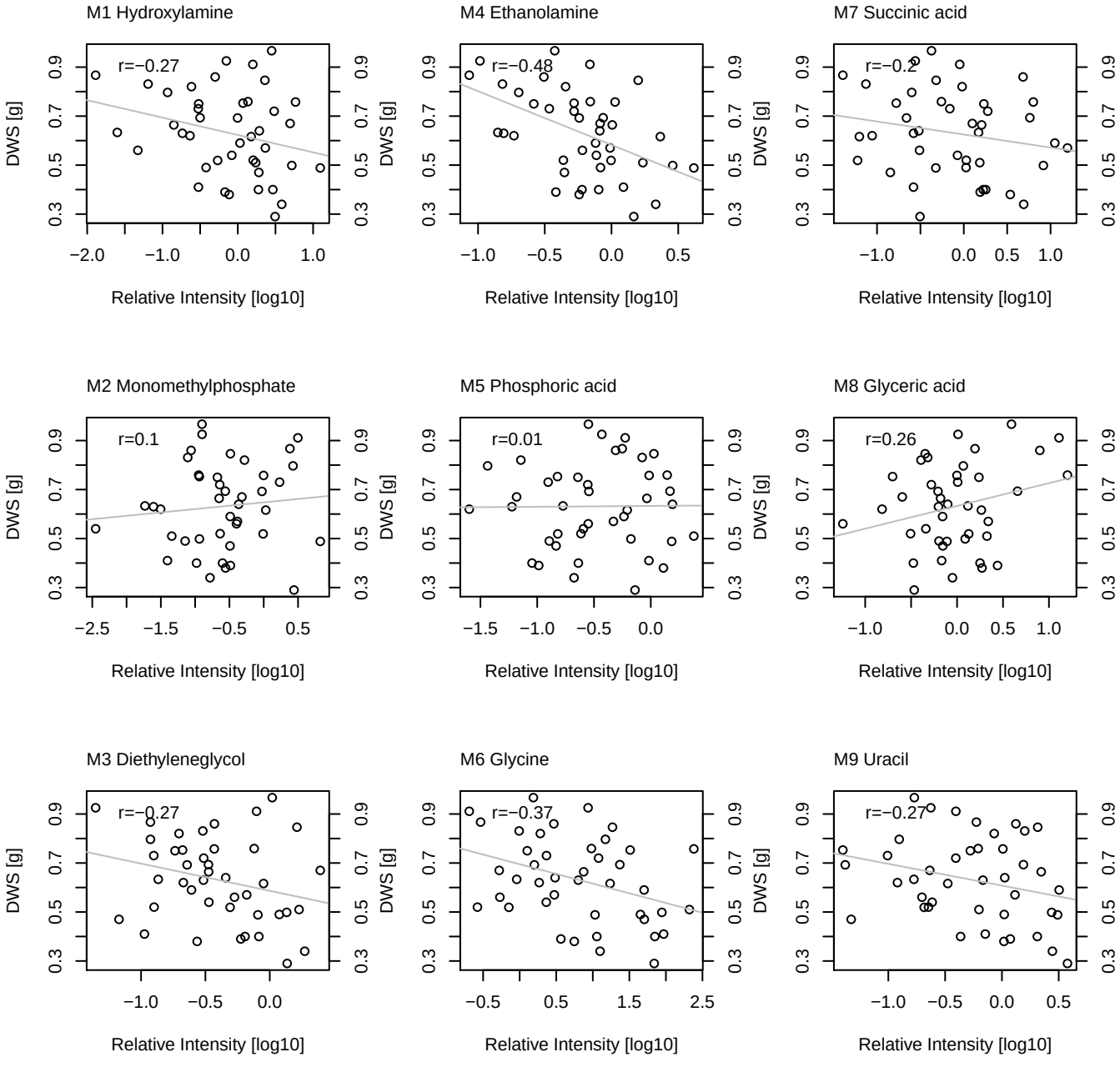
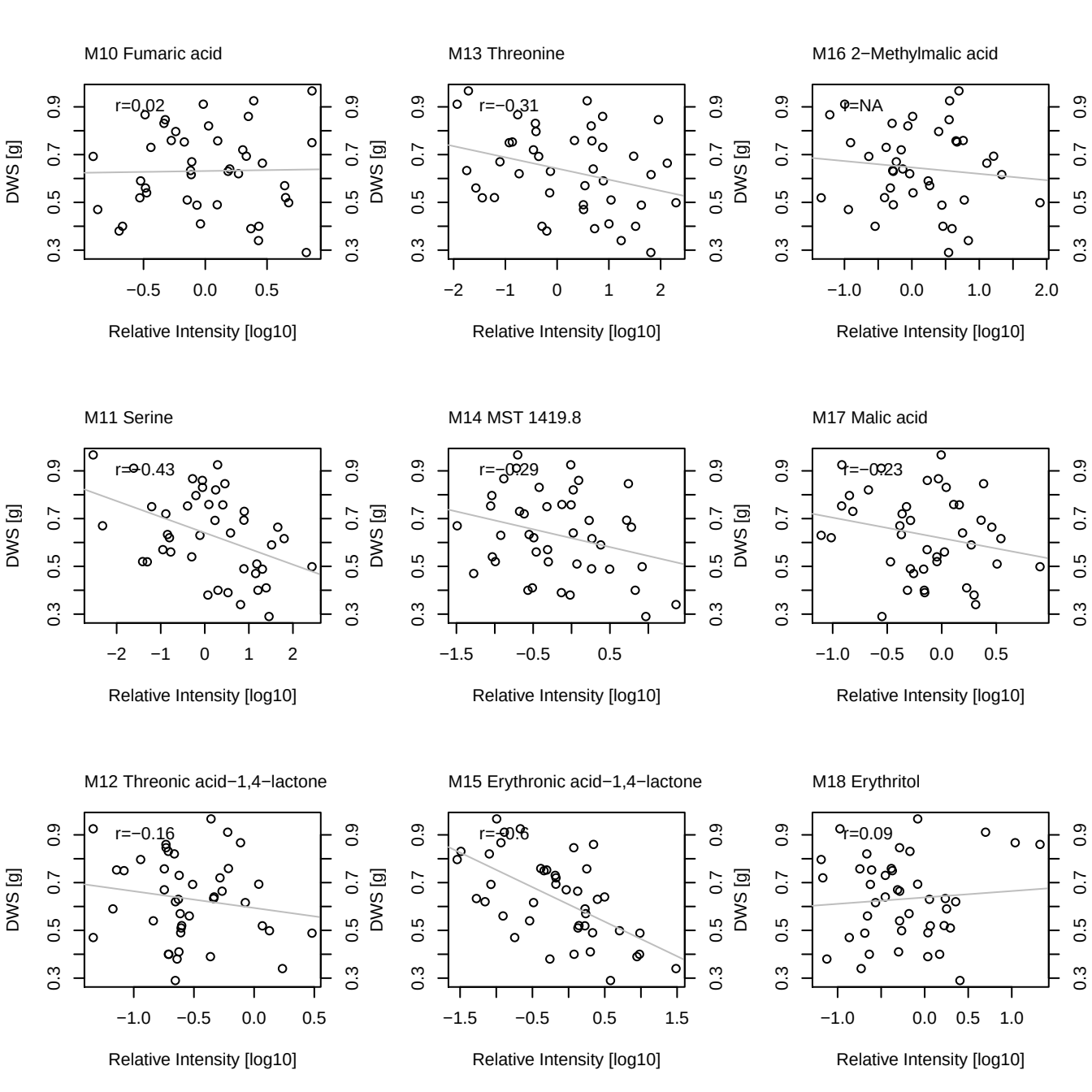
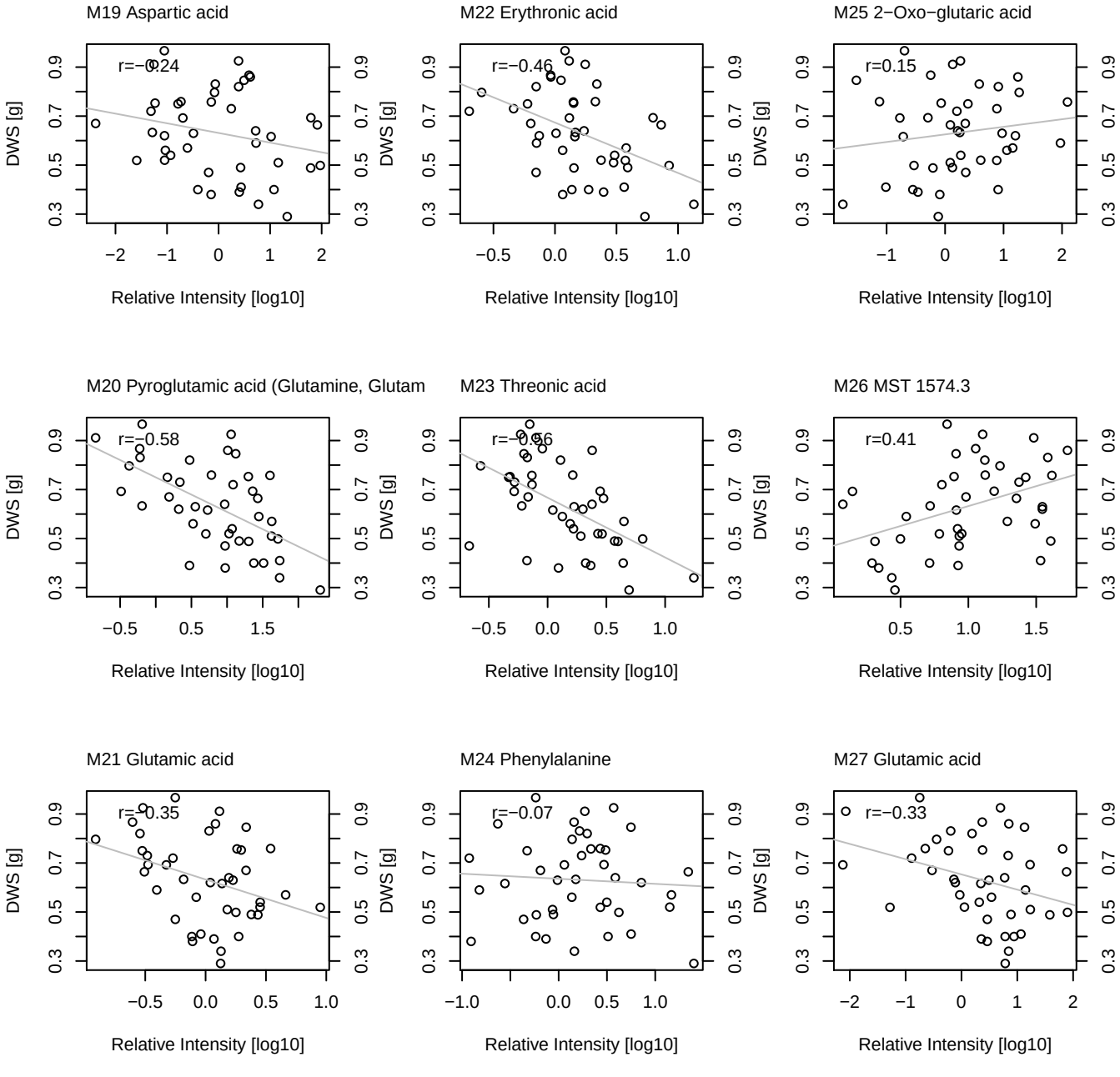
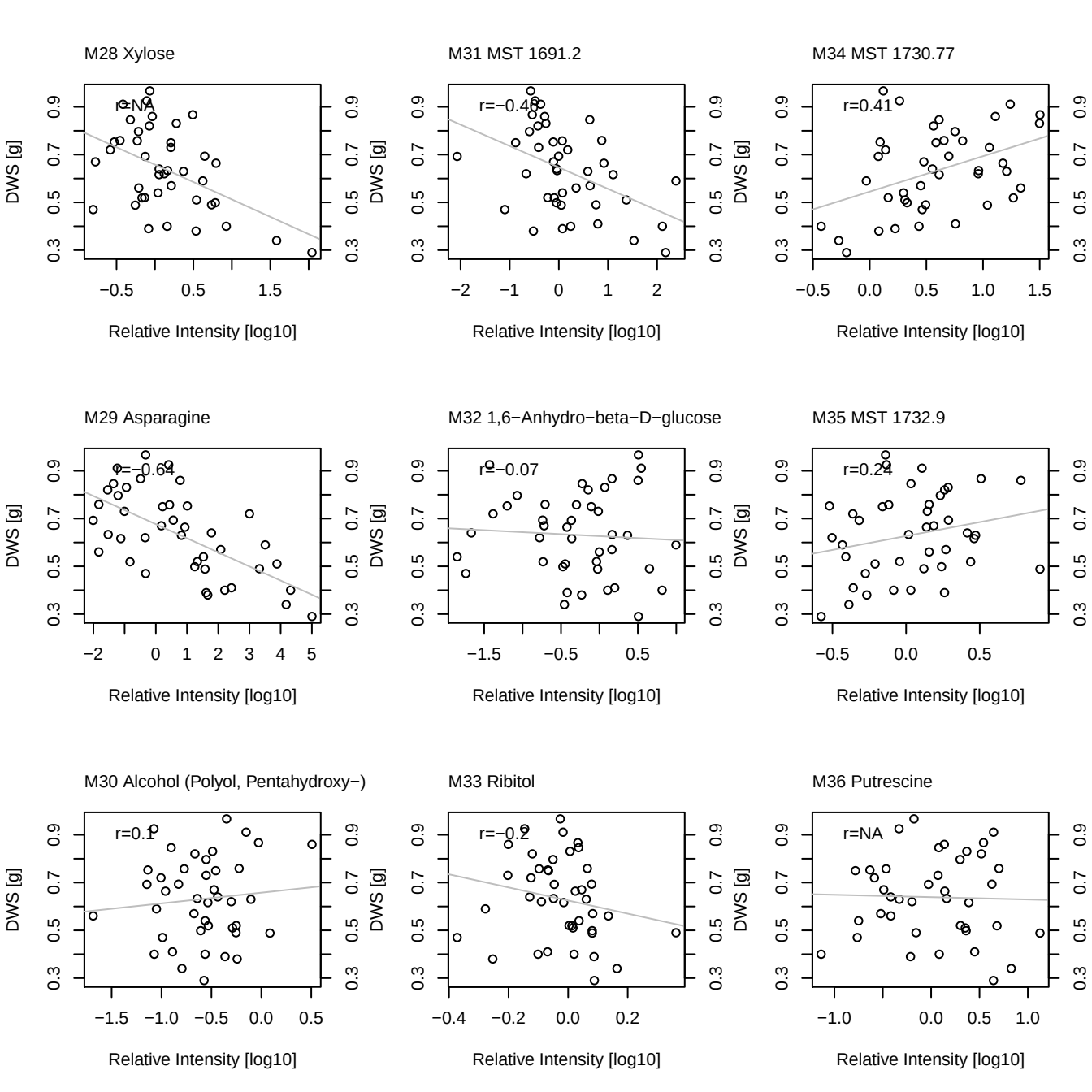
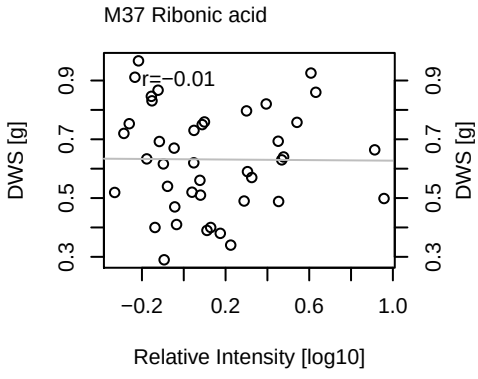
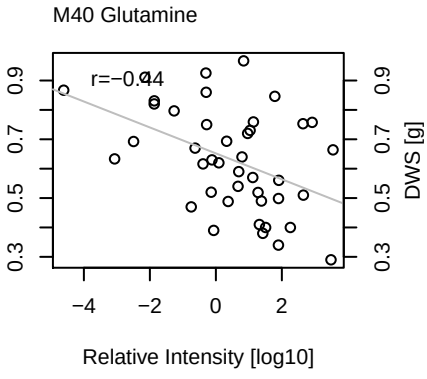

M1 Hydroxylamine
r=−0.27
M4 Ethanolamine
r=−0.48
M7 Succinic acid
r=−0.2
M2 Monomethylphosphate
r=0.1
M5 Phosphoric acid
r=0.01
M8 Glyceric acid
r=0.26
M3 Diethyleneglycol
r=−0.27
M6 Glycine
r=−0.37
M9 Uracil
r=−0.27
DWS [g]
Relative Intensity [log10]

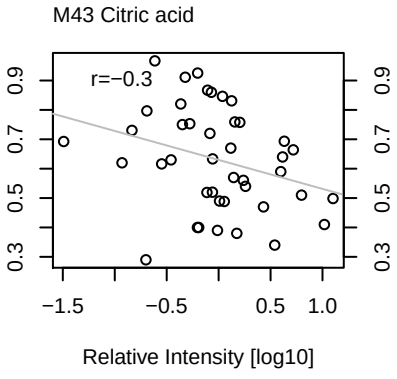

M10 Fumaric acid
r=0.02
M13 Threonine
r=−0.31
M16 2−Methylmalic acid
r=NA
M11 Serine
r=−0.43
M14 MST 1419.8
r=−0.29
M17 Malic acid
r=−0.23
M12 Threonic acid−1,4−lactone
r=−0.16
M15 Erythronic acid−1,4−lactone
r=−0.6
M18 Erythritol
r=0.09
DWS [g]
Relative Intensity [log10]

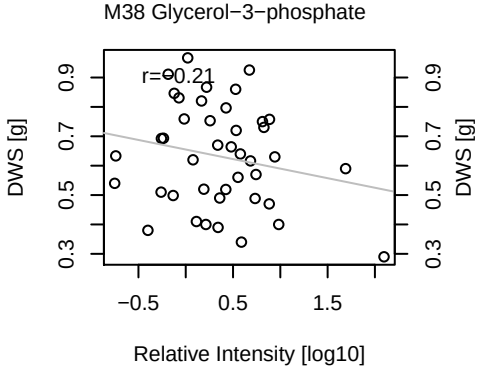

M19 Aspartic acid
r=−0.24
M22 Erythronic acid
r=−0.46
M25 2−Oxo−glutaric acid
r=0.15
M20 Pyroglutamic acid (Glutamine, Glutam
r=−0.58
M23 Threonic acid
r=−0.56
M26 MST 1574.3
r=0.41
M21 Glutamic acid
r=−0.35
M24 Phenylalanine
r=−0.07
M27 Glutamic acid
r=−0.33
DWS [g]
Relative Intensity [log10]

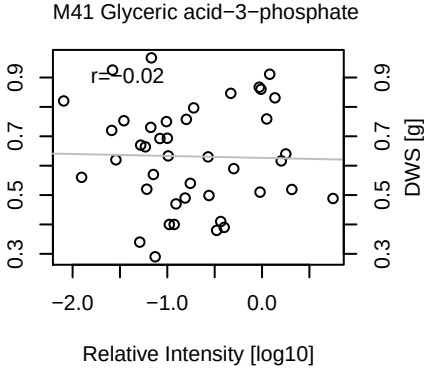

M28 Xylose
r=NA
M31 MST 1691.2
r=−0.46
M34 MST 1730.77
r=0.41
M29 Asparagine
r=−0.64
M32 1,6−Anhydro−beta−D−glucose
r=−0.07
M35 MST 1732.9
r=0.24
M30 Alcohol (Polyol, Pentahydroxy−)
r=0.1
M33 Ribitol
r=−0.2
M36 Putrescine
r=NA
DWS [g]
Relative Intensity [log10]

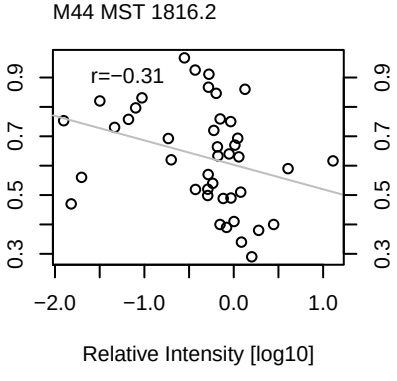

M37 Ribonic acid
r=−0.01
DWS [g]
Relative Intensity [log10]

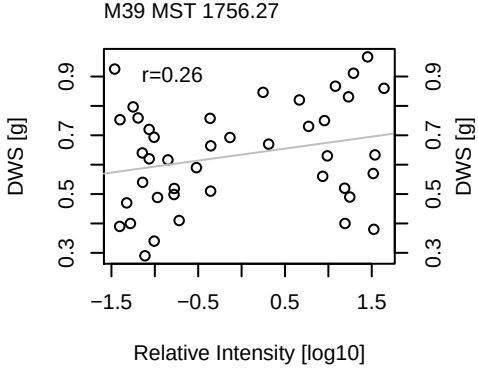

M40 Glutamine
r=−0.44
DWS [g]
Relative Intensity [log10]

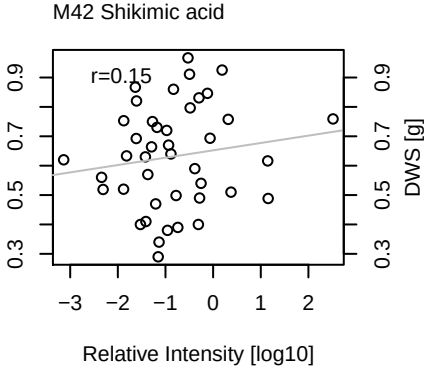

M43 Citric acid
r=−0.3
DWS [g]
Relative Intensity [log10]

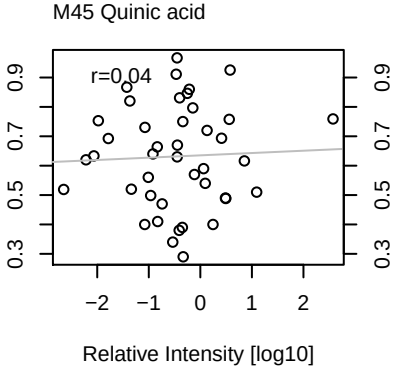

M38 Glycerol−3−phosphate
r=−0.21
DWS [g]
Relative Intensity [log10]

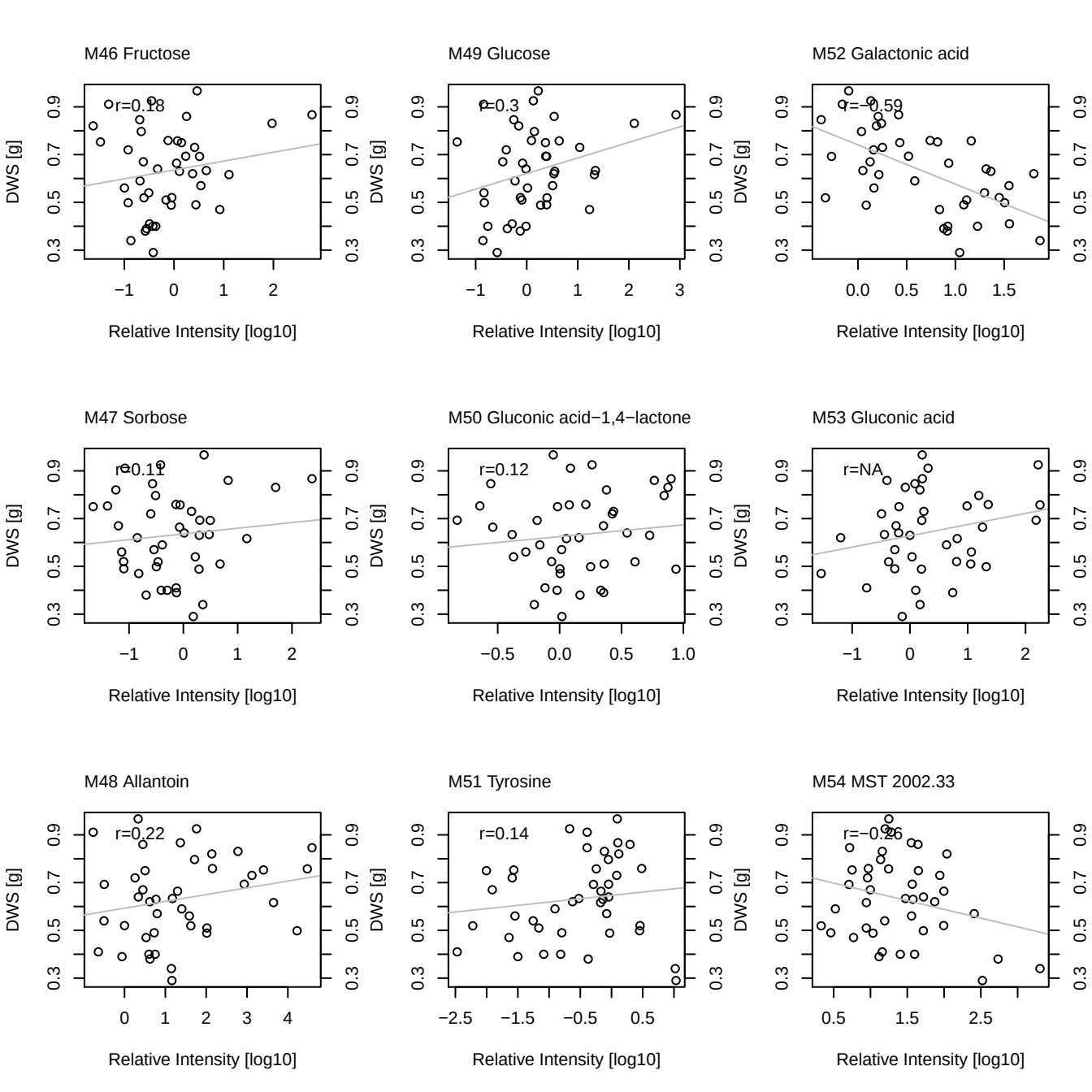

M41 Glyceric acid−3−phosphate
r=−0.02
DWS [g]
Relative Intensity [log10]

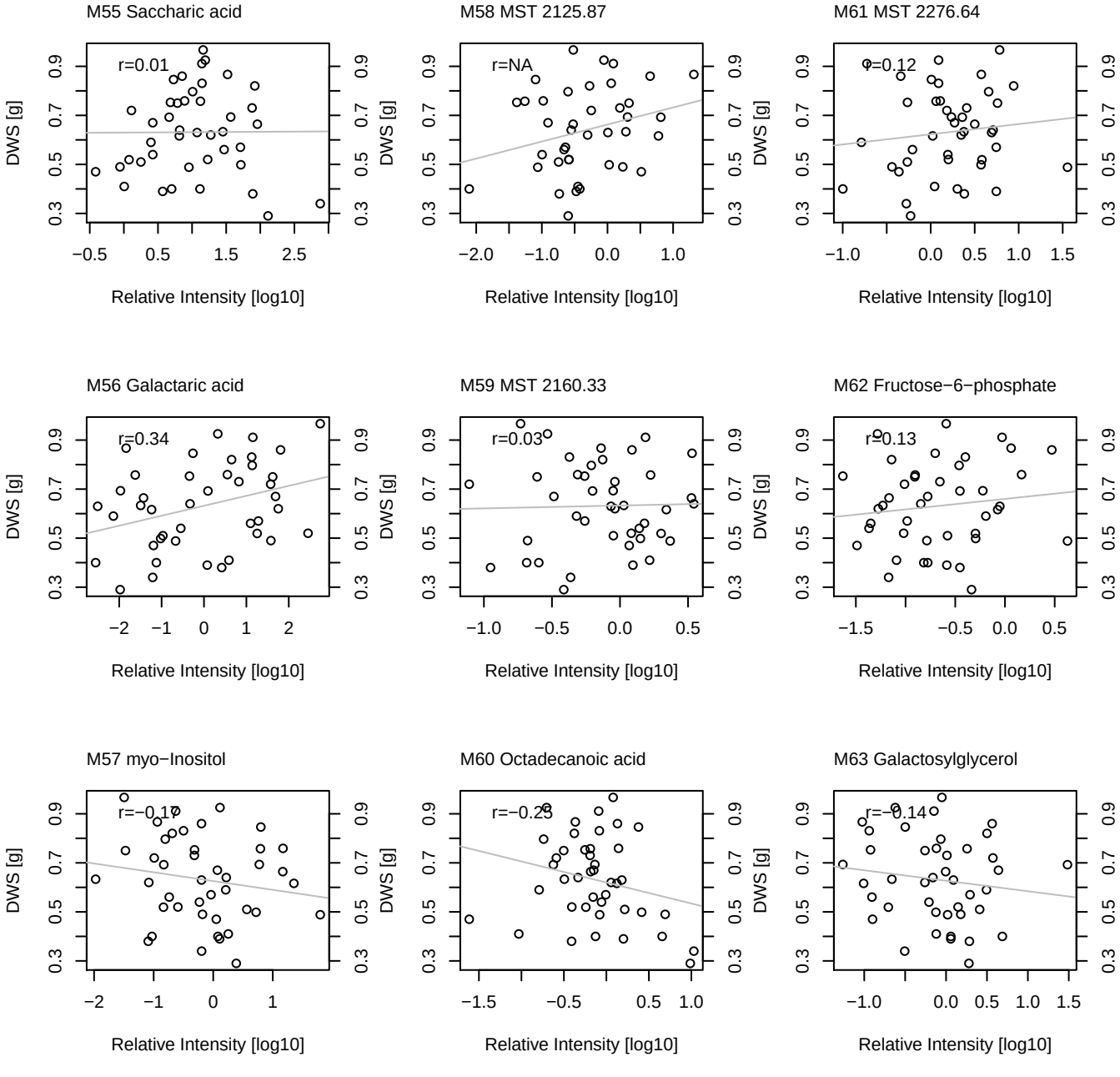

M44 MST 1816.2
r=−0.31
DWS [g]
Relative Intensity [log10]

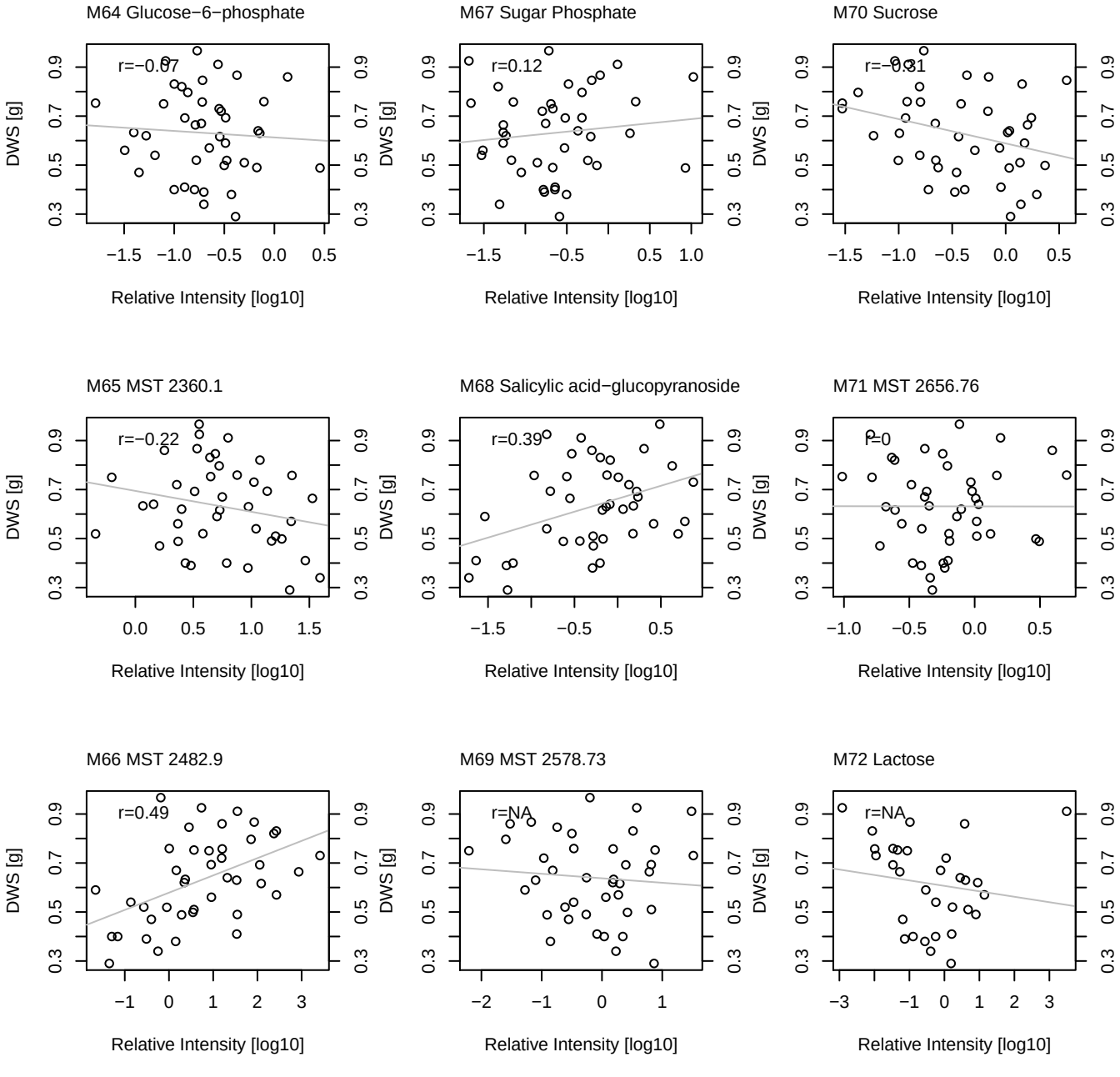

M39 MST 1756.27
r=0.26
DWS [g]
Relative Intensity [log10]

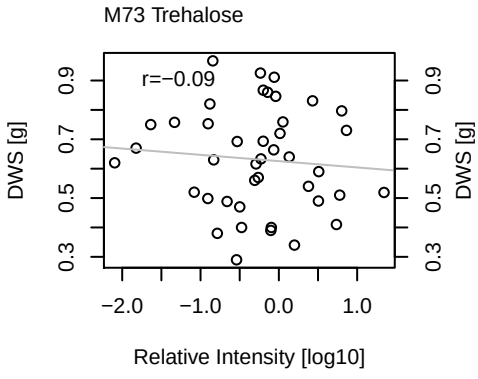

M42 Shikimic acid
r=0.15
DWS [g]
Relative Intensity [log10]

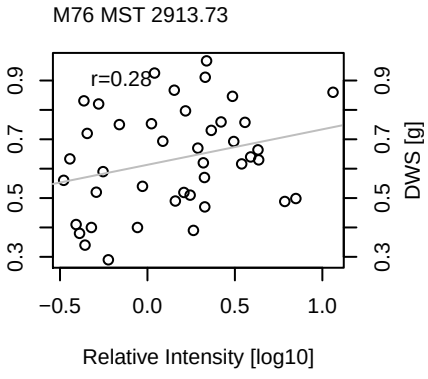

M45 Quinic acid
r=0.04
DWS [g]
Relative Intensity [log10]

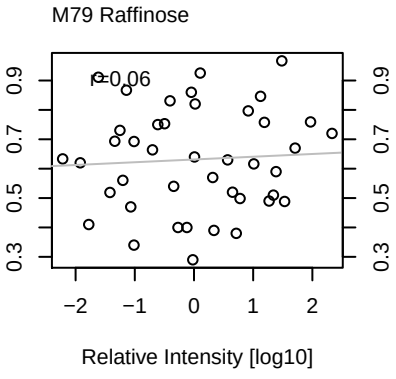

M46 Fructose
r=0.18
M49 Glucose
r=0.3
M52 Galactonic acid
r=−0.59
M47 Sorbose
r=0.11
M50 Gluconic acid−1,4−lactone
r=0.12
M53 Gluconic acid
r=NA
M48 Allantoin
r=0.22
M51 Tyrosine
r=0.14
M54 MST 2002.33
r=−0.26
DWS [g]
Relative Intensity [log10]

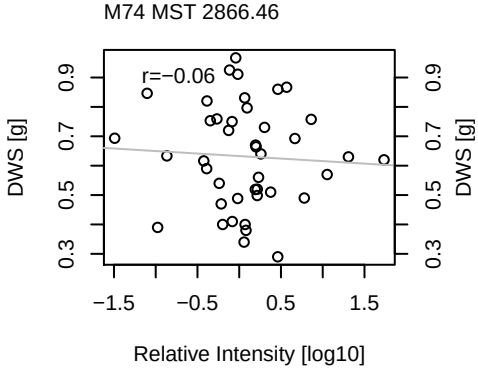

M55 Saccharic acid
r=0.01
M58 MST 2125.87
r=NA
M61 MST 2276.64
r=0.12
M56 Galactaric acid
r=0.34
M59 MST 2160.33
r=0.03
M62 Fructose−6−phosphate
r=0.13
M57 myo−Inositol
r=−0.17
M60 Octadecanoic acid
r=−0.23
M63 Galactosylglycerol
r=−0.14
DWS [g]
Relative Intensity [log10]

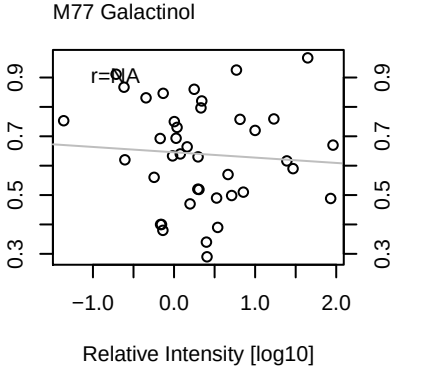

M64 Glucose−6−phosphate
r=−0.07
M67 Sugar Phosphate
r=0.12
M70 Sucrose
r=−0.31
M65 MST 2360.1
r=−0.22
M68 Salicylic acid−glucopyranoside
r=0.39
M71 MST 2656.76
r=0
M66 MST 2482.9
r=0.49
M69 MST 2578.73
r=NA
M72 Lactose
r=NA
DWS [g]
Relative Intensity [log10]

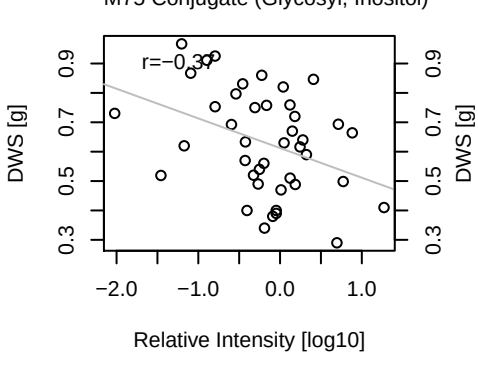

M73 Trehalose
r=−0.09
DWS [g]
Relative Intensity [log10]

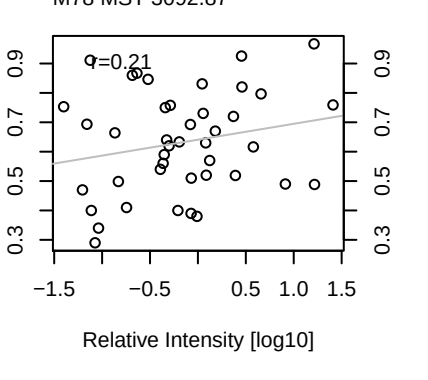

M76 MST 2913.73
r=0.28
DWS [g]
Relative Intensity [log10]


M79 Raffinose
r=0.06
DWS [g]
Relative Intensity [log10]


M74 MST 2866.46
r=−0.06
DWS [g]
Relative Intensity [log10]


M77 Galactinol
r=NA
DWS [g]
Relative Intensity [log10]


M75 Conjugate (Glycosyl, Inositol)
r=−0.37
DWS [g]
Relative Intensity [log10]


M78 MST 3092.87
r=0.21
DWS [g]
Relative Intensity [log10]