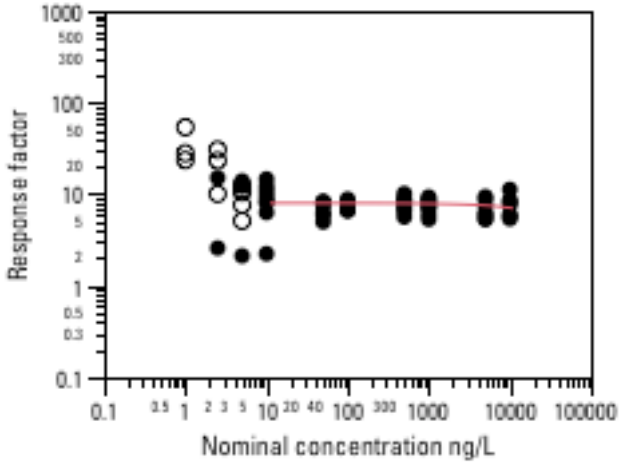
Sulfonylurea and Urea

Parent=Chlorimuron-ethyl, Compound Name=Chlorimuron-ethyl



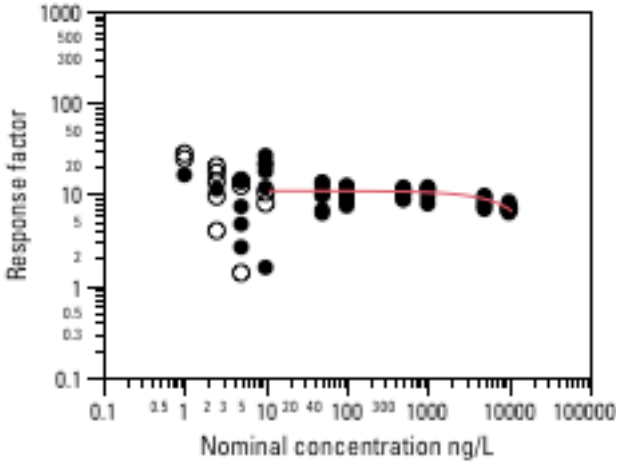
Linear fit: Response factor = 12.977182 - 0.0003267*Nominal concentration ng/L

Parent=Diflufenzopyr, Compound Name=Diflufenzopyr



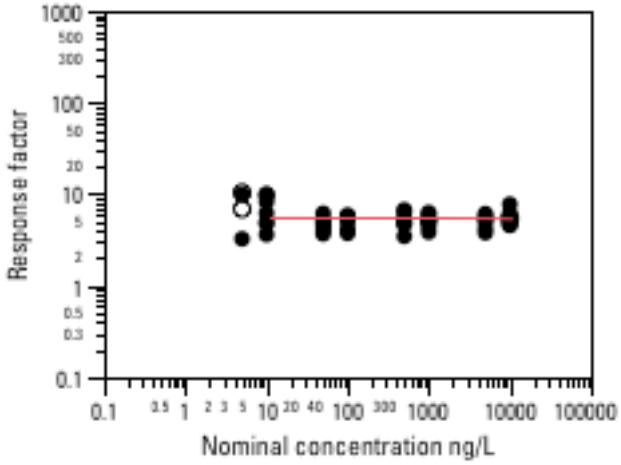
Linear fit: Response factor = 7.9826309 - 0.0000885*Nominal concentration ng/L

Parent=Chlorsulfuron, Compound Name=Chlorsulfuron



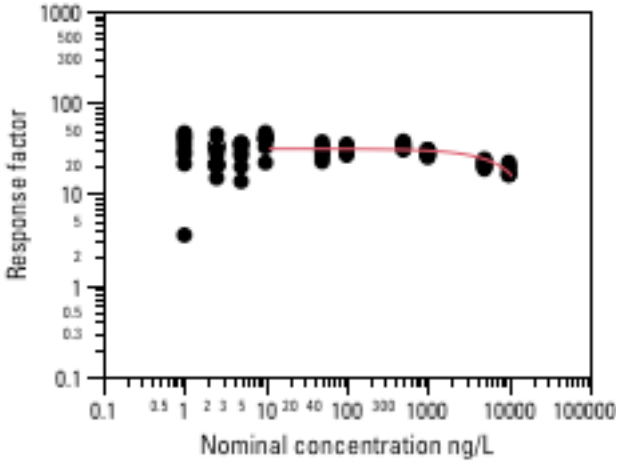
Linear fit: Response factor = 10.856142 - 0.000396*Nominal concentration ng/L

Parent=Halosulfuron-methyl, Compound Name=Chlorosulfonamide acid



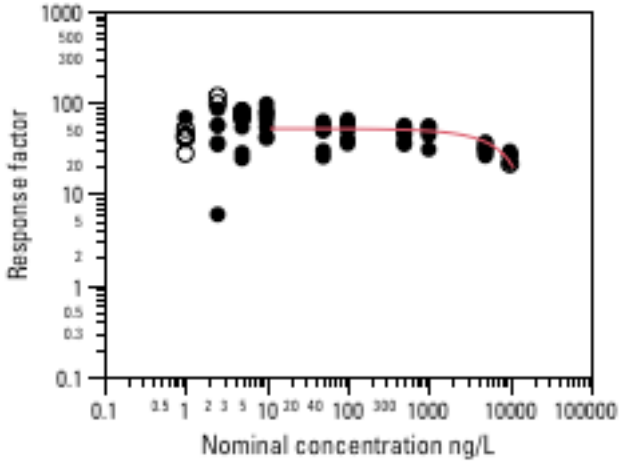
Linear fit: Response factor = 5.4721873 - 0.0000111*Nominal concentration ng/L

Parent=Novaluron, Compound Name=Novaluron



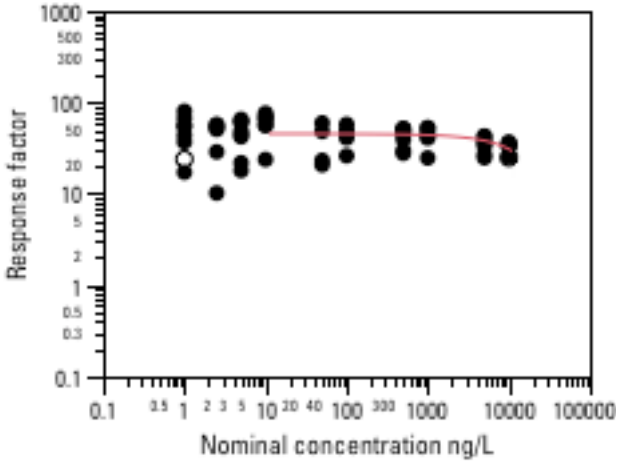
Linear fit: Response factor = 31.00688 - 0.001396*Nominal concentration ng/L

Parent=Sulfentrazone, Compound Name=Sulfentrazone



Linear fit: Response factor = 51.641898 - 0.0029372*Nominal concentration ng/L

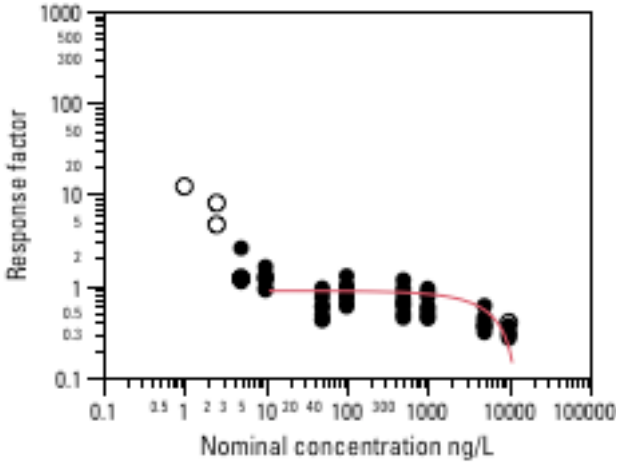
Parent=Prosulfuron, Compound Name=Prosulfuron



Linear fit: Response factor = 45.402284 - 0.0014527*Nominal concentration ng/L

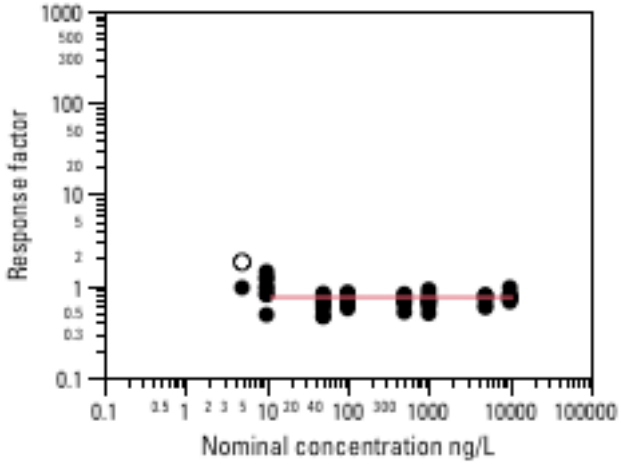
Triazine

Parent=Atrazine, Compound Name=Ammelide



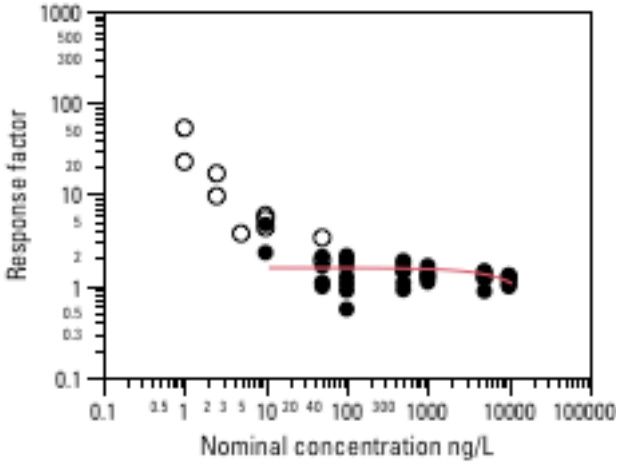
Linear fit: Response factor = 0.879167 - 0.0000668*Nominal concentration ng/L

Parent=Hexazinone, Compound Name=Hexazinone TP E



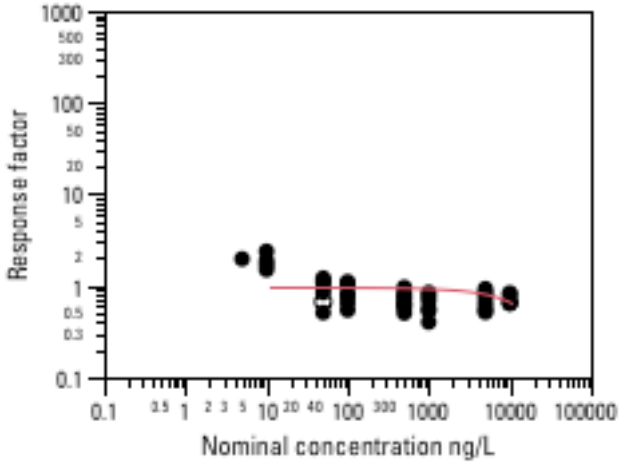
Linear fit: Response factor = 0.7492955 - 2.3082e-7*Nominal concentration ng/L

Parent=Hexazinone, Compound Name=Hexazinone TP D



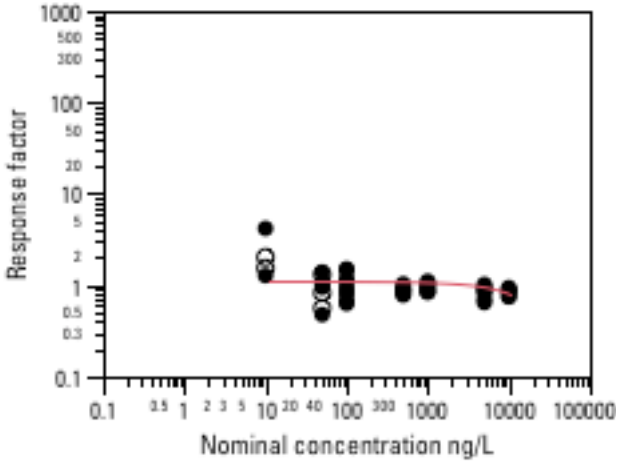
Linear fit: Response factor = 1.5682254 - 4.6285e-5*Nominal concentration ng/L

Parent=Metribuzin, Compound Name=Metribuzin DADK



Linear fit: Response factor = 0.9498801 - 2.9138e-5*Nominal concentration ng/L

Parent=Metribuzin, Compound Name=Metribuzin DK



Linear fit: Response factor = 1.08671 - 2.8737e-5*Nominal concentration ng/L