

Metabolomic profile of systemic sclerosis patients

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Supplementary Materials

Fig S1. Signal assignments of the serum metabolites in an NMR spectrum.

1. Lipid 1; 2. 2-OH-butyrate; 3. Isoleucine; 4. Leucine; 5. Valine; 6. 3-OH-butyrate; 7. Lipid 2; 8. Lactate; 9. Alanine; 10. Lysine; 11. Acetate; 12. Proline; 13. N-acetyl-groups; 14. Methionine; 15. Glutamate; 16. Pyroglutamate; 17. Glutamine; 18. Citrate; 19. Aspartate; 20. Sarcosine; 21. Asparagine; 22. Creatinine; 23. Creatine; 24. Ornithine; 25. Choline; 26. Glucose; 27. Betaine; 28. 1,3-Dimethylurate*; 29. Methanol**; 30. Glycine; 31. Glycerol; 32. Glucitol*; 33. Glycylproline*; 34. Fructose; 35. Threonine; 36. Tyrosine; 37. Histidine; 38. tryptophan; 39. Phenylalanine; 40. τ -methylhistidine; 41. Oxypurinol*; 42. Adenosine*; 43. Inosine*; 44. Formate. * = **uncertain attribution**; ** = **extraction contaminant**.

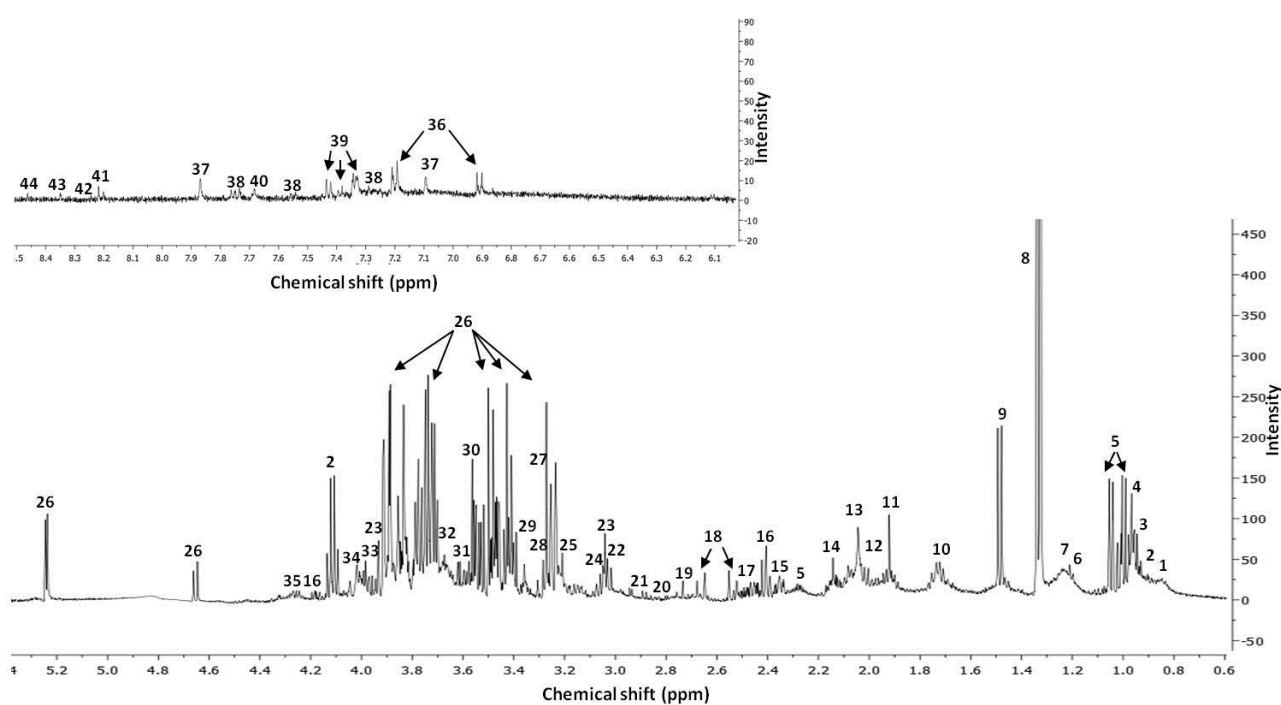


Table S1: Attributions of the metabolites identified in the NMR spectra with the corresponding chemical shifts.

Compound Name	Chemical Shifts [± 0.03 ppm]
1,3-Dimethylurate*	3.31; 3.43
2-Hydroxybutyrate	0.89; 1.64; 1.73; 3.98
3-Hydroxybutyrate	1.19; 2.30; 2.39; 4.14
Acetate	1.91
Adenosine*	8.33; 8.25; 6.06; 4.43; 4.29; 3.91; 3.83
Alanine	1.47; 3.78
Asparagine	2.85; 2.94; 4.00; 6.91; 7.62
Aspartate	2.68; 2.80; 3.89
Choline	3.20; 3.51; 4.06
Citrate	2.53; 2.69
Creatine	3.03; 3.92
Creatinine	3.03; 4.05
Formate	8.45
Fructose	3.55; 3.56; 3.59; 3.67; 3.70; 3.70; 3.79; 3.79; 3.82; 3.89; 3.99; 4.01; 4.10; 4.11
Glucitol*	3.63; 3.65; 3.72; 3.75; 3.77; 3.84
Glucose	3.24; 3.39; 3.40; 3.46; 3.48; 3.53; 3.70; 3.72; 3.76; 3.82; 3.84; 3.89; 4.64; 5.24
Glutamate	2.04; 2.12; 2.33; 2.36; 3.75
Glutamine	2.11; 2.14; 2.43; 2.46; 3.77; 6.87; 7.59
Glycerol	3.55; 3.65; 3.78
Glycine	3.55
Glycylproline*	1.97; 2.12; 2.24; 2.32; 3.53; 3.58; 3.95; 4.27;
Histidine	3.14; 3.24; 3.98; 7.09; 7.88
Inosine*	8.33; 8.23; 6.09; 4.43; 4.27; 3.91; 3.83
Isoleucine	0.93; 1.00; 1.25; 1.46; 1.97; 3.66
Lactate	1.32; 4.12
Leucine	0.94; 0.95; 1.67; 1.70; 1.73; 3.72
Lipid 1	0.82

Lipid 2	1.22
Lysine	1.43; 1.50; 1.72; 1.88; 1.91; 3.02; 3.75
Methanol**	3.36
Methionine	2.11; 2.13; 2.19; 2.63; 3.85
N-acetylgroups	2.02
Ornithine	1.74; 1.82; 1.93; 3.05; 3.78
Oxypurinol*	8.22
Phenylalanine	3.11; 3.27; 3.99; 7.32; 7.37; 7.42
Proline	1.98; 2.02; 2.34; 3.33; 3.41; 4.12
Pyroglutamate	2.02; 2.39; 2.50; 4.17
Sarcosine	2.74; 3.6
Threonine	1.32; 3.58; 4.25
Tryptophan	7.73; 7.53; 7.31; 7.27; 7.19; 4.05; 3.48; 3.30
Tyrosine	3.04; 3.19; 3.93; 6.89; 7.18
Valine	0.98; 1.03; 2.26; 3.60
τ -methylhistidine	7.76; 7.0; 3.96; 3.68; 3.16; 3.06

* = uncertain attribution; ** = extraction contaminant

Fig. S2 GC-MS chromatogram with the attributions of the metabolites in a serum sample

1. Lactic acid; 2 Valine; Retention Standard (R.S.); 3. 2-Hydroxybutyric acid; 4. Acetic acid; 5. 3-Hydroxybutyric acid; 6. Butanoic acid; 7. Urea; 8. Glycerol; 9. Phospahte; 10. Threonine; 11. Glycine; 12. Glyceric acid; 13. Glutaric acid; 14. Aspartic acid; 15. 2-Pyrrolidone; 16. D-Threitol; 17. Glutamic acid; 18. Threonic acid; 19. Citric acid; 20. 1,5-Anhydro-Sorbitol; 21. Sugars; 22. Myo-inositol; 23. Oleamide.

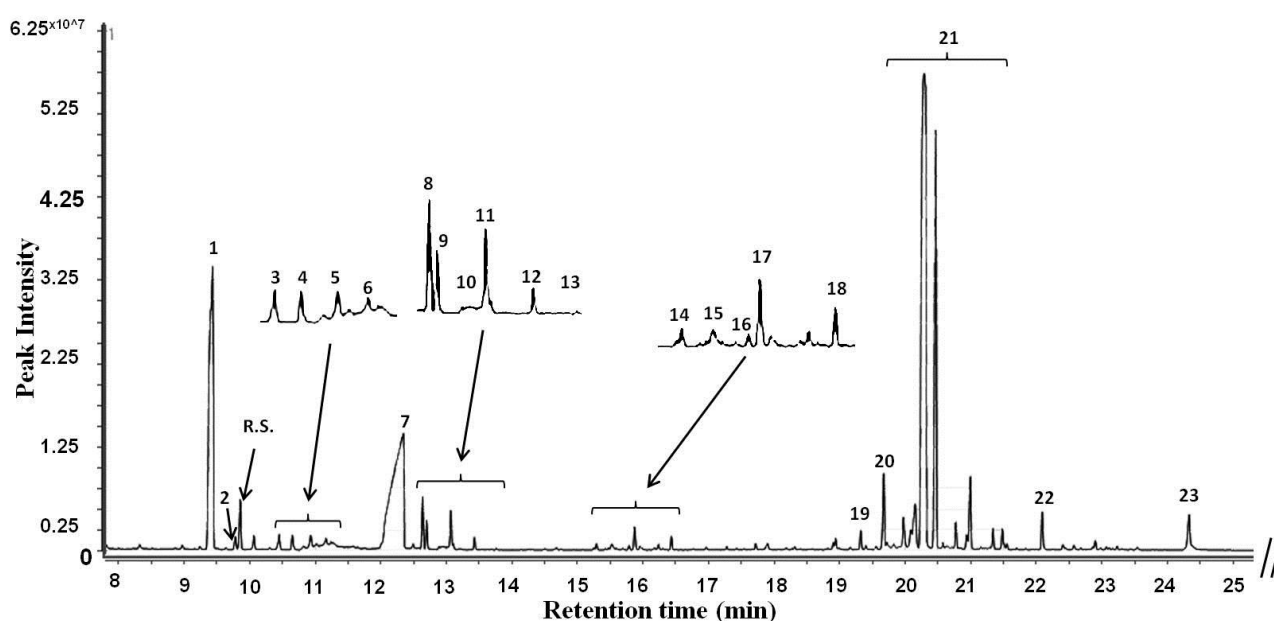


Fig. S3 PCA score plots resulting from the ^1H -NMR analysis and GC-MS analysis of Healthy Control (HC) and Systemic Sclerosis (SSc) samples, and of diffused cutaneous SSc (dcSSc) and limited cutaneous SSc (lcSSc) samples. A) PCA model of HC and SSc samples generated using the NMR serum spectra. B). PCA model of dcSSc and lcSSc samples generated using the NMR serum spectra C-D) PCA model of HC and and SSc samples generated using the GC-MS analysis. D. PCA model of dcSSc and lcSSc samples generated using the GC-MS analysis.

