

# Supplementary Information

## Ehrlich and Sarcoma 180 Tumour Characterisation and Early Detection by <sup>1</sup>H NMR-Based Metabonomics of Mice Serum

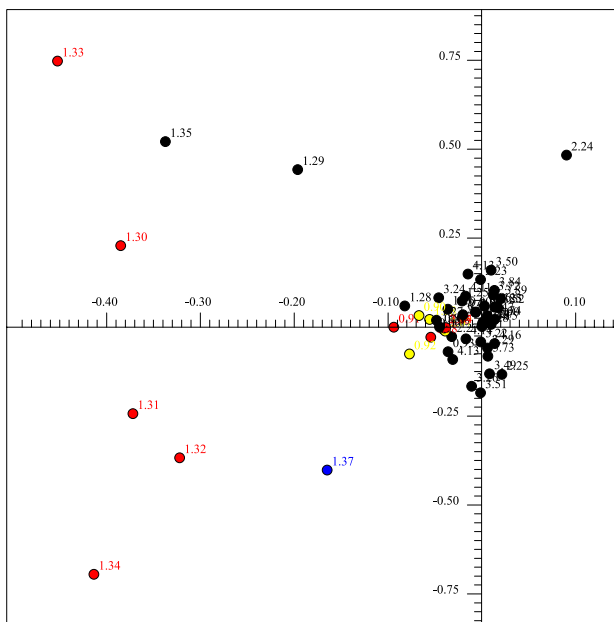
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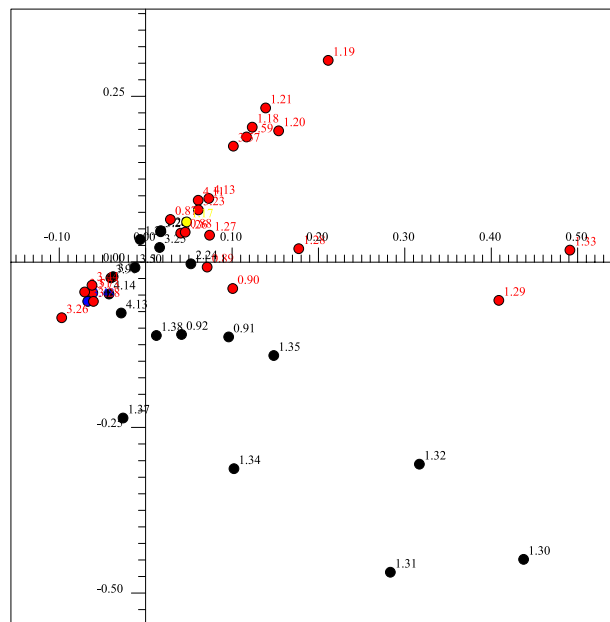
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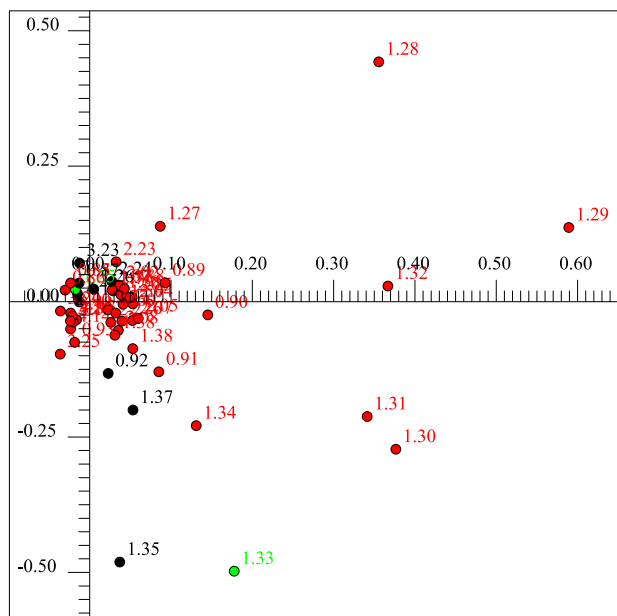


**Figure S1.** X-loading plot from PLS-DA analyses of <sup>1</sup>H NMR spectra of serum from three days post-incubation Ehrlich tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket *p*-values as follows:  
*p*-value >  $8.47 \times 10^{-4}$  (black)  
zone 1:  $6.36 \times 10^{-4}$ - $8.47 \times 10^{-4}$  (blue)  
zone 2:  $4.24 \times 10^{-4}$ - $6.36 \times 10^{-4}$  (green)  
zone 3:  $2.13 \times 10^{-4}$ - $4.24 \times 10^{-4}$  (yellow)  
zone 4: 0.00- $2.13 \times 10^{-4}$  (red)

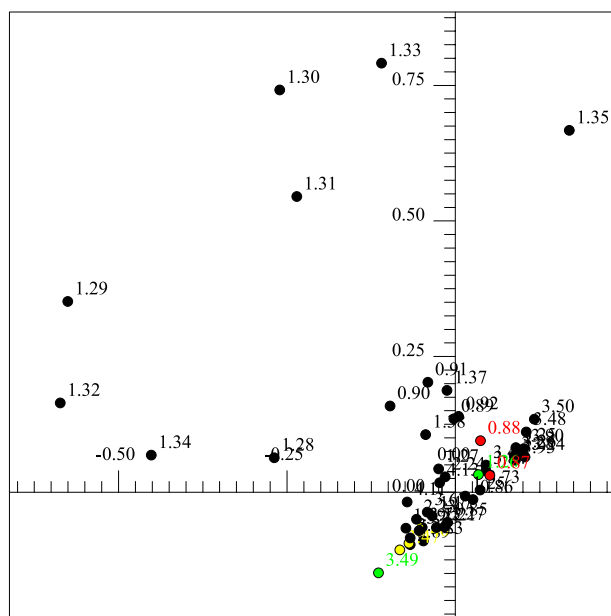


**Figure S2.** X-loading plot from PLS-DA analyses of <sup>1</sup>H NMR spectra of serum from five days post-incubation Ehrlich tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket *p*-values as follows:  
*p*-value >  $1.14 \times 10^{-3}$  (black)  
zone 1:  $8.52 \times 10^{-4}$ - $1.14 \times 10^{-3}$  (blue)  
zone 2:  $5.68 \times 10^{-4}$ - $8.52 \times 10^{-4}$  (green)  
zone 3:  $2.84 \times 10^{-4}$ - $5.68 \times 10^{-4}$  (yellow)  
zone 4: 0.00- $2.84 \times 10^{-4}$  (red)

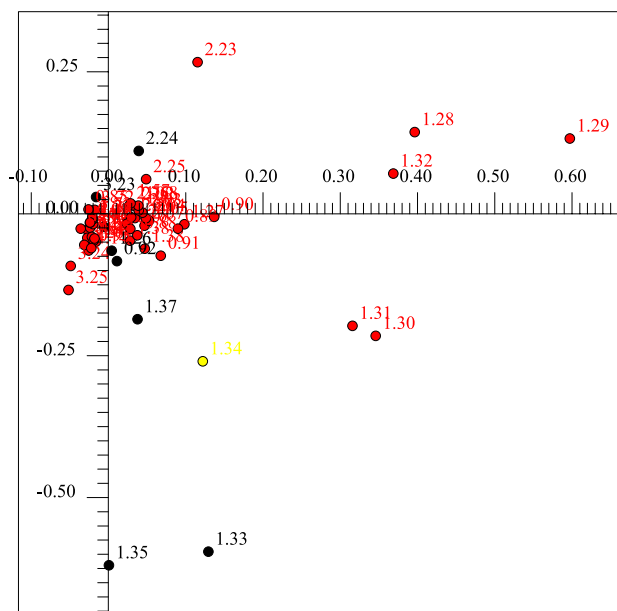
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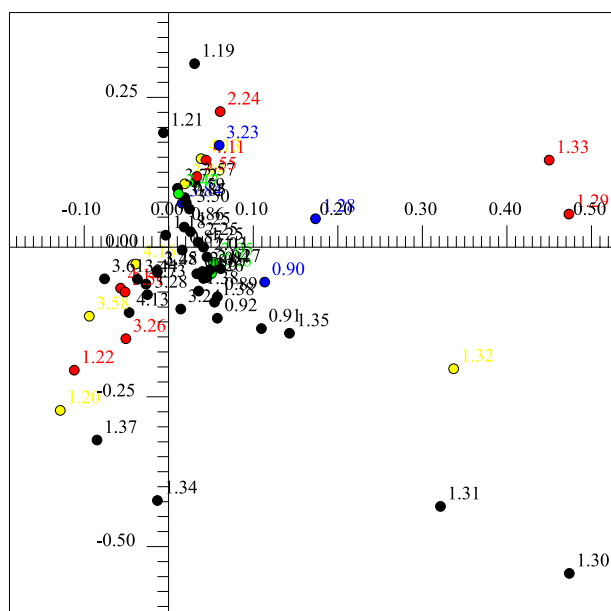
**Figure S3.** X-loading plot from PLS-DA analyses of <sup>1</sup>H NMR spectra of serum from seven days post-incubation Ehrlich tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket *p*-values as follows:  
*p*-value >  $9.62 \times 10^{-4}$  (black)  
 zone 1:  $7.21 \times 10^{-4}$ - $9.62 \times 10^{-4}$  (blue)  
 zone 2:  $4.81 \times 10^{-4}$ - $7.21 \times 10^{-4}$  (green)  
 zone 3:  $2.40 \times 10^{-4}$ - $4.81 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.40 \times 10^{-4}$  (red)



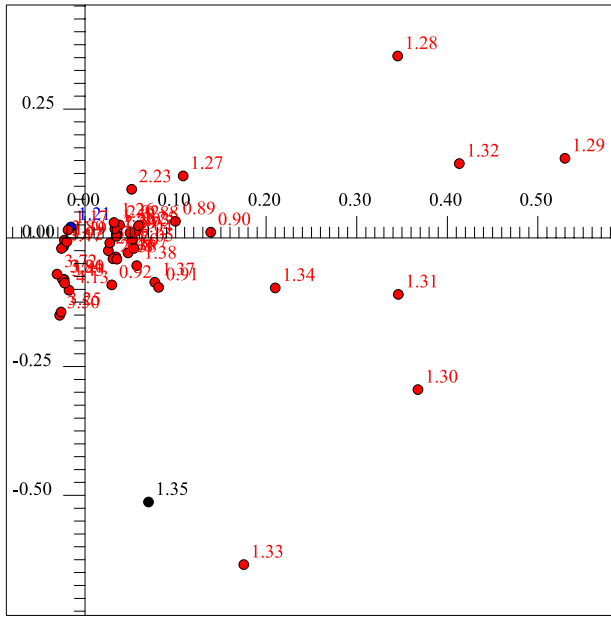
**Figure S5.** X-loading plot from PLS-DA analyses of <sup>1</sup>H NMR spectra of serum from three days post-incubation Ehrlich tumour-inoculated Balb-C mice and matched control group. X-loadings plot points are heat map color-coded according to bucket *p*-values as follows:  
*p*-value >  $1.02 \times 10^{-3}$  (black)  
 zone 1:  $7.68 \times 10^{-4}$ - $1.02 \times 10^{-3}$  (blue)  
 zone 2:  $5.15 \times 10^{-4}$ - $7.68 \times 10^{-4}$  (green)  
 zone 3:  $2.63 \times 10^{-4}$ - $5.15 \times 10^{-4}$  (yellow)  
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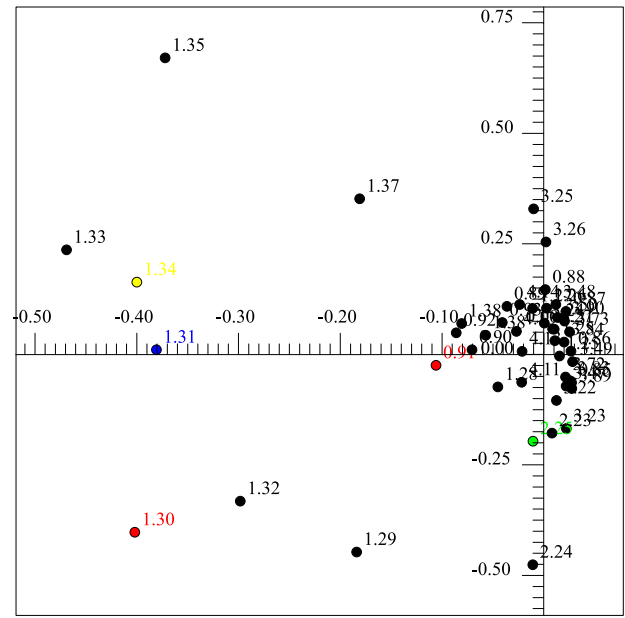
**Figure S4.** X-loading plot from PLS-DA analyses of <sup>1</sup>H NMR spectra of serum from ten days post-incubation Ehrlich tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket *p*-values as follows:  
*p*-value >  $8.33 \times 10^{-4}$  (black)  
 zone 1:  $6.25 \times 10^{-4}$ - $8.33 \times 10^{-4}$  (blue)  
 zone 2:  $4.17 \times 10^{-4}$ - $6.25 \times 10^{-4}$  (green)  
 zone 3:  $2.08 \times 10^{-4}$ - $4.17 \times 10^{-4}$  (yellow)  
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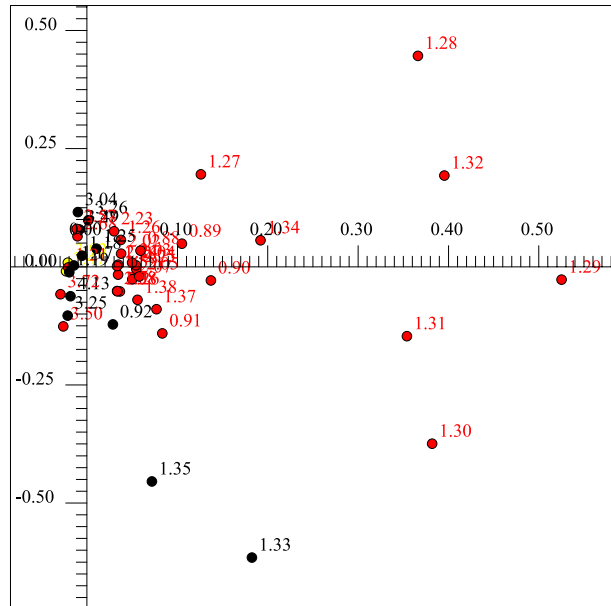
**Figure S6.** X-loading plot from PLS-DA analyses of <sup>1</sup>H NMR spectra of serum from five days post-incubation Ehrlich tumour-inoculated Balb-C mice and matched control group. X-loadings plot points are heat map color-coded according to bucket *p*-values as follows:  
*p*-value >  $8.33 \times 10^{-4}$  (black)  
 zone 1:  $6.27 \times 10^{-4}$ - $8.33 \times 10^{-4}$  (blue)  
 zone 2:  $4.20 \times 10^{-4}$ - $6.27 \times 10^{-4}$  (green)  
 zone 3:  $2.14 \times 10^{-4}$ - $4.20 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.14 \times 10^{-4}$  (red)



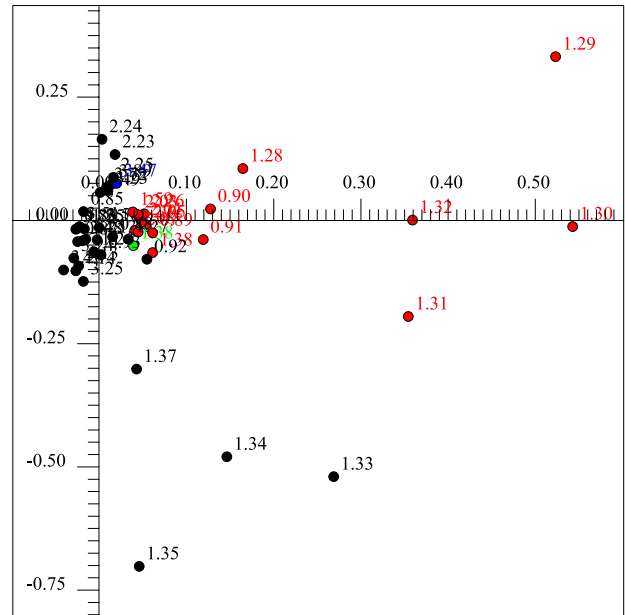
**Figure S7.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from seven days post-incubation Ehrlich tumour-inoculated Balb-C mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 1.12 \times 10^{-3}$  (black)  
 zone 1:  $8.33 \times 10^{-4}$ - $1.12 \times 10^{-3}$  (blue)  
 zone 2:  $5.56 \times 10^{-4}$ - $8.33 \times 10^{-4}$  (green)  
 zone 3:  $2.78 \times 10^{-4}$ - $5.56 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.78 \times 10^{-4}$  (red)



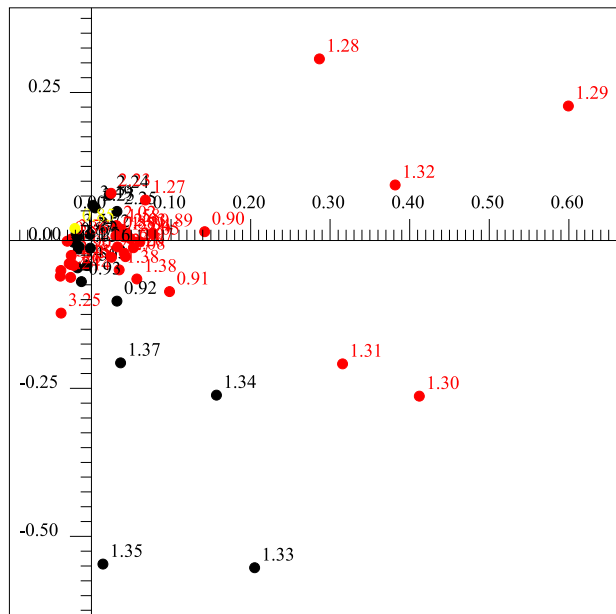
**Figure S9.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from three days post-incubation Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 1.04 \times 10^{-3}$  (black)  
 zone 1:  $7.96 \times 10^{-4}$ - $1.04 \times 10^{-3}$  (blue)  
 zone 2:  $5.51 \times 10^{-4}$ - $7.96 \times 10^{-4}$  (green)  
 zone 3:  $3.06 \times 10^{-4}$ - $5.51 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $3.06 \times 10^{-4}$  (red)



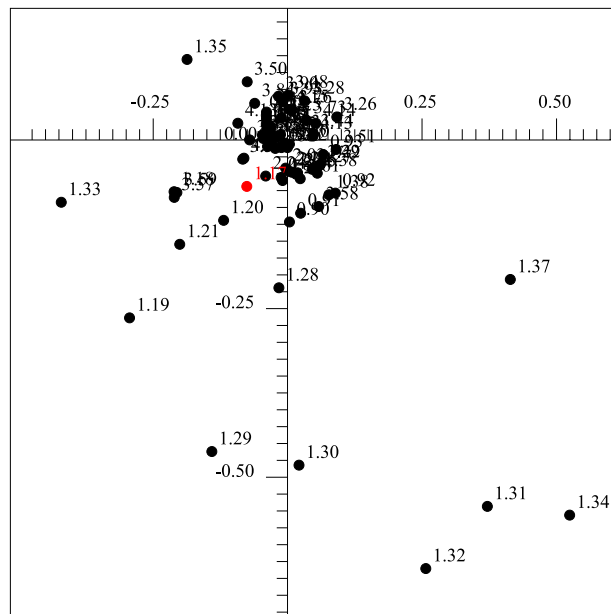
**Figure S8.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from ten days post-incubation Ehrlich tumour-inoculated Balb-C mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 1.06 \times 10^{-3}$  (black)  
 zone 1:  $7.98 \times 10^{-4}$ - $1.06 \times 10^{-3}$  (blue)  
 zone 2:  $5.32 \times 10^{-4}$ - $7.98 \times 10^{-4}$  (green)  
 zone 3:  $2.66 \times 10^{-4}$ - $5.32 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.66 \times 10^{-4}$  (red)



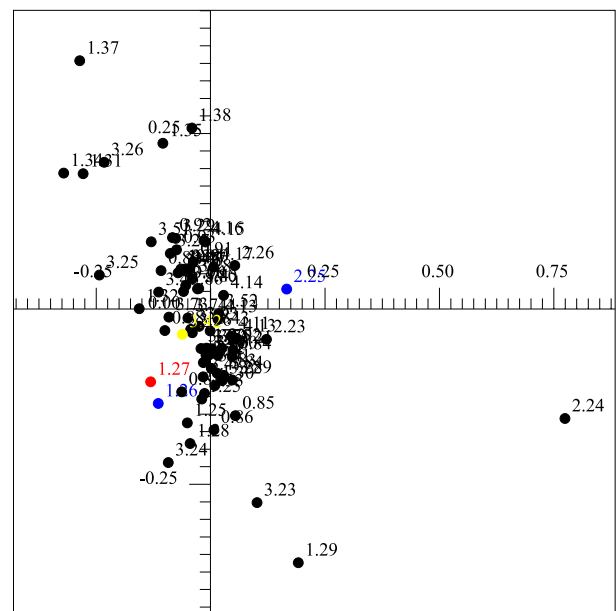
**Figure S10.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from seven days post-incubation Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 1.02 \times 10^{-3}$  (black)  
 zone 1:  $7.65 \times 10^{-4}$ - $1.02 \times 10^{-3}$  (blue)  
 zone 2:  $5.10 \times 10^{-4}$ - $7.65 \times 10^{-4}$  (green)  
 zone 3:  $2.55 \times 10^{-4}$ - $5.10 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.55 \times 10^{-4}$  (red)



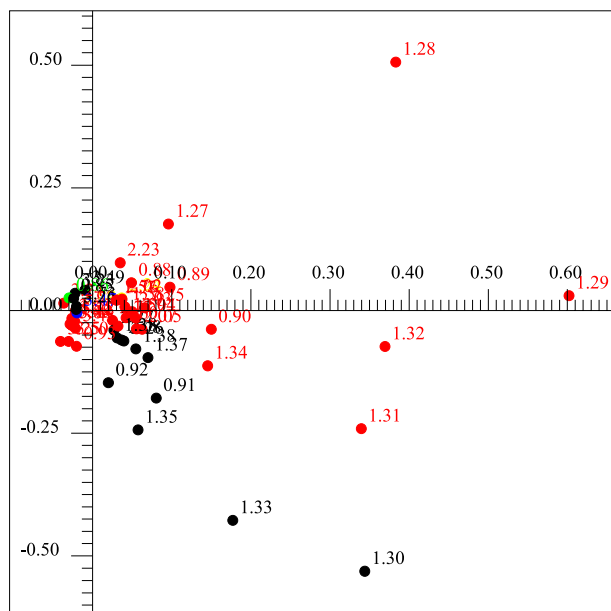
**Figure S11.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from ten days post-incubation Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 9.26 \times 10^{-4}$  (black)  
 zone 1:  $6.94 \times 10^{-4}$ - $9.26 \times 10^{-4}$  (blue)  
 zone 2:  $4.63 \times 10^{-4}$ - $6.94 \times 10^{-4}$  (green)  
 zone 3:  $2.31 \times 10^{-4}$ - $4.63 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.31 \times 10^{-4}$  (red)



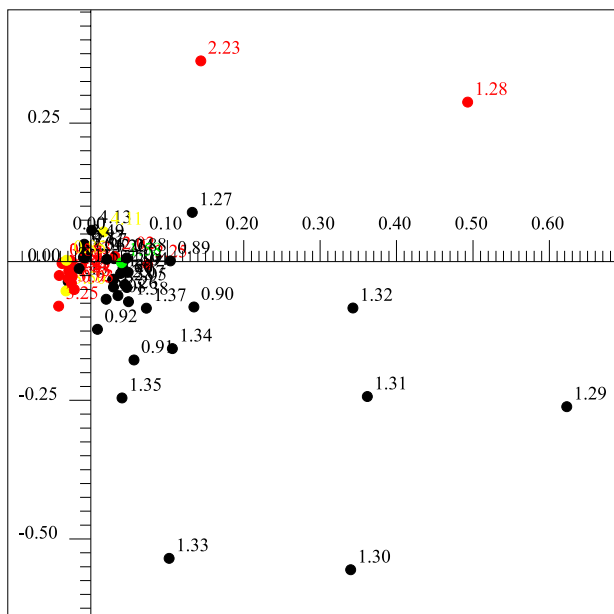
**Figure S13.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from five days post-incubation Ehrlich and Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 6.58 \times 10^{-4}$  (black)  
 zone 1:  $6.09 \times 10^{-4}$ - $6.58 \times 10^{-4}$  (blue)  
 zone 2:  $5.60 \times 10^{-4}$ - $6.09 \times 10^{-4}$  (green)  
 zone 3:  $5.12 \times 10^{-4}$ - $5.60 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $5.12 \times 10^{-4}$  (red)



**Figure S12.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from three days post-incubation Ehrlich and Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 6.41 \times 10^{-4}$  (black)  
 zone 1:  $4.99 \times 10^{-4}$ - $6.41 \times 10^{-4}$  (blue)  
 zone 2:  $3.58 \times 10^{-4}$ - $4.99 \times 10^{-4}$  (green)  
 zone 3:  $2.16 \times 10^{-4}$ - $3.58 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.16 \times 10^{-4}$  (red)



**Figure S14.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from seven days post-incubation Ehrlich and Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 9.26 \times 10^{-4}$  (black)  
 zone 1:  $6.94 \times 10^{-4}$ - $9.26 \times 10^{-4}$  (blue)  
 zone 2:  $4.63 \times 10^{-4}$ - $6.94 \times 10^{-4}$  (green)  
 zone 3:  $2.31 \times 10^{-4}$ - $4.63 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.31 \times 10^{-4}$  (red)



**Figure S15.** X-loading plot from PLS-DA analyses of  $^1\text{H}$  NMR spectra of serum from ten days post-incubation Ehrlich and Sarcoma 180 tumour-inoculated Swiss mice and matched control group. X-loadings plot points are heat map color-coded according to bucket  $p$ -values as follows:  
 $p$ -value  $> 8.77 \times 10^{-4}$  (black)  
 zone 1:  $6.58 \times 10^{-4}$ - $8.77 \times 10^{-4}$  (blue)  
 zone 2:  $4.39 \times 10^{-4}$ - $6.58 \times 10^{-4}$  (green)  
 zone 3:  $2.19 \times 10^{-4}$ - $4.39 \times 10^{-4}$  (yellow)  
 zone 4:  $0.00$ - $2.19 \times 10^{-4}$  (red)