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visualEPR: a fast and easy-to-use web tool for visualizing and simulating EPR spectra

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SPEKTROSKOPIJA ELEKTRONSKE PARAMAGNETSKE REZONANCIJE (EPR SPEKTROSKOPIJA)

EPR — spektroskopska metoda kojom se istražuje struktura i dinamika čestica koje posjeduju nespareni elektron (paramagnetske čestice) → najčešće slobodni radikali

EPR — jedina metoda koja izravno detektira slobodne radikale

► brojne primjene

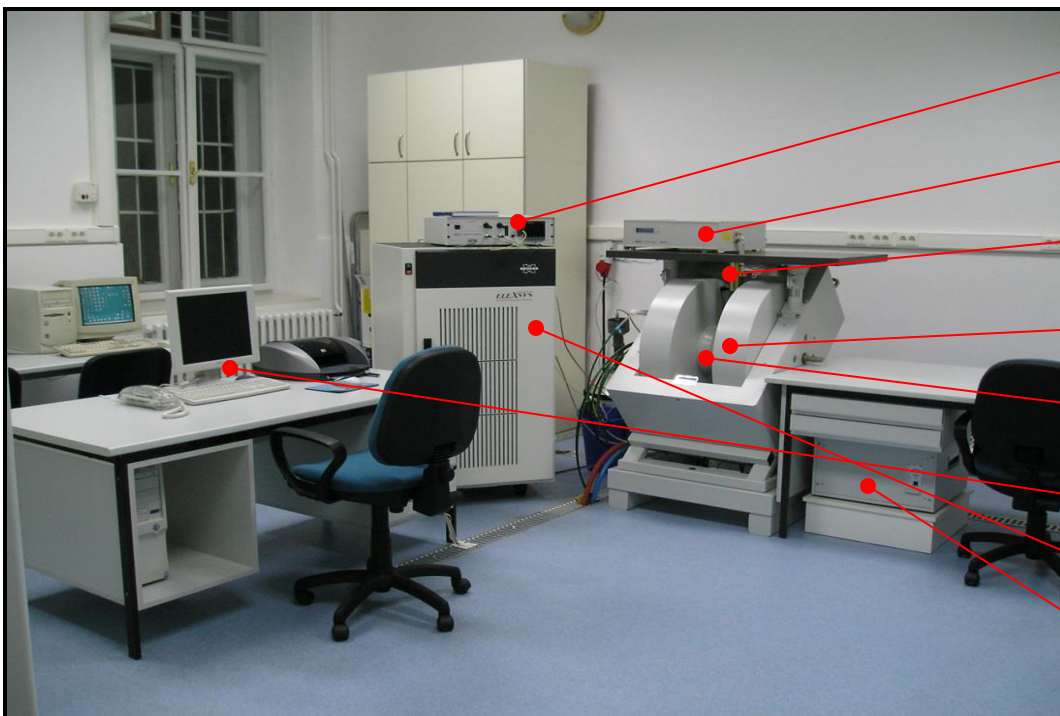
- poluvodička svojstva materijala
 - supravodička svojstva materijala
 - struktura radikala
 - kinetika kemijskih reakcija
 - oksidacija lipoproteina (LDL)
 - antioksidacijska svojstva flavonoida (vino, propolis), vitamina (E i C), ljekovitog bilja
 - dinamika lipidnog dvosloja staničnih membrana
- FIZIKA
- spin trapping
 - EPR oxometry
 - DPPH scavenging
 - spin labeling
- BIOFIZIKA
-

EPR spektrometar

EPR SPEKTROMETAR ELEXSYS E500

Laboratorij za slobodne radikale
Farmaceutsko–biokemijski fakultet, Zagreb

spin trapping / radical produced by UV light (GZ11, GZ16)
DPPH scavenging (ferrocenes)
low temperature measurements (Fe^{3+} –transferrin)



- temperaturna jedinica
- izvor mikrovalnog zračenja
- valovod
- polovi elektromagneta
- rezonantna šupljina
- računalo
- elektronički dio (konzola)
- napajanje magneta

Temeljna načela EPR spektroskopije

$$U = -\vec{\mu}_s \cdot \vec{B} \quad \hat{H} \cdot \psi = E \cdot \psi$$

... $E = m_s g \mu_B B$ energija spinskog sistema

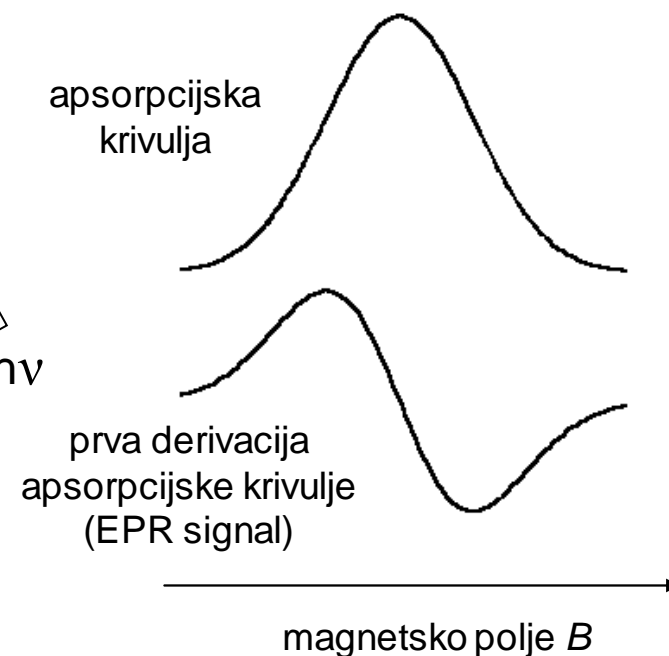
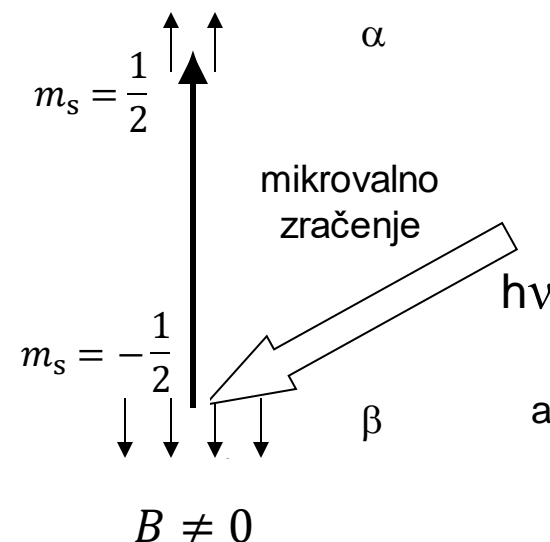
g → g -vrijednost (g -faktor)

μ_B → Bohrov magneton

$$E_\alpha = \frac{1}{2} g \mu_B B \quad E_\beta = -\frac{1}{2} g \mu_B B \quad B = 0$$

$$\Delta E = g \mu_B B \quad \text{uvjet rezonancije}$$

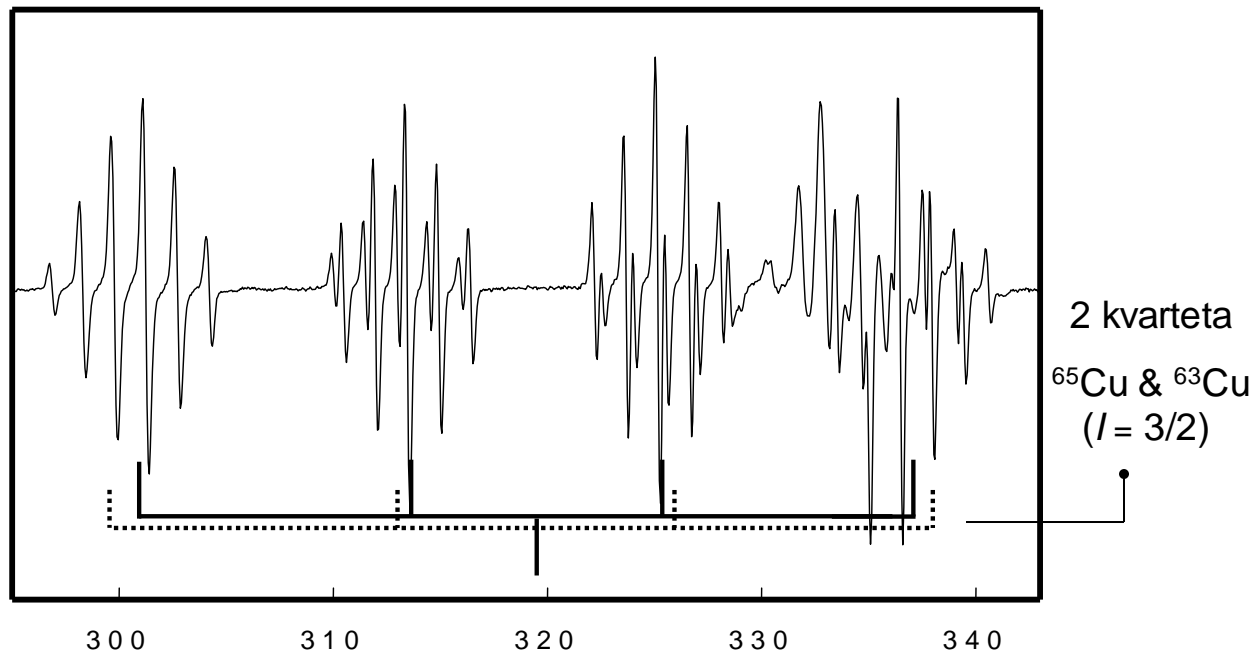
Zeemanovo cijepanje



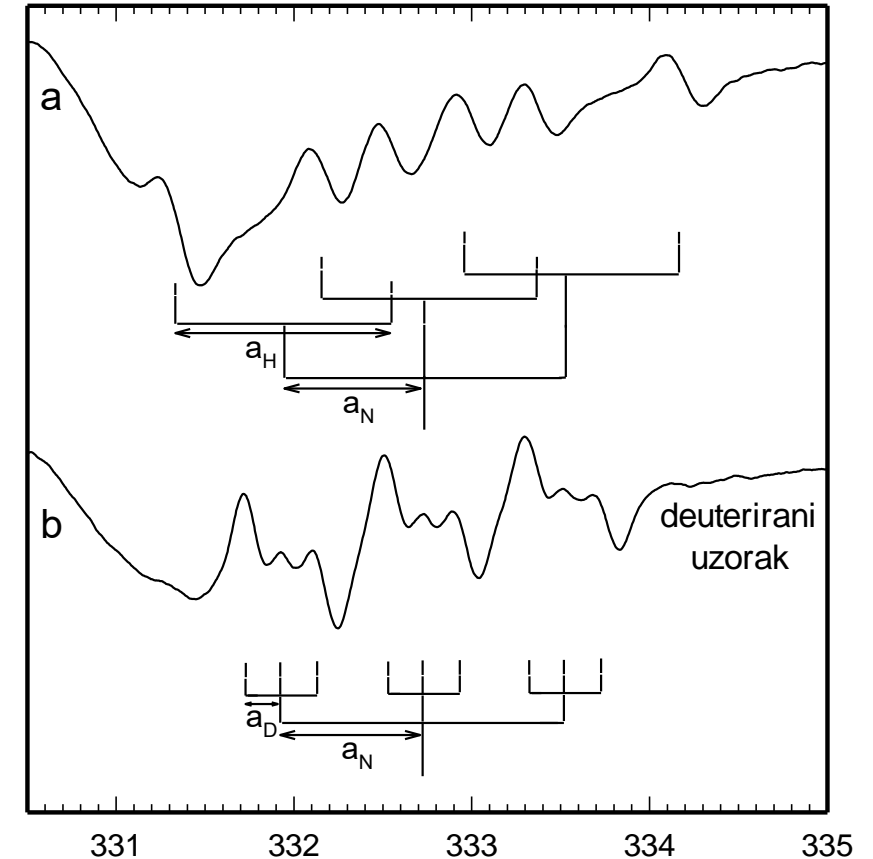
EPR spektri

► EPR spektri mogu biti kompleksni

paramagnetski kompleks Cu(II)–2-tiotimin



paramagnetski kompleks V(IV)–hidroksiurea



visual EPR

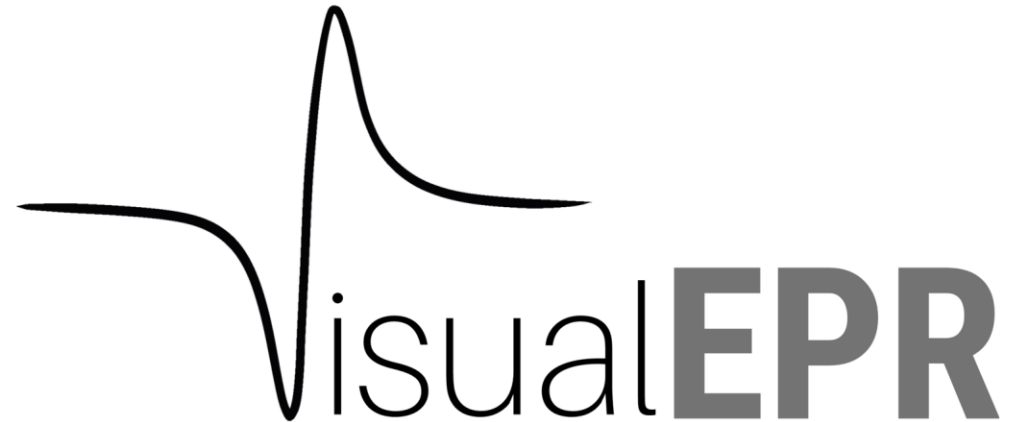
javascript spectra visualisation

LOAD EPR SPECTRA

PROCESSING

SIMULATION

EXPORT



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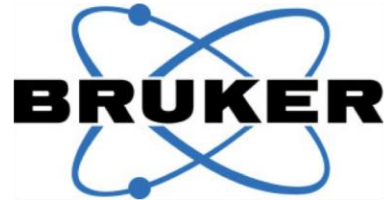
² Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

³ University of York, Department of Chemistry, Heslington, York, YO10 5DD, UK

VIEWER

Nije odabrana niti jedna datoteka.

visualEPR — DATA IMPORT



Bruker format

- .PAR + .SPC
- Little endian
- Windows or linux based

Bruker BES³T

- .DSC + .DTA
- .YGF (2D)
- Big endian
- Linux based



LINEV ADANI

- .JSON
- Human readable
- Windows based



Bruker Magnetech

- .XML
- base64 compression
- Windows based



magnetech
by Freiberg Instruments



JEOL

- proprietary
- Little endian
- Windows based

visualEPR — PROCESSING

LOAD EPR SPECTRA

PROCESSING

OPTIONS

BASELINE

FILTERING

INTEG/DERIV

MANIPULATION

SIMULATION

EXPORT

INTEG/DERIV

Apply to last trace:

1st derivation

1st integration

Baseline correction

Normalize

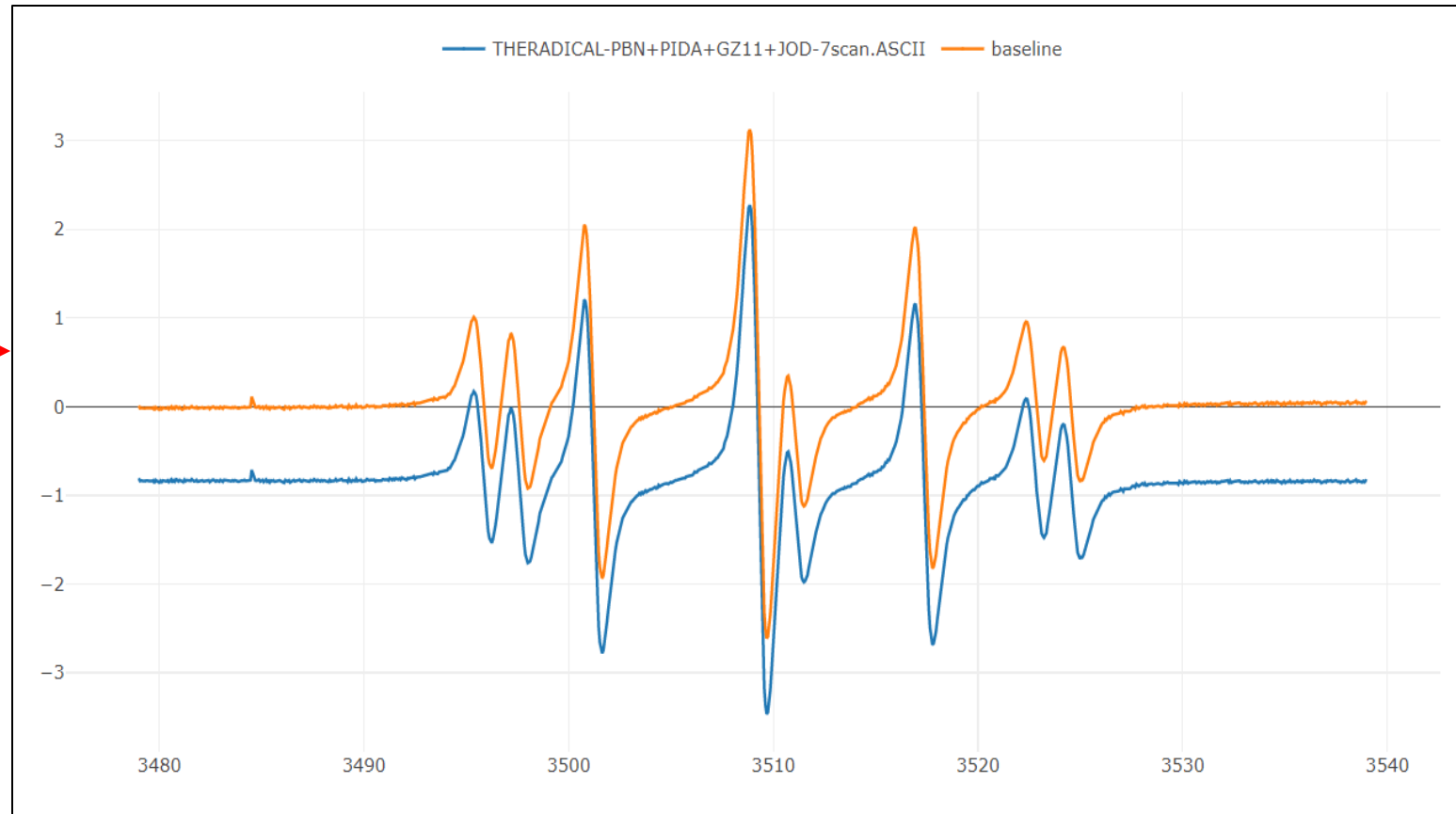
FILTERING

Apply to last trace:

Moving average

Savitzky-Golay

Noise reduction



visualEPR — SIMULATION

SIMULATION

MANUAL INPUT

Frequency (GHz)

intensity a.u.

Add radical

Remove radical

Radical 1:

relative amount (%):

g(iso):

Lorentzian (%):

line width (G):

No. equiv. nuclei:

nuclear spin:

hyperfine (G):

Radical 2:

relative amount (%):

g(iso):

Lorentzian (%):

line width (G):

No. equiv. nuclei:

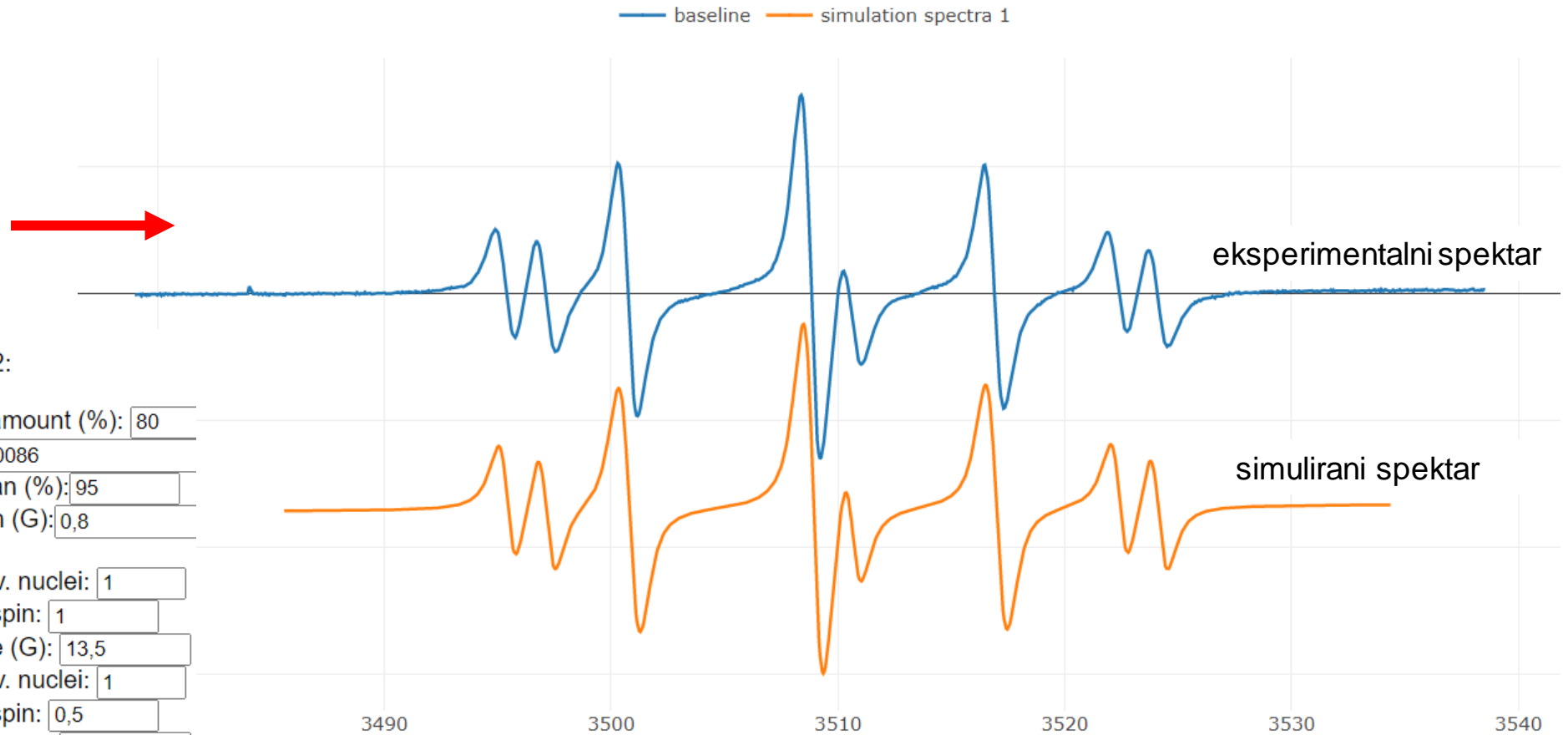
nuclear spin:

hyperfine (G):

No. equiv. nuclei:

nuclear spin:

hyperfine (G):



visualEPR — MANIPULATION

MANIPULATION

Reset Annot.

Replot

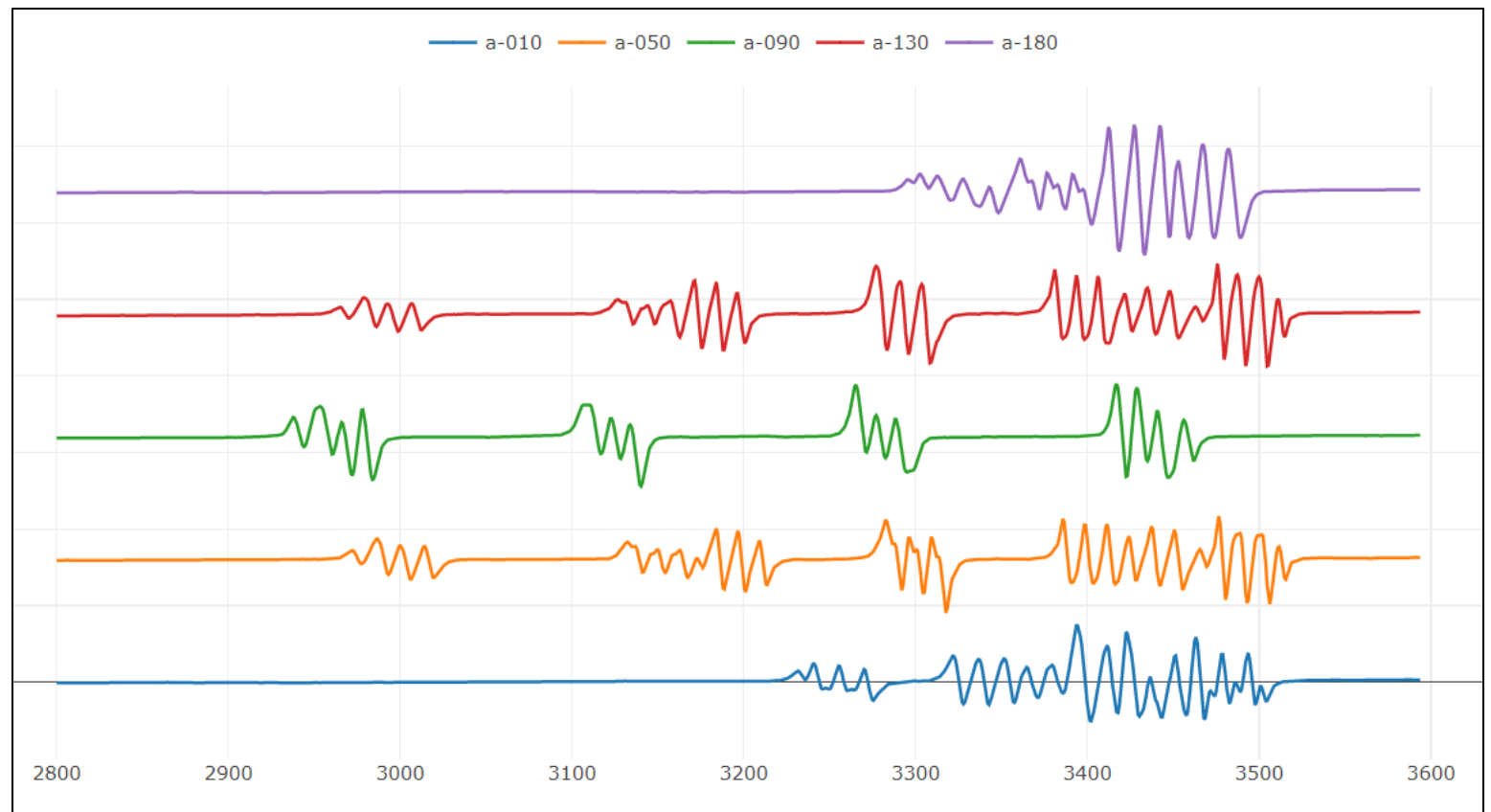
Remove last trace

Remove first trace

Resample to 1024

Overlap/panorama

Refresh page



visualEPR — EXPORT

EXPORT

GRAPH

SVG

PNG

Height:

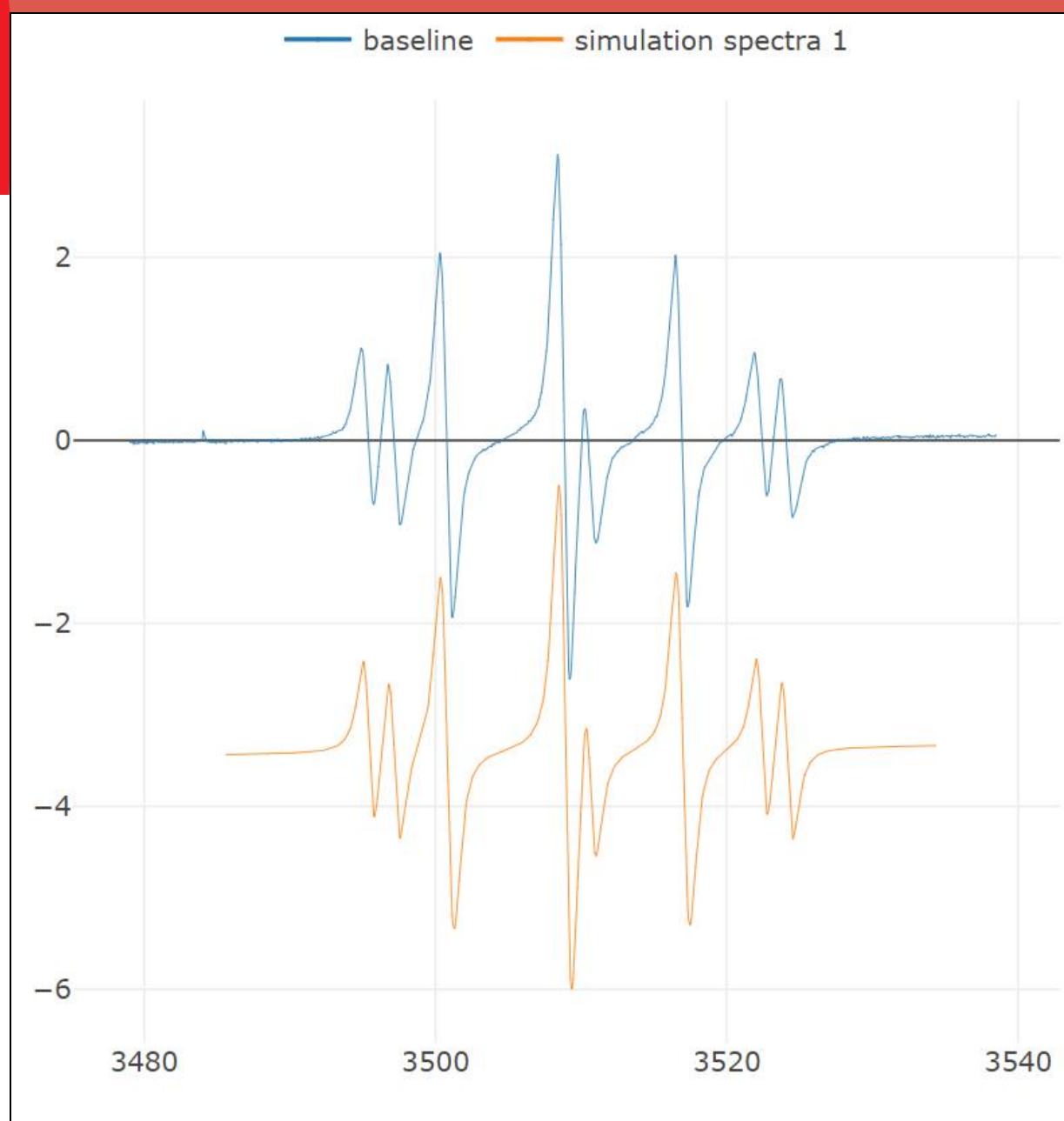
Width:

Scale:

Filename:

Show legend

Download graph



visualEPR — PREDNOSTI

- ▶ ONLINE, FREE
- ▶ IMPORTS RAW DATA FROM CURRENTLY MOST USED EPR SPECTROMETERS
- ▶ EASY-TO-RUN → pogodan za starije generacije (50+)

detalji i informacije u svezi programa visualEPR:

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