

Results of full automatic measurements for human blood serum All the measurements, incorporating solvent signal suppression, are automatically set up and accomplished.

| | | 2 | <u></u> |
|--------------|---|---------------|------------|
| Filename: | [| | |
| Comment: | [| | |
| Slot: | I | Sample Status | EJECTED |
| Temp. Set: | 25[dC] | Curr. Temp. | O[dC] |
| Temp. State: | TEMP OFF | Lock Status | OFF |
| Solvent: | NO SOLVENT P-DIOXANE-D8 PYRIDINE-D5 TETRACHLOROE | THANE-D2 | |
| Notify: | [| | 01 |
| — metabonom | ics.auto2 | Single P | - Remove - |
| T2 filter | | J-resolved | |
| Diff | usion filter | | |
| | | | |

<u>Upper left</u>: ¹H spectrum with solvent signal suppression, where sharp signals and broad signals are overlapped.

<u>Upper right</u>: T₂-filter spectrum using CPMG technique, where broad signals are filtered out, leaving small molecule components.

Lower left: Diffusion-filter spectrum using BPP-LED technique, where signals having large diffusion coefficients are filtered out, leaving large molecule components.

<u>Lower right</u>: Summation spectrum of J-resolved 2D spectrum, where J couplings are removed, simplifying the spectrum.

Interface for full automatic measurements (Left)

Template for the above four measurements, which are specified by COMET (COnsortium for MEtabonomic Toxicology) project* and can also be customized on request.

* J. C. Lindon et al., Toxicology and Applied Pharmacology, 187, (2003) 137-146.

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