

# Adaptive Wavelet Noise Suppression

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- License
  - AWNS is provided under the GNU General Public License.
  - (C) Dadi Zhao, University of Birmingham & University College London.
  - AWNS is not for commercial use.
  - AWNS is not for clinical use at the current stage.
- Publication
  - D Zhao et al., Noise suppression of proton magnetic resonance spectroscopy improves childhood brain tumour classification. NMR Biomed, 2023
- Version
  - Version 0.1, October 2023

## Contents

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- [Settings](#)
- [Processing](#)
- [Functions \(DO NOT TOUCH\)](#)

## Settings

---

```
clear
LsMtd = {"f", "cs", "dd", "cplx", "ddd"};
LsF = {'db1', 'db2', 'db3', 'db4', 'db5', 'db6', 'db7', 'db8', 'db9', 'db10'};
LsCS = {'db1', 'db2', 'db3', 'db4', 'db5', 'db6', 'db7', 'db8', 'db9', 'db10'};
LsDD = {'filters1', 'filters2'};
LsCplx = {'dtf1', 'dtf2', 'dtf3', 'dtf4'};
LsDDD = {'dddtf1'};
LsMtd = [repmat(LsMtd{1}, length(LsF), 1);
         repelem(LsMtd{2}, length(LsCS), 1);
         repelem(LsMtd{3}, length(LsDD), 1);
         repelem(LsMtd{4}, length(LsCplx), 1);
         repelem(LsMtd{5}, length(LsDDD), 1)];
LsWv = [LsF, LsCS, LsDD, LsCplx, LsDDD];
FNLCM = 'WS.raw';
NMetab = 38;
FWHMTolerance = 1.5;
TqFS = 2000;
TqFT = 127800000;
TqTE = 0.03;
TqBasis = '1h_brain_full';
TqLoc = '/Applications/TARQUIN.app';
save('SettingsAWNS.mat')
```

## Processing

---

```
if exist(FNLCM, 'file') == 2
    AWNSPartI;
    AWNSPartII;
    AWNSPartIII;
end
```

## Functions (DO NOT TOUCH)

---

```
function AWNSPartI
load('SettingsAWNS.mat', 'LsF');
load('SettingsAWNS.mat', 'LsCS');
load('SettingsAWNS.mat', 'LsDD');
load('SettingsAWNS.mat', 'LsCplx');
load('SettingsAWNS.mat', 'LsDDD');
load('SettingsAWNS.mat', 'FNLCM');
[SpecX, H] = ReadLCMRaw(FNLCM);
LocTemp = 'Temporary';
if ~exist(LocTemp, 'dir')
    mkdir(LocTemp);
end
mkdir('Temporary/f')
mkdir('Temporary/cs')
mkdir('Temporary/dd')
mkdir('Temporary/cplx')
mkdir('Temporary/ddd')
LsWv = LsF;
for iWv = 1:length(LsWv)
    SpecY = ifft(WaveletDecomp(fft(SpecX), 'wv', 'Lvd', LsWv{iWv}, 1));
    WriteLCMRaw(['Temporary/f/', LsWv{iWv}, '.raw'], SpecY, H);
end
fclose('all');
LsWv = LsCS;
for iWv = 1:length(LsWv)
    SpecY = ifft(WaveletDecompCriticallySampled(fft(SpecX), LsWv{iWv}, 1));
    WriteLCMRaw(['Temporary/cs/', LsWv{iWv}, '.raw'], SpecY, H);
end
fclose('all');
```

```

LsWv = LsDD;
for iWv = 1:length(LsWv)
    SpecY = ifft(WaveletDecompDoubleDensity(fft(SpecX),LsWv{iWv},1));
    FO = ['Temporary/dd/',LsWv{iWv},'.raw'];
    WriteLCMRaw(FO, SpecY, H);
end
fclose('all');
LsWv = LsCplx;
for iWv = 1:length(LsWv)
    SpecY = ifft(WaveletDecompComplex(fft(SpecX),LsWv{iWv},1));
    FO = ['Temporary/cplx/',LsWv{iWv},'.raw'];
    WriteLCMRaw(FO, SpecY(:,1), H);
end
fclose('all');
LsWv = LsDDD;
for iWv = 1:length(LsWv)
    SpecY = ifft(WaveletDecompComplex(fft(SpecX),LsWv{iWv},1));
    FO = ['Temporary/ddd/',LsWv{iWv},'.raw'];
    WriteLCMRaw(FO, SpecY(:,1), H);
end
fclose('all');
end
function AWNSPartII
disp('Please make sure you are using macOS or Linux.')
load('SettingsAWNS.mat', 'LsWv');
load('SettingsAWNS.mat', 'LsMtd');
load('SettingsAWNS.mat', 'TqFS');
load('SettingsAWNS.mat', 'TqFT');
load('SettingsAWNS.mat', 'TqTE');
load('SettingsAWNS.mat', 'TqLoc');
load('SettingsAWNS.mat', 'TqBasis');
fileID = fopen('TARQUIN4AWNS.sh', 'w');
fprintf(fileID, ['export PATH=$PATH:', TqLoc, '/Contents/MacOS \n'];
fprintf(fileID, ['tarquin',...
    ' --input WS.raw',...
    ' --input_w W.raw',...
    ' --format lcm',...
    ' --fs ', num2str(TqFS),...
    ' --ft ', num2str(TqFT),...
    ' --echo ', num2str(TqTE),...
    ' --int_basis ', TqBasis,...
    ' --output_txt d0.txt \n']);
for iWv = 1:length(LsWv)
    fprintf(fileID, ['tarquin',...
        ' --input Temporary/', LsMtd{iWv}, '/', LsWv{iWv}, '.raw',...
        ' --input_w W.raw',...
        ' --format lcm',...
        ' --fs ', num2str(TqFS),...
        ' --ft ', num2str(TqFT),...
        ' --echo ', num2str(TqTE),...
        ' --int_basis ', TqBasis,...
        ' --output_txt Temporary/', LsMtd{iWv}, '/', LsWv{iWv}, '.txt \n']);
end
fclose(fileID);
system('sh TARQUIN4AWNS.sh')
delete('TARQUIN4AWNS.sh')
end
function AWNSPartIII
load('SettingsAWNS.mat', 'LsWv');
load('SettingsAWNS.mat', 'LsMtd');
load('SettingsAWNS.mat', 'FWHMTolerance');
load('SettingsAWNS.mat', 'FNLCM');
[~, FWHM0] = ObtainQC(FNLCM);
[LsfSNR, LsFWHM] = ObtainQCList;
[~, Index] = sort(LsfSNR, 'descend');
iS = 1;
iD = Index(iS);
while (LsFWHM(iD) > FWHM0*FWHMTolerance)
    iS = iS + 1;
    iD = Index(iS);
end
MtdS = LsMtd{iD};
BasS = LsWv{iD};
copyfile(['Temporary/', MtdS, '/', BasS, '.raw'], 'd1.raw')
copyfile(['Temporary/', MtdS, '/', BasS, '.txt'], 'd1.txt')
rmdir('Temporary', 's')
end
function [LsfSNR, LsFWHM] = ObtainQCList
load('SettingsAWNS.mat', 'LsWv');
load('SettingsAWNS.mat', 'LsMtd');
LsfSNR = zeros(length(LsWv),1);
LsFWHM = zeros(length(LsWv),1);
for iWv = 1:length(LsWv)
    TqTxt = ['Temporary/', LsMtd{iWv}, '/', LsWv{iWv}, '.txt'];
    [LsfSNR(iWv), LsFWHM(iWv)] = ObtainQC(TqTxt);
end
end
function [X, H] = ReadLCMRaw( FNLCM )
[~,~,Ext] = fileparts(FNLCM);
if isempty(Ext) == 1
    FNLCM = [FNLCM, '.RAW'];
end
F = fopen(FNLCM, 'r');
C = textscan(F, '%f', 4096*2, 'headerlines', 5);
D = reshape(C{1,1},2,[],[]);
fclose(F);
F = fopen(FNLCM, 'r');

```

```

temp = textscan(F, '%s', 'delimiter', '\n');
content = temp{1,1};
H = content(1:5,1);
fclose(F);
X = transpose(D(1,:)) + 1i.*transpose(D(2,:));
end
function WriteLCMRaw( FNLCM, X, H )
F = fopen(FNLCM, 'w');
fprintf(F, ' $NMID\n');
fprintf(F, [' $FMTDAT=', char(39), '(2E15.6)', char(39), '\n']);
fprintf(F, [' ', H{3}, ' \n']);
fprintf(F, [' ', H{4}, ' \n']);
fprintf(F, ' $END\n');
res = zeros(length(X),2);
res(:,1) = real(X);
res(:,2) = imag(X);
for i = 1:length(X)
    if res(i,1) > 0 && res(i,2) > 0
        T = [' ', num2str(res(i,1), '%5d'), ' ', num2str(res(i,2), '%5d'), '\n'];
        fprintf(F, T);
    elseif res(i,1) < 0 && res(i,2) < 0
        T = [' ', num2str(res(i,1), '%5d'), ' ', num2str(res(i,2), '%5d'), '\n'];
        fprintf(F, T);
    elseif res(i,1) > 0 && res(i,2) < 0
        T = [' ', num2str(res(i,1), '%5d'), ' ', num2str(res(i,2), '%5d'), '\n'];
        fprintf(F, T);
    else
        T = [' ', num2str(res(i,1), '%5d'), ' ', num2str(res(i,2), '%5d'), '\n'];
        fprintf(F, T);
    end
end
fclose('all');
end
function [SNRO, FWHM] = ObtainQC(TQOutputTxt)
load('SettingsAWNS.mat', 'NMetab');
F = fopen (TQOutputTxt, 'r');
T = textscan(F, '%s', 'delimiter', '\n');
T = T{1,1};
T1 = T{NMetab+7,1};
FWHM = str2double(T1(20:length(T1)));
T1 = T{NMetab+8,1};
SNRO = str2double(T1(20:length(T1)));
fclose(F);
end
function Y = WaveletDecompDoubleDensity( X, DTBasis, Lv )
YR = dddtree('ddt', real(X), Lv, DTBasis);
YR = YR.cfs{2};
YI = dddtree('ddt', imag(X), Lv, DTBasis);
YI = YI.cfs{2};
Y = YR + 1i* YI;
end
function Y = WaveletDecompComplex( X, DTBasis, Lv )
YR = dddtree('cplxdt', real(X), Lv, DTBasis);
YR = YR.cfs{2};
YI = dddtree('cplxdt', imag(X), Lv, DTBasis);
YI = YI.cfs{2};
Y = YR + 1i* YI;
end
function Y = WaveletDecomp( X, WvPT, Thr, WvN, Lv )
[c,l] = wavedec(real(X), Lv, WvN);
[threshold, sorh, keepapp] = ddencmp('den', WvPT, detcoef(c,l,Lv));
if strcmp(Thr, 'gbl')
    YR = wdencmp('gbl', real(X), WvN, Lv, threshold, sorh, keepapp);
else
    threshold = zeros(1, Lv);
    keepapp = zeros(1, Lv);
    for i = 1:Lv
        [threshold(i), ~, keepapp(i)] = ddencmp('den', WvPT, detcoef(c,l,i));
    end
    YR = wdencmp('lvd', real(X), WvN, Lv, threshold, sorh);
end
[c,l] = wavedec(imag(X), Lv, WvN);
[threshold, sorh, keepapp] = ddencmp('den', WvPT, detcoef(c,l,Lv));
if strcmp(Thr, 'gbl')
    YI = wdencmp('gbl', imag(X), WvN, Lv, threshold, sorh, keepapp);
else
    threshold = zeros(1, Lv);
    keepapp = zeros(1, Lv);
    for i = 1:Lv
        [threshold(i), ~, keepapp(i)] = ddencmp('den', WvPT, detcoef(c,l,i));
    end
    YI = wdencmp('lvd', imag(X), WvN, Lv, threshold, sorh);
end
Y = YR + 1i*YI;
end
function Y = WaveletDecompCriticallySampled( X, DTBasis, Lv )
YR = dddtree('dwt', real(X), Lv, DTBasis);
YR = YR.cfs{2};
YI = dddtree('dwt', imag(X), Lv, DTBasis);
YI = YI.cfs{2};
Y = YR + 1i* YI;
end

```

Warning: Perfect reconstruction is not guaranteed.  
Warning: Perfect reconstruction is not guaranteed.  
Please make sure you are using macOS or Linux.

2023-Oct-27 06:24:21 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:21 INFO : Loading data file : WS.raw  
2023-Oct-27 06:24:21 INFO : nStart = 20  
2023-Oct-27 06:24:21 INFO : nEnd = 512  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:21 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:21 INFO : nStart = 20  
2023-Oct-27 06:24:21 INFO : nEnd = 512

Parameters Before Preprocessing

-----  
Input file: WS.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:21 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:21 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:21 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:21 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:21 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:21 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:21 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:21 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:21 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:21 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:22 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:22 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:22 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:22 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:22 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:22 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:22 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:22 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:22 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:22 INFO : Ref new = 4.667193 ppm  
2023-Oct-27 06:24:22 DEBUG : Width pts : 35.58  
2023-Oct-27 06:24:22 DEBUG : Width Hz est : 5.79  
2023-Oct-27 06:24:22 DEBUG : Init beta est : 81.68  
2023-Oct-27 06:24:22 INFO : Ymax = 0.021505  
2023-Oct-27 06:24:22 INFO : sdev noise = 0.000294  
2023-Oct-27 06:24:22 INFO : SNR guess = 36.5890  
2023-Oct-27 06:24:22 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: WS.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.66719 ppm

2023-Oct-27 06:24:22 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:22 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:22 INFO : Running optimiser  
2023-Oct-27 06:24:22 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:22 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:22 INFO : 31 group vectors in total  
2023-Oct-27 06:24:22 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:22 INFO : Final nStart = 20  
2023-Oct-27 06:24:22 INFO : Final nEnd = 512  
2023-Oct-27 06:24:22 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:22 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:22 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:22 INFO : Adjusting basis set to 4.667193 ppm  
2023-Oct-27 06:24:22 INFO : Time domain noise = 0.000009  
2023-Oct-27 06:24:22 DEBUG : Using init\_beta: 81.683640  
2023-Oct-27 06:24:22 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:22 DEBUG : Initial phase fit completed.....

2023-Oct-27 06:24:23 INFO : done.  
2023-Oct-27 06:24:23 DEBUG : Final Beta: 101.48  
2023-Oct-27 06:24:23 DEBUG : Final Phi0: -0.14  
2023-Oct-27 06:24:23 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:23 INFO : FWHM right ppm = 2.000367  
2023-Oct-27 06:24:23 INFO : FWHM left ppm = 2.046215  
2023-Oct-27 06:24:23 INFO : Metabolite FWHM (ppm) = 0.045848  
2023-Oct-27 06:24:23 INFO : Spec noise = 0.000010  
2023-Oct-27 06:24:23 INFO : sdev noise = 0.000405  
2023-Oct-27 06:24:23 INFO : SNR residual = 24.750225  
2023-Oct-27 06:24:23 INFO : SNR max = 32.254437  
2023-Oct-27 06:24:23 INFO : Ymax = 0.020035  
2023-Oct-27 06:24:23 INFO : Ymax metab = 0.020035  
2023-Oct-27 06:24:23 INFO : Fit quality = 1.303198  
2023-Oct-27 06:24:23 INFO : Baseline dev = 0.028852  
2023-Oct-27 06:24:23 INFO : Ymax = 0.020035  
2023-Oct-27 06:24:23 INFO : BSL = 0.040535  
2023-Oct-27 06:24:23 INFO : Computing CRLBs.  
2023-Oct-27 06:24:23 DEBUG : Sigma: 9.013012e-11  
2023-Oct-27 06:24:23 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 2.62852  
l2 norm of error at final p = 1.63672  
l2 norm of J.\*e at final p = 260.934  
l2 norm of D\*p at final p = 7.88326e-12  
number of iterations = 18  
number of function evaluations = 2  
number of Jacobian evaluations = 194  
stopped by small D\*p

2023-Oct-27 06:24:23 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:23 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:23 INFO : Loading data file : Temporary/f/db1.raw  
2023-Oct-27 06:24:23 INFO : nStart = 20  
2023-Oct-27 06:24:23 INFO : nEnd = 512  
TARQUIN Version 4.3.11

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2023-Oct-27 06:24:23 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:23 INFO : nStart = 20  
2023-Oct-27 06:24:23 INFO : nEnd = 512  
Parameters Before Preprocessing

-----  
Input file: Temporary/f/db1.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:23 INFO : Starting 'Preprocessing'  
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2023-Oct-27 06:24:23 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:23 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:23 INFO : Ref new = 4.667193 ppm  
2023-Oct-27 06:24:23 DEBUG : Width pts : 37.16  
2023-Oct-27 06:24:23 DEBUG : Width Hz est : 6.05  
2023-Oct-27 06:24:23 DEBUG : Init beta est : 90.73  
2023-Oct-27 06:24:23 INFO : Ymax = 0.022243  
2023-Oct-27 06:24:23 INFO : sdev noise = 0.000193  
2023-Oct-27 06:24:23 INFO : SNR guess = 57.6965  
2023-Oct-27 06:24:23 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/f/db1.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.66719 ppm

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2023-Oct-27 06:24:23 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:23 INFO : Adjusting basis set to 4.667193 ppm  
2023-Oct-27 06:24:23 INFO : Time domain noise = 0.000003  
2023-Oct-27 06:24:23 DEBUG : Using init\_beta: 90.729856  
2023-Oct-27 06:24:23 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:23 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:25 INFO : done.  
2023-Oct-27 06:24:25 DEBUG : Final Beta: 106.58  
2023-Oct-27 06:24:25 DEBUG : Final Phi0: -0.25  
2023-Oct-27 06:24:25 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:25 INFO : FWHM right ppm = 1.996547  
2023-Oct-27 06:24:25 INFO : FWHM left ppm = 2.046215  
2023-Oct-27 06:24:25 INFO : Metabolite FWHM (ppm) = 0.049669  
2023-Oct-27 06:24:25 INFO : Spec noise = 0.000006  
2023-Oct-27 06:24:25 INFO : sdev noise = 0.000442  
2023-Oct-27 06:24:25 INFO : SNR residual = 22.865112  
2023-Oct-27 06:24:25 INFO : SNR max = 55.202181  
2023-Oct-27 06:24:25 INFO : Ymax = 0.020196  
2023-Oct-27 06:24:25 INFO : Ymax metab = 0.020196  
2023-Oct-27 06:24:25 INFO : Fit quality = 2.414254  
2023-Oct-27 06:24:25 INFO : Baseline dev = 0.033406  
2023-Oct-27 06:24:25 INFO : Ymax = 0.020196  
2023-Oct-27 06:24:25 INFO : BSL = 0.060913  
2023-Oct-27 06:24:25 INFO : Computing CRLBs.  
2023-Oct-27 06:24:25 DEBUG : Sigma: 8.842851e-12  
2023-Oct-27 06:24:25 INFO : done.

Optimisation details

-----  
l2 norm of error at initial p = 2.46666  
l2 norm of error at final p = 1.26772  
l2 norm of J.\*e at final p = 49.1529  
l2 norm of D\*p at final p = 2.61881e-33  
number of iterations = 18  
number of function evaluations = 2  
number of Jacobian evaluations = 421  
stopped by small D\*p

2023-Oct-27 06:24:25 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:25 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:25 INFO : Loading data file : Temporary/f/db2.raw  
2023-Oct-27 06:24:25 INFO : nStart = 20  
2023-Oct-27 06:24:25 INFO : nEnd = 512  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:25 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:25 INFO : nStart = 20  
2023-Oct-27 06:24:25 INFO : nEnd = 512

Parameters Before Preprocessing

-----  
Input file: Temporary/f/db2.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s

Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:25 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:25 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:25 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:25 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:25 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:25 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:25 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:25 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:25 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:25 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:25 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:25 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:25 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:25 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:25 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:25 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:25 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:25 DEBUG : Max Phi0 : 0.31  
2023-Oct-27 06:24:25 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:25 INFO : Ref new = 4.667193 ppm  
2023-Oct-27 06:24:25 DEBUG : Width pts : 37.94  
2023-Oct-27 06:24:25 DEBUG : Width Hz est : 6.17  
2023-Oct-27 06:24:25 DEBUG : Init beta est : 95.32  
2023-Oct-27 06:24:25 INFO : Ymax = 0.021338  
2023-Oct-27 06:24:25 INFO : sdev noise = 0.000204  
2023-Oct-27 06:24:25 INFO : SNR guess = 52.3005  
2023-Oct-27 06:24:25 INFO : Finished 'Preprocessing'

#### Parameters After Preprocessing

-----  
Input file: Temporary/f/db2.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.66719 ppm

2023-Oct-27 06:24:25 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:25 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:25 INFO : Running optimiser  
2023-Oct-27 06:24:25 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:25 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:25 INFO : 31 group vectors in total  
2023-Oct-27 06:24:25 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:25 INFO : Final nStart = 20  
2023-Oct-27 06:24:25 INFO : Final nEnd = 512  
2023-Oct-27 06:24:25 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:25 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:25 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:25 INFO : Adjusting basis set to 4.667193 ppm  
2023-Oct-27 06:24:25 INFO : Time domain noise = 0.000003  
2023-Oct-27 06:24:25 DEBUG : Using init\_beta: 95.317843  
2023-Oct-27 06:24:25 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:25 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:26 INFO : done.  
2023-Oct-27 06:24:26 DEBUG : Final Beta: 137.99  
2023-Oct-27 06:24:26 DEBUG : Final Phi0: -0.29  
2023-Oct-27 06:24:26 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:26 INFO : FWHM right ppm = 1.996547  
2023-Oct-27 06:24:26 INFO : FWHM left ppm = 2.046215  
2023-Oct-27 06:24:26 INFO : Metabolite FWHM (ppm) = 0.049669  
2023-Oct-27 06:24:26 INFO : Spec noise = 0.000005  
2023-Oct-27 06:24:26 INFO : sdev noise = 0.000368  
2023-Oct-27 06:24:26 INFO : SNR residual = 26.651609  
2023-Oct-27 06:24:26 INFO : SNR max = 57.710707  
2023-Oct-27 06:24:26 INFO : Ymax = 0.019607  
2023-Oct-27 06:24:26 INFO : Ymax metab = 0.019607  
2023-Oct-27 06:24:26 INFO : Fit quality = 2.165374  
2023-Oct-27 06:24:26 INFO : Baseline dev = 0.038555  
2023-Oct-27 06:24:26 INFO : Ymax = 0.019607  
2023-Oct-27 06:24:26 INFO : BSL = 0.070530  
2023-Oct-27 06:24:26 INFO : Computing CRLBs.  
2023-Oct-27 06:24:26 DEBUG : Sigma: 9.128884e-12  
2023-Oct-27 06:24:26 INFO : done.

Optimisation details

-----  
l2 norm of error at initial p = 2.38997  
l2 norm of error at final p = 1.13992  
l2 norm of J.\*e at final p = 219.778  
l2 norm of D\*p at final p = 1.19789e-08  
number of iterations = 12  
number of function evaluations = 2  
number of Jacobian evaluations = 36  
stopped by small D\*p

2023-Oct-27 06:24:26 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:26 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:26 INFO : Loading data file : Temporary/f/db3.raw  
2023-Oct-27 06:24:26 INFO : nStart = 20  
2023-Oct-27 06:24:26 INFO : nEnd = 512  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:26 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:26 INFO : nStart = 20  
2023-Oct-27 06:24:26 INFO : nEnd = 512

Parameters Before Preprocessing

-----  
Input file: Temporary/f/db3.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:26 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:26 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:26 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:26 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:26 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:26 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:26 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:26 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:26 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:26 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:26 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:26 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:26 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:26 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:26 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:26 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:26 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:26 DEBUG : Max Phi0 : -0.06  
2023-Oct-27 06:24:26 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:26 INFO : Ref new = 4.669103 ppm  
2023-Oct-27 06:24:26 DEBUG : Width pts : 27.85  
2023-Oct-27 06:24:26 DEBUG : Width Hz est : 4.53  
2023-Oct-27 06:24:26 DEBUG : Init beta est : 44.43  
2023-Oct-27 06:24:26 INFO : Ymax = 0.017535  
2023-Oct-27 06:24:26 INFO : sdev noise = 0.000209  
2023-Oct-27 06:24:26 INFO : SNR guess = 41.9804  
2023-Oct-27 06:24:26 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/f/db3.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.6691 ppm

```
2023-Oct-27 06:24:26 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:26 INFO : All simulation threads stopped.
2023-Oct-27 06:24:26 INFO : Running optimiser
2023-Oct-27 06:24:26 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:26 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:26 INFO : 31 group vectors in total
2023-Oct-27 06:24:26 INFO : 31 basis vectors in total
2023-Oct-27 06:24:26 INFO : Final nStart = 20
2023-Oct-27 06:24:26 INFO : Final nEnd = 512
2023-Oct-27 06:24:26 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:26 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:26 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:26 INFO : Adjusting basis set to 4.669103 ppm
2023-Oct-27 06:24:26 INFO : Time domain noise = 0.000003
2023-Oct-27 06:24:26 DEBUG : Using init_beta: 44.427239
2023-Oct-27 06:24:26 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:26 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:27 INFO : done.
2023-Oct-27 06:24:27 DEBUG : Final Beta: 141.77
2023-Oct-27 06:24:27 DEBUG : Final Phi0: -0.38
2023-Oct-27 06:24:27 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:27 INFO : FWHM right ppm = 1.994636
2023-Oct-27 06:24:27 INFO : FWHM left ppm = 2.044305
2023-Oct-27 06:24:27 INFO : Metabolite FWHM (ppm) = 0.049669
2023-Oct-27 06:24:27 INFO : Spec noise = 0.000006
2023-Oct-27 06:24:27 INFO : sdev noise = 0.000369
2023-Oct-27 06:24:27 INFO : SNR residual = 26.704832
2023-Oct-27 06:24:27 INFO : SNR max = 55.192983
2023-Oct-27 06:24:27 INFO : Ymax = 0.019732
2023-Oct-27 06:24:27 INFO : Ymax metab = 0.019732
2023-Oct-27 06:24:27 INFO : Fit quality = 2.066779
2023-Oct-27 06:24:27 INFO : Baseline dev = 0.036925
2023-Oct-27 06:24:27 INFO : Ymax = 0.019732
2023-Oct-27 06:24:27 INFO : BSL = 0.022194
2023-Oct-27 06:24:27 INFO : Computing CRLBs.
2023-Oct-27 06:24:27 DEBUG : Sigma: 8.687861e-12
2023-Oct-27 06:24:27 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 3.97555
l2 norm of error at final p = 1.15165
l2 norm of J.*e at final p = 422.109
l2 norm of D*p at final p = 1.53408e-09
number of iterations = 12
number of function evaluations = 2
number of Jacobian evaluations = 166
stopped by small D*p
```

```
2023-Oct-27 06:24:27 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:27 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:27 INFO : Loading data file : Temporary/f/db4.raw
2023-Oct-27 06:24:27 INFO : nStart = 20
2023-Oct-27 06:24:27 INFO : nEnd = 512
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:27 INFO : Loading data file : W.raw
2023-Oct-27 06:24:27 INFO : nStart = 20
2023-Oct-27 06:24:27 INFO : nEnd = 512
Parameters Before Preprocessing
```

```
-----
Input file: Temporary/f/db4.raw
Water reference file: W.raw
Data points: 1024
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 512
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:27 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:27 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:27 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:27 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:27 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:27 INFO : Ref new = 4.636628 ppm
2023-Oct-27 06:24:27 INFO : Residual water freq. (Hz) : -1.708984
2023-Oct-27 06:24:27 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:27 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:27 INFO : Starting 'SVD of LP matrix'
```

```
2023-Oct-27 06:24:28 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:28 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:28 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:28 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:28 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:28 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:28 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:28 DEBUG : Max Phi0 : 0.50
2023-Oct-27 06:24:28 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:28 INFO : Ref new = 4.667193 ppm
2023-Oct-27 06:24:28 DEBUG : Width pts : 39.71
2023-Oct-27 06:24:28 DEBUG : Width Hz est : 6.46
2023-Oct-27 06:24:28 DEBUG : Init beta est : 106.26
2023-Oct-27 06:24:28 INFO : Ymax = 0.020277
2023-Oct-27 06:24:28 INFO : sdev noise = 0.000206
2023-Oct-27 06:24:28 INFO : SNR guess = 49.1441
2023-Oct-27 06:24:28 INFO : Finished 'Preprocessing'
```

#### Parameters After Preprocessing

```
-----
Input file: Temporary/f/db4.raw
Water reference file: W.raw
Data points: 1024
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 512
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.66719 ppm
```

```
2023-Oct-27 06:24:28 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:28 INFO : All simulation threads stopped.
2023-Oct-27 06:24:28 INFO : Running optimiser
2023-Oct-27 06:24:28 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:28 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:28 INFO : 31 group vectors in total
2023-Oct-27 06:24:28 INFO : 31 basis vectors in total
2023-Oct-27 06:24:28 INFO : Final nStart = 20
2023-Oct-27 06:24:28 INFO : Final nEnd = 512
2023-Oct-27 06:24:28 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:28 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:28 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:28 INFO : Adjusting basis set to 4.667193 ppm
2023-Oct-27 06:24:28 INFO : Time domain noise = 0.000002
2023-Oct-27 06:24:28 DEBUG : Using init_beta: 106.260046
2023-Oct-27 06:24:28 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:28 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:28 INFO : done.
2023-Oct-27 06:24:28 DEBUG : Final Beta: 143.97
2023-Oct-27 06:24:28 DEBUG : Final Phi0: -0.04
2023-Oct-27 06:24:28 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:28 INFO : FWHM right ppm = 1.992726
2023-Oct-27 06:24:28 INFO : FWHM left ppm = 2.046215
2023-Oct-27 06:24:28 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:28 INFO : Spec noise = 0.000006
2023-Oct-27 06:24:28 INFO : sdev noise = 0.000352
2023-Oct-27 06:24:28 INFO : SNR residual = 27.414364
2023-Oct-27 06:24:28 INFO : SNR max = 50.263414
2023-Oct-27 06:24:28 INFO : Ymax = 0.019274
2023-Oct-27 06:24:28 INFO : Ymax metab = 0.019274
2023-Oct-27 06:24:28 INFO : Fit quality = 1.833470
2023-Oct-27 06:24:28 INFO : Baseline dev = 0.034776
2023-Oct-27 06:24:28 INFO : Ymax = 0.019274
2023-Oct-27 06:24:28 INFO : BSL = 0.049220
2023-Oct-27 06:24:28 INFO : Computing CRLBs.
2023-Oct-27 06:24:28 DEBUG : Sigma: 5.508932e-12
2023-Oct-27 06:24:28 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.10197
l2 norm of error at final p = 1.17504
l2 norm of J.'*e at final p = 358.258
l2 norm of D*p at final p = 7.89963e-12
number of iterations = 9
number of function evaluations = 2
number of Jacobian evaluations = 180
stopped by small D*p
```

```
2023-Oct-27 06:24:28 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:28 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:28 INFO : Loading data file : Temporary/f/db5.raw
2023-Oct-27 06:24:28 INFO : nStart = 20
```

2023-Oct-27 06:24:28 INFO : nEnd = 512  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:28 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:28 INFO : nStart = 20  
2023-Oct-27 06:24:28 INFO : nEnd = 512  
Parameters Before Preprocessing

-----  
Input file: Temporary/f/db5.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:28 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:28 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:28 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:28 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:28 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:28 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:28 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:28 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:28 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:28 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:29 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:29 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:29 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:29 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:29 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:29 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:29 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:29 DEBUG : Max Phi0 : 0.50  
2023-Oct-27 06:24:29 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:29 INFO : Ref new = 4.688207 ppm  
2023-Oct-27 06:24:29 DEBUG : Width pts : 25.63  
2023-Oct-27 06:24:29 DEBUG : Width Hz est : 4.17  
2023-Oct-27 06:24:29 DEBUG : Init beta est : 35.80  
2023-Oct-27 06:24:29 INFO : Ymax = 0.015448  
2023-Oct-27 06:24:29 INFO : sdev noise = 0.000204  
2023-Oct-27 06:24:29 INFO : SNR guess = 37.7937  
2023-Oct-27 06:24:29 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/f/db5.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.68821 ppm

2023-Oct-27 06:24:29 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:29 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:29 INFO : Running optimiser  
2023-Oct-27 06:24:29 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:29 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:29 INFO : 31 group vectors in total  
2023-Oct-27 06:24:29 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:29 INFO : Final nStart = 20  
2023-Oct-27 06:24:29 INFO : Final nEnd = 512  
2023-Oct-27 06:24:29 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:29 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:29 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:29 INFO : Adjusting basis set to 4.688207 ppm  
2023-Oct-27 06:24:29 INFO : Time domain noise = 0.000001  
2023-Oct-27 06:24:29 DEBUG : Using init\_beta: 35.796025  
2023-Oct-27 06:24:29 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:29 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:30 INFO : done.  
2023-Oct-27 06:24:30 DEBUG : Final Beta: 149.18  
2023-Oct-27 06:24:30 DEBUG : Final Phi0: -0.08  
2023-Oct-27 06:24:30 DEBUG : Final Phi1: 0.00

```
2023-Oct-27 06:24:30 INFO : FWHM right ppm = 2.013740
2023-Oct-27 06:24:30 INFO : FWHM left ppm = 2.067229
2023-Oct-27 06:24:30 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:30 INFO : Spec noise = 0.000007
2023-Oct-27 06:24:30 INFO : sdev noise = 0.000352
2023-Oct-27 06:24:30 INFO : SNR residual = 26.872211
2023-Oct-27 06:24:30 INFO : SNR max = 40.395607
2023-Oct-27 06:24:30 INFO : Ymax = 0.018934
2023-Oct-27 06:24:30 INFO : Ymax metab = 0.018934
2023-Oct-27 06:24:30 INFO : Fit quality = 1.503248
2023-Oct-27 06:24:30 INFO : Baseline dev = 0.033196
2023-Oct-27 06:24:30 INFO : Ymax = 0.018934
2023-Oct-27 06:24:30 INFO : BSL = 0.019327
2023-Oct-27 06:24:30 INFO : Computing CRLBs.
2023-Oct-27 06:24:30 DEBUG : Sigma: 2.192569e-12
2023-Oct-27 06:24:30 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 8.55605
l2 norm of error at final p = 1.20814
l2 norm of J.*e at final p = 321.611
l2 norm of D*p at final p = 8.01671e-11
number of iterations = 10
number of function evaluations = 2
number of Jacobian evaluations = 166
stopped by small D*p
```

```
2023-Oct-27 06:24:30 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:30 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:30 INFO : Loading data file : Temporary/f/db6.raw
2023-Oct-27 06:24:30 INFO : nStart = 20
2023-Oct-27 06:24:30 INFO : nEnd = 512
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:30 INFO : Loading data file : W.raw
2023-Oct-27 06:24:30 INFO : nStart = 20
2023-Oct-27 06:24:30 INFO : nEnd = 512
Parameters Before Preprocessing
```

```
-----
Input file: Temporary/f/db6.raw
Water reference file: W.raw
Data points: 1024
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 512
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:30 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:30 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:30 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:30 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:30 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:30 INFO : Ref new = 4.636628 ppm
2023-Oct-27 06:24:30 INFO : Residual water freq. (Hz) : -1.708984
2023-Oct-27 06:24:30 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:30 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:30 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:30 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:30 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:30 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:30 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:30 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:30 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:30 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:30 DEBUG : Max Phi0 : 0.57
2023-Oct-27 06:24:30 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:30 INFO : Ref new = 4.667193 ppm
2023-Oct-27 06:24:30 DEBUG : Width pts : 38.24
2023-Oct-27 06:24:30 DEBUG : Width Hz est : 6.22
2023-Oct-27 06:24:30 DEBUG : Init beta est : 97.15
2023-Oct-27 06:24:30 INFO : Ymax = 0.021290
2023-Oct-27 06:24:30 INFO : sdev noise = 0.000207
2023-Oct-27 06:24:30 INFO : SNR guess = 51.4652
2023-Oct-27 06:24:30 INFO : Finished 'Preprocessing'
```

#### Parameters After Preprocessing

```
-----
Input file: Temporary/f/db6.raw
```

Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.66719 ppm

2023-Oct-27 06:24:30 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:30 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:30 INFO : Running optimiser  
2023-Oct-27 06:24:30 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:30 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:30 INFO : 31 group vectors in total  
2023-Oct-27 06:24:30 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:30 INFO : Final nStart = 20  
2023-Oct-27 06:24:30 INFO : Final nEnd = 512  
2023-Oct-27 06:24:30 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:30 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:30 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:30 INFO : Adjusting basis set to 4.667193 ppm  
2023-Oct-27 06:24:30 INFO : Time domain noise = 0.000001  
2023-Oct-27 06:24:30 DEBUG : Using init\_beta: 97.145905  
2023-Oct-27 06:24:30 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:30 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:31 INFO : done.  
2023-Oct-27 06:24:31 DEBUG : Final Beta: 138.09  
2023-Oct-27 06:24:31 DEBUG : Final Phi0: 0.09  
2023-Oct-27 06:24:31 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:31 INFO : FWHM right ppm = 1.992726  
2023-Oct-27 06:24:31 INFO : FWHM left ppm = 2.046215  
2023-Oct-27 06:24:31 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:31 INFO : Spec noise = 0.000006  
2023-Oct-27 06:24:31 INFO : sdev noise = 0.000343  
2023-Oct-27 06:24:31 INFO : SNR residual = 27.608464  
2023-Oct-27 06:24:31 INFO : SNR max = 46.064708  
2023-Oct-27 06:24:31 INFO : Ymax = 0.018958  
2023-Oct-27 06:24:31 INFO : Ymax metab = 0.018958  
2023-Oct-27 06:24:31 INFO : Fit quality = 1.668499  
2023-Oct-27 06:24:31 INFO : Baseline dev = 0.035385  
2023-Oct-27 06:24:31 INFO : Ymax = 0.018958  
2023-Oct-27 06:24:31 INFO : BSL = 0.057305  
2023-Oct-27 06:24:31 INFO : Computing CRLBs.  
2023-Oct-27 06:24:31 DEBUG : Sigma: 1.035453e-12  
2023-Oct-27 06:24:31 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 2.37755  
l2 norm of error at final p = 1.20269  
l2 norm of J.'\*e at final p = 399.633  
l2 norm of D\*p at final p = 2.79864e-11  
number of iterations = 7  
number of function evaluations = 2  
number of Jacobian evaluations = 168  
stopped by small D\*p

2023-Oct-27 06:24:31 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:31 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:31 INFO : Loading data file : Temporary/f/db7.raw  
2023-Oct-27 06:24:31 INFO : nStart = 20  
2023-Oct-27 06:24:31 INFO : nEnd = 512  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:31 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:31 INFO : nStart = 20  
2023-Oct-27 06:24:31 INFO : nEnd = 512  
Parameters Before Preprocessing

-----  
Input file: Temporary/f/db7.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512

Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:31 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:31 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:31 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:31 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:31 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:31 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:31 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:31 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:31 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:31 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:31 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:31 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:31 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:31 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:31 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:31 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:31 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:31 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:31 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:31 INFO : Ref new = 4.669103 ppm  
2023-Oct-27 06:24:31 DEBUG : Width pts : 38.40  
2023-Oct-27 06:24:31 DEBUG : Width Hz est : 6.25  
2023-Oct-27 06:24:31 DEBUG : Init beta est : 98.13  
2023-Oct-27 06:24:31 INFO : Ymax = 0.020455  
2023-Oct-27 06:24:31 INFO : sdev noise = 0.000196  
2023-Oct-27 06:24:31 INFO : SNR guess = 52.2321  
2023-Oct-27 06:24:31 INFO : Finished 'Preprocessing'

#### Parameters After Preprocessing

-----  
Input file: Temporary/f/db7.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.6691 ppm

2023-Oct-27 06:24:31 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:31 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:31 INFO : Running optimiser  
2023-Oct-27 06:24:31 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:31 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:31 INFO : 31 group vectors in total  
2023-Oct-27 06:24:31 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:31 INFO : Final nStart = 20  
2023-Oct-27 06:24:31 INFO : Final nEnd = 512  
2023-Oct-27 06:24:31 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:31 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:31 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:31 INFO : Adjusting basis set to 4.669103 ppm  
2023-Oct-27 06:24:31 INFO : Time domain noise = 0.000001  
2023-Oct-27 06:24:31 DEBUG : Using init\_beta: 98.129365  
2023-Oct-27 06:24:31 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:32 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:32 INFO : done.  
2023-Oct-27 06:24:32 DEBUG : Final Beta: 136.88  
2023-Oct-27 06:24:32 DEBUG : Final Phi0: -0.24  
2023-Oct-27 06:24:32 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:32 INFO : FWHM right ppm = 1.994636  
2023-Oct-27 06:24:32 INFO : FWHM left ppm = 2.048126  
2023-Oct-27 06:24:32 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:32 INFO : Spec noise = 0.000007  
2023-Oct-27 06:24:32 INFO : sdev noise = 0.000328  
2023-Oct-27 06:24:32 INFO : SNR residual = 28.729662  
2023-Oct-27 06:24:32 INFO : SNR max = 44.950828  
2023-Oct-27 06:24:32 INFO : Ymax = 0.018865  
2023-Oct-27 06:24:32 INFO : Ymax metab = 0.018865  
2023-Oct-27 06:24:32 INFO : Fit quality = 1.564614  
2023-Oct-27 06:24:32 INFO : Baseline dev = 0.035331  
2023-Oct-27 06:24:32 INFO : Ymax = 0.018865  
2023-Oct-27 06:24:32 INFO : BSL = 0.053894  
2023-Oct-27 06:24:32 INFO : Computing CRLBs.  
2023-Oct-27 06:24:32 DEBUG : Sigma: 1.419568e-12  
2023-Oct-27 06:24:32 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 2.48105  
l2 norm of error at final p = 1.19317

l2 norm of J.'\*e at final p = 553.822  
l2 norm of D\*p at final p = 2.30516e-10  
number of iterations = 7  
number of function evaluations = 2  
number of Jacobian evaluations = 158  
stopped by small D\*p

2023-Oct-27 06:24:32 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:32 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:32 INFO : Loading data file : Temporary/f/db8.raw  
2023-Oct-27 06:24:32 INFO : nStart = 20  
2023-Oct-27 06:24:32 INFO : nEnd = 512  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:32 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:32 INFO : nStart = 20  
2023-Oct-27 06:24:32 INFO : nEnd = 512  
Parameters Before Preprocessing

-----  
Input file: Temporary/f/db8.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:32 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:32 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:32 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:32 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:32 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:32 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:32 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:32 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:32 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:32 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:32 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:32 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:32 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:32 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:32 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:32 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:32 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:32 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:32 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:32 INFO : Ref new = 4.667193 ppm  
2023-Oct-27 06:24:32 DEBUG : Width pts : 38.16  
2023-Oct-27 06:24:32 DEBUG : Width Hz est : 6.21  
2023-Oct-27 06:24:32 DEBUG : Init beta est : 96.68  
2023-Oct-27 06:24:32 INFO : Ymax = 0.021067  
2023-Oct-27 06:24:32 INFO : sdev noise = 0.000197  
2023-Oct-27 06:24:32 INFO : SNR guess = 53.4853  
2023-Oct-27 06:24:32 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/f/db8.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.66719 ppm

2023-Oct-27 06:24:32 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:33 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:33 INFO : Running optimiser  
2023-Oct-27 06:24:33 INFO : Setting metab shift limit to 0.030000 ppm

```
2023-Oct-27 06:24:33 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:33 INFO : 31 group vectors in total
2023-Oct-27 06:24:33 INFO : 31 basis vectors in total
2023-Oct-27 06:24:33 INFO : Final nStart = 20
2023-Oct-27 06:24:33 INFO : Final nEnd = 512
2023-Oct-27 06:24:33 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:33 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:33 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:33 INFO : Adjusting basis set to 4.667193 ppm
2023-Oct-27 06:24:33 INFO : Time domain noise = 0.000001
2023-Oct-27 06:24:33 DEBUG : Using init_beta: 96.679759
2023-Oct-27 06:24:33 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:33 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:33 INFO : done.
2023-Oct-27 06:24:33 DEBUG : Final Beta: 139.04
2023-Oct-27 06:24:33 DEBUG : Final Phi0: -0.28
2023-Oct-27 06:24:33 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:33 INFO : FWHM right ppm = 1.992726
2023-Oct-27 06:24:33 INFO : FWHM left ppm = 2.046215
2023-Oct-27 06:24:33 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:33 INFO : Spec noise = 0.000006
2023-Oct-27 06:24:33 INFO : sdev noise = 0.000328
2023-Oct-27 06:24:33 INFO : SNR residual = 28.920168
2023-Oct-27 06:24:33 INFO : SNR max = 50.280139
2023-Oct-27 06:24:33 INFO : Ymax = 0.018959
2023-Oct-27 06:24:33 INFO : Ymax metab = 0.018959
2023-Oct-27 06:24:33 INFO : Fit quality = 1.738584
2023-Oct-27 06:24:33 INFO : Baseline dev = 0.038056
2023-Oct-27 06:24:33 INFO : Ymax = 0.018959
2023-Oct-27 06:24:33 INFO : BSL = 0.068767
2023-Oct-27 06:24:33 INFO : Computing CRLBs.
2023-Oct-27 06:24:33 DEBUG : Sigma: 1.088629e-12
2023-Oct-27 06:24:33 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.17037
l2 norm of error at final p = 1.1835
l2 norm of J.*e at final p = 352.016
l2 norm of D*p at final p = 4.26269e-11
number of iterations = 7
number of function evaluations = 2
number of Jacobian evaluations = 166
stopped by small D*p
```

```
2023-Oct-27 06:24:33 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:33 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:33 INFO : Loading data file : Temporary/f/db9.raw
2023-Oct-27 06:24:33 INFO : nStart = 20
2023-Oct-27 06:24:33 INFO : nEnd = 512
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:33 INFO : Loading data file : W.raw
2023-Oct-27 06:24:33 INFO : nStart = 20
2023-Oct-27 06:24:33 INFO : nEnd = 512
```

#### Parameters Before Preprocessing

```
-----
Input file: Temporary/f/db9.raw
Water reference file: W.raw
Data points: 1024
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 512
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:33 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:33 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:33 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:33 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:33 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:33 INFO : Ref new = 4.636628 ppm
2023-Oct-27 06:24:33 INFO : Residual water freq. (Hz) : -1.708984
2023-Oct-27 06:24:33 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:33 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:33 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:34 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:34 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:34 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:34 INFO : Starting 'estimating LP amplitudes'
```

```
2023-Oct-27 06:24:34 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:34 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:34 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:34 DEBUG : Max Phi0 : 0.31
2023-Oct-27 06:24:34 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:34 INFO : Ref new = 4.667193 ppm
2023-Oct-27 06:24:34 DEBUG : Width pts : 37.27
2023-Oct-27 06:24:34 DEBUG : Width Hz est : 6.07
2023-Oct-27 06:24:34 DEBUG : Init beta est : 91.36
2023-Oct-27 06:24:34 INFO : Ymax = 0.021480
2023-Oct-27 06:24:34 INFO : sdev noise = 0.000207
2023-Oct-27 06:24:34 INFO : SNR guess = 51.9287
2023-Oct-27 06:24:34 INFO : Finished 'Preprocessing'
```

#### Parameters After Preprocessing

```
-----
Input file: Temporary/f/db9.raw
Water reference file: W.raw
Data points: 1024
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 512
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.66719 ppm
```

```
2023-Oct-27 06:24:34 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:34 INFO : All simulation threads stopped.
2023-Oct-27 06:24:34 INFO : Running optimiser
2023-Oct-27 06:24:34 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:34 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:34 INFO : 31 group vectors in total
2023-Oct-27 06:24:34 INFO : 31 basis vectors in total
2023-Oct-27 06:24:34 INFO : Final nStart = 20
2023-Oct-27 06:24:34 INFO : Final nEnd = 512
2023-Oct-27 06:24:34 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:34 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:34 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:34 INFO : Adjusting basis set to 4.667193 ppm
2023-Oct-27 06:24:34 INFO : Time domain noise = 0.000002
2023-Oct-27 06:24:34 DEBUG : Using init_beta: 91.355366
2023-Oct-27 06:24:34 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:34 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:35 INFO : done.
2023-Oct-27 06:24:35 DEBUG : Final Beta: 137.95
2023-Oct-27 06:24:35 DEBUG : Final Phi0: -0.20
2023-Oct-27 06:24:35 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:35 INFO : FWHM right ppm = 1.992726
2023-Oct-27 06:24:35 INFO : FWHM left ppm = 2.046215
2023-Oct-27 06:24:35 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:35 INFO : Spec noise = 0.000005
2023-Oct-27 06:24:35 INFO : sdev noise = 0.000319
2023-Oct-27 06:24:35 INFO : SNR residual = 30.193981
2023-Oct-27 06:24:35 INFO : SNR max = 55.473527
2023-Oct-27 06:24:35 INFO : Ymax = 0.019293
2023-Oct-27 06:24:35 INFO : Ymax metab = 0.019293
2023-Oct-27 06:24:35 INFO : Fit quality = 1.837238
2023-Oct-27 06:24:35 INFO : Baseline dev = 0.038667
2023-Oct-27 06:24:35 INFO : Ymax = 0.019293
2023-Oct-27 06:24:35 INFO : BSL = 0.069557
2023-Oct-27 06:24:35 INFO : Computing CRLBs.
2023-Oct-27 06:24:35 DEBUG : Sigma: 2.938942e-12
2023-Oct-27 06:24:35 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.40166
l2 norm of error at final p = 1.17967
l2 norm of J.*e at final p = 354.046
l2 norm of D*p at final p = 2.79684e-11
number of iterations = 7
number of function evaluations = 2
number of Jacobian evaluations = 168
stopped by small D*p
```

```
2023-Oct-27 06:24:35 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:35 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:35 INFO : Loading data file : Temporary/f/db10.raw
2023-Oct-27 06:24:35 INFO : nStart = 20
2023-Oct-27 06:24:35 INFO : nEnd = 512
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

2023-Oct-27 06:24:35 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:35 INFO : nStart = 20  
2023-Oct-27 06:24:35 INFO : nEnd = 512

Parameters Before Preprocessing

-----  
Input file: Temporary/f/db10.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:35 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:35 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:35 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:35 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:35 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:35 INFO : Ref new = 4.636628 ppm  
2023-Oct-27 06:24:35 INFO : Residual water freq. (Hz) : -1.708984  
2023-Oct-27 06:24:35 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:35 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:35 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:35 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:35 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:35 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:35 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:35 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:35 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:35 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:35 DEBUG : Max Phi0 : 0.00  
2023-Oct-27 06:24:35 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:35 INFO : Ref new = 4.669103 ppm  
2023-Oct-27 06:24:35 DEBUG : Width pts : 39.14  
2023-Oct-27 06:24:35 DEBUG : Width Hz est : 6.37  
2023-Oct-27 06:24:35 DEBUG : Init beta est : 102.70  
2023-Oct-27 06:24:35 INFO : Ymax = 0.019711  
2023-Oct-27 06:24:35 INFO : sdev noise = 0.000199  
2023-Oct-27 06:24:35 INFO : SNR guess = 49.6453  
2023-Oct-27 06:24:35 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/f/db10.raw  
Water reference file: W.raw  
Data points: 1024  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 512  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.6691 ppm

2023-Oct-27 06:24:35 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:35 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:35 INFO : Running optimiser  
2023-Oct-27 06:24:35 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:35 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:35 INFO : 31 group vectors in total  
2023-Oct-27 06:24:35 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:35 INFO : Final nStart = 20  
2023-Oct-27 06:24:35 INFO : Final nEnd = 512  
2023-Oct-27 06:24:35 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:35 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:35 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:35 INFO : Adjusting basis set to 4.669103 ppm  
2023-Oct-27 06:24:35 INFO : Time domain noise = 0.000002  
2023-Oct-27 06:24:35 DEBUG : Using init\_beta: 102.698029  
2023-Oct-27 06:24:35 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:35 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:36 INFO : done.  
2023-Oct-27 06:24:36 DEBUG : Final Beta: 132.98  
2023-Oct-27 06:24:36 DEBUG : Final Phi0: -0.45  
2023-Oct-27 06:24:36 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:36 INFO : FWHM right ppm = 1.994636  
2023-Oct-27 06:24:36 INFO : FWHM left ppm = 2.044305  
2023-Oct-27 06:24:36 INFO : Metabolite FWHM (ppm) = 0.049669  
2023-Oct-27 06:24:36 INFO : Spec noise = 0.000005

```
2023-Oct-27 06:24:36 INFO : sdev noise = 0.000307
2023-Oct-27 06:24:36 INFO : SNR residual = 31.499185
2023-Oct-27 06:24:36 INFO : SNR max = 56.646065
2023-Oct-27 06:24:36 INFO : Ymax = 0.019343
2023-Oct-27 06:24:36 INFO : Ymax metab = 0.019343
2023-Oct-27 06:24:36 INFO : Fit quality = 1.798334
2023-Oct-27 06:24:36 INFO : Baseline dev = 0.034101
2023-Oct-27 06:24:36 INFO : Ymax = 0.019343
2023-Oct-27 06:24:36 INFO : BSL = 0.045994
2023-Oct-27 06:24:36 INFO : Computing CRLBs.
2023-Oct-27 06:24:36 DEBUG : Sigma: 2.704908e-12
2023-Oct-27 06:24:36 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.45516
l2 norm of error at final p = 1.16766
l2 norm of J.*e at final p = 9.74717
l2 norm of D*p at final p = 1.44211e-12
number of iterations = 7
number of function evaluations = 2
number of Jacobian evaluations = 160
stopped by small D*p
```

```
2023-Oct-27 06:24:36 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:36 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:36 INFO : Loading data file : Temporary/cs/db1.raw
2023-Oct-27 06:24:36 INFO : nStart = 20
2023-Oct-27 06:24:36 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:36 INFO : Loading data file : W.raw
2023-Oct-27 06:24:36 INFO : nStart = 20
2023-Oct-27 06:24:36 INFO : nEnd = 500
```

#### Parameters Before Preprocessing

```
-----
Input file: Temporary/cs/db1.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:36 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:36 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:36 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:36 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:36 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:36 INFO : Ref new = 4.630897 ppm
2023-Oct-27 06:24:36 INFO : Residual water freq. (Hz) : -2.441406
2023-Oct-27 06:24:36 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:36 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:36 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:36 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:36 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:36 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:36 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:36 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:36 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:36 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:36 DEBUG : Max Phi0 : 0.25
2023-Oct-27 06:24:36 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:36 INFO : Ref new = 4.657641 ppm
2023-Oct-27 06:24:36 DEBUG : Width pts : 18.47
2023-Oct-27 06:24:36 DEBUG : Width Hz est : 6.01
2023-Oct-27 06:24:36 DEBUG : Init beta est : 89.49
2023-Oct-27 06:24:36 INFO : Ymax = 0.028211
2023-Oct-27 06:24:36 INFO : sdev noise = 0.000298
2023-Oct-27 06:24:36 INFO : SNR guess = 47.3361
2023-Oct-27 06:24:36 INFO : Finished 'Preprocessing'
```

#### Parameters After Preprocessing

```
-----
Input file: Temporary/cs/db1.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
```

Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65764 ppm

2023-Oct-27 06:24:36 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:36 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:36 INFO : Running optimiser  
2023-Oct-27 06:24:36 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:36 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:36 INFO : 31 group vectors in total  
2023-Oct-27 06:24:36 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:36 INFO : Final nStart = 20  
2023-Oct-27 06:24:36 INFO : Final nEnd = 500  
2023-Oct-27 06:24:36 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:36 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:36 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:36 INFO : Adjusting basis set to 4.657641 ppm  
2023-Oct-27 06:24:36 INFO : Time domain noise = 0.000015  
2023-Oct-27 06:24:36 DEBUG : Using init\_beta: 89.487163  
2023-Oct-27 06:24:36 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:36 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:37 INFO : done.  
2023-Oct-27 06:24:37 DEBUG : Final Beta: 129.72  
2023-Oct-27 06:24:37 DEBUG : Final Phi0: -0.32  
2023-Oct-27 06:24:37 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:37 INFO : FWHM right ppm = 1.998457  
2023-Oct-27 06:24:37 INFO : FWHM left ppm = 2.044305  
2023-Oct-27 06:24:37 INFO : Metabolite FWHM (ppm) = 0.045848  
2023-Oct-27 06:24:37 INFO : Spec noise = 0.000012  
2023-Oct-27 06:24:37 INFO : sdev noise = 0.000630  
2023-Oct-27 06:24:37 INFO : SNR residual = 19.941532  
2023-Oct-27 06:24:37 INFO : SNR max = 45.859835  
2023-Oct-27 06:24:37 INFO : Ymax = 0.025128  
2023-Oct-27 06:24:37 INFO : Ymax metab = 0.025128  
2023-Oct-27 06:24:37 INFO : Fit quality = 2.299715  
2023-Oct-27 06:24:37 INFO : Baseline dev = 0.035653  
2023-Oct-27 06:24:37 INFO : Ymax = 0.025128  
2023-Oct-27 06:24:37 INFO : BSL = 0.058953  
2023-Oct-27 06:24:37 INFO : Computing CRLBs.  
2023-Oct-27 06:24:37 DEBUG : Sigma: 2.122786e-10  
2023-Oct-27 06:24:37 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 2.76424  
l2 norm of error at final p = 1.85615  
l2 norm of J.\*e at final p = 224.05  
l2 norm of D\*p at final p = 2.74527e-12  
number of iterations = 9  
number of function evaluations = 2  
number of Jacobian evaluations = 181  
stopped by small D\*p

2023-Oct-27 06:24:37 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:37 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:37 INFO : Loading data file : Temporary/cs/db2.raw  
2023-Oct-27 06:24:37 INFO : nStart = 20  
2023-Oct-27 06:24:37 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:37 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:37 INFO : nStart = 20  
2023-Oct-27 06:24:37 INFO : nEnd = 500  
Parameters Before Preprocessing

-----  
Input file: Temporary/cs/db2.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes

Reference: 4.65 ppm

```
2023-Oct-27 06:24:37 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:37 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:37 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:37 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:37 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:37 INFO : Ref new = 4.642359 ppm
2023-Oct-27 06:24:37 INFO : Residual water freq. (Hz) : -0.976562
2023-Oct-27 06:24:37 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:37 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:37 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:37 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:37 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:37 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:37 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:37 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:37 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:37 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:37 DEBUG : Max Phi0 : 0.38
2023-Oct-27 06:24:37 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:37 INFO : Ref new = 4.672924 ppm
2023-Oct-27 06:24:37 DEBUG : Width pts : 19.01
2023-Oct-27 06:24:37 DEBUG : Width Hz est : 6.19
2023-Oct-27 06:24:37 DEBUG : Init beta est : 95.87
2023-Oct-27 06:24:37 INFO : Ymax = 0.029113
2023-Oct-27 06:24:37 INFO : sdev noise = 0.000298
2023-Oct-27 06:24:37 INFO : SNR guess = 48.9096
2023-Oct-27 06:24:37 INFO : Finished 'Preprocessing'
```

Parameters After Preprocessing

```
-----
Input file: Temporary/cs/db2.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.67292 ppm
```

```
2023-Oct-27 06:24:37 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:37 INFO : All simulation threads stopped.
2023-Oct-27 06:24:37 INFO : Running optimiser
2023-Oct-27 06:24:37 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:37 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:37 INFO : 31 group vectors in total
2023-Oct-27 06:24:37 INFO : 31 basis vectors in total
2023-Oct-27 06:24:37 INFO : Final nStart = 20
2023-Oct-27 06:24:37 INFO : Final nEnd = 500
2023-Oct-27 06:24:37 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:37 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:37 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:37 INFO : Adjusting basis set to 4.672924 ppm
2023-Oct-27 06:24:37 INFO : Time domain noise = 0.000014
2023-Oct-27 06:24:37 DEBUG : Using init_beta: 95.868201
2023-Oct-27 06:24:37 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:37 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:37 INFO : done.
2023-Oct-27 06:24:37 DEBUG : Final Beta: 129.62
2023-Oct-27 06:24:37 DEBUG : Final Phi0: 0.20
2023-Oct-27 06:24:37 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:37 INFO : FWHM right ppm = 1.998457
2023-Oct-27 06:24:37 INFO : FWHM left ppm = 2.044305
2023-Oct-27 06:24:37 INFO : Metabolite FWHM (ppm) = 0.045848
2023-Oct-27 06:24:37 INFO : Spec noise = 0.000012
2023-Oct-27 06:24:37 INFO : sdev noise = 0.000724
2023-Oct-27 06:24:37 INFO : SNR residual = 17.602508
2023-Oct-27 06:24:37 INFO : SNR max = 45.091780
2023-Oct-27 06:24:37 INFO : Ymax = 0.025504
2023-Oct-27 06:24:37 INFO : Ymax metab = 0.025504
2023-Oct-27 06:24:37 INFO : Fit quality = 2.561668
2023-Oct-27 06:24:37 INFO : Baseline dev = 0.026585
2023-Oct-27 06:24:37 INFO : Ymax = 0.025504
2023-Oct-27 06:24:37 INFO : BSL = 0.034625
2023-Oct-27 06:24:37 INFO : Computing CRLBs.
2023-Oct-27 06:24:37 DEBUG : Sigma: 1.963764e-10
2023-Oct-27 06:24:37 INFO : done.
```

Optimisation details

```
-----
l2 norm of error at initial p = 2.78101
l2 norm of error at final p = 1.75154
l2 norm of J.*e at final p = 53.3233
l2 norm of D*p at final p = 2.32912e-10
number of iterations = 8
number of function evaluations = 2
```

number of Jacobian evaluations = 157  
stopped by small D\*p

2023-Oct-27 06:24:37 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:37 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:37 INFO : Loading data file : Temporary/cs/db3.raw  
2023-Oct-27 06:24:37 INFO : nStart = 20  
2023-Oct-27 06:24:37 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:37 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:37 INFO : nStart = 20  
2023-Oct-27 06:24:37 INFO : nEnd = 500

Parameters Before Preprocessing

-----  
Input file: Temporary/cs/db3.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:37 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:37 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:37 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:37 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:37 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:37 INFO : Ref new = 4.653821 ppm  
2023-Oct-27 06:24:37 INFO : Residual water freq. (Hz) : 0.488281  
2023-Oct-27 06:24:37 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:37 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:37 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:37 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:37 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:37 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:37 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:37 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:37 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:37 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:37 DEBUG : Max Phi0 : 0.00  
2023-Oct-27 06:24:37 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:37 INFO : Ref new = 4.676745 ppm  
2023-Oct-27 06:24:37 DEBUG : Width pts : 19.56  
2023-Oct-27 06:24:37 DEBUG : Width Hz est : 6.37  
2023-Oct-27 06:24:37 DEBUG : Init beta est : 102.53  
2023-Oct-27 06:24:37 INFO : Ymax = 0.027685  
2023-Oct-27 06:24:37 INFO : sdev noise = 0.000301  
2023-Oct-27 06:24:37 INFO : SNR guess = 45.9732  
2023-Oct-27 06:24:37 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/cs/db3.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.67674 ppm

2023-Oct-27 06:24:37 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:38 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:38 INFO : Running optimiser  
2023-Oct-27 06:24:38 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:38 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:38 INFO : 31 group vectors in total  
2023-Oct-27 06:24:38 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:38 INFO : Final nStart = 20

```
2023-Oct-27 06:24:38 INFO : Final nEnd = 500
2023-Oct-27 06:24:38 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:38 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:38 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:38 INFO : Adjusting basis set to 4.676745 ppm
2023-Oct-27 06:24:38 INFO : Time domain noise = 0.000014
2023-Oct-27 06:24:38 DEBUG : Using init_beta: 102.525783
2023-Oct-27 06:24:38 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:38 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:38 INFO : done.
2023-Oct-27 06:24:38 DEBUG : Final Beta: 137.05
2023-Oct-27 06:24:38 DEBUG : Final Phi0: -0.30
2023-Oct-27 06:24:38 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:38 INFO : FWHM right ppm = 1.986995
2023-Oct-27 06:24:38 INFO : FWHM left ppm = 2.040484
2023-Oct-27 06:24:38 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:38 INFO : Spec noise = 0.000013
2023-Oct-27 06:24:38 INFO : sdev noise = 0.000688
2023-Oct-27 06:24:38 INFO : SNR residual = 19.461898
2023-Oct-27 06:24:38 INFO : SNR max = 46.484677
2023-Oct-27 06:24:38 INFO : Ymax = 0.026771
2023-Oct-27 06:24:38 INFO : Ymax metab = 0.026771
2023-Oct-27 06:24:38 INFO : Fit quality = 2.388497
2023-Oct-27 06:24:38 INFO : Baseline dev = 0.028486
2023-Oct-27 06:24:38 INFO : Ymax = 0.026771
2023-Oct-27 06:24:38 INFO : BSL = 0.044878
2023-Oct-27 06:24:38 INFO : Computing CRLBs.
2023-Oct-27 06:24:38 DEBUG : Sigma: 1.999252e-10
2023-Oct-27 06:24:38 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.54508
l2 norm of error at final p = 1.71764
l2 norm of J.*e at final p = 56.0698
l2 norm of D*p at final p = 2.38502e-15
number of iterations = 7
number of function evaluations = 2
number of Jacobian evaluations = 209
stopped by small D*p
```

```
2023-Oct-27 06:24:38 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:38 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:38 INFO : Loading data file : Temporary/cs/db4.raw
2023-Oct-27 06:24:38 INFO : nStart = 20
2023-Oct-27 06:24:38 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:38 INFO : Loading data file : W.raw
2023-Oct-27 06:24:38 INFO : nStart = 20
2023-Oct-27 06:24:38 INFO : nEnd = 500
Parameters Before Preprocessing
```

```
-----
Input file: Temporary/cs/db4.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:38 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:38 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:38 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:38 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:38 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:38 INFO : Ref new = 4.665283 ppm
2023-Oct-27 06:24:38 INFO : Residual water freq. (Hz) : 1.953125
2023-Oct-27 06:24:38 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:38 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:38 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:38 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:38 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:38 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:38 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:38 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:38 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:38 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:38 DEBUG : Max Phi0 : 0.13
```

```
2023-Oct-27 06:24:38 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:38 INFO : Ref new = 4.699669 ppm
2023-Oct-27 06:24:38 DEBUG : Width pts : 19.48
2023-Oct-27 06:24:38 DEBUG : Width Hz est : 6.34
2023-Oct-27 06:24:38 DEBUG : Init beta est : 101.51
2023-Oct-27 06:24:38 INFO : Ymax = 0.027741
2023-Oct-27 06:24:38 INFO : sdev noise = 0.000310
2023-Oct-27 06:24:38 INFO : SNR guess = 44.6776
2023-Oct-27 06:24:38 INFO : Finished 'Preprocessing'
```

#### Parameters After Preprocessing

```
-----
Input file: Temporary/cs/db4.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.69967 ppm
```

```
2023-Oct-27 06:24:38 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:38 INFO : All simulation threads stopped.
2023-Oct-27 06:24:38 INFO : Running optimiser
2023-Oct-27 06:24:38 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:38 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:38 INFO : 31 group vectors in total
2023-Oct-27 06:24:38 INFO : 31 basis vectors in total
2023-Oct-27 06:24:38 INFO : Final nStart = 20
2023-Oct-27 06:24:38 INFO : Final nEnd = 500
2023-Oct-27 06:24:38 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:38 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:38 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:38 INFO : Adjusting basis set to 4.699669 ppm
2023-Oct-27 06:24:38 INFO : Time domain noise = 0.000013
2023-Oct-27 06:24:38 DEBUG : Using init_beta: 101.510052
2023-Oct-27 06:24:38 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:38 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:39 INFO : done.
2023-Oct-27 06:24:39 DEBUG : Final Beta: 120.71
2023-Oct-27 06:24:39 DEBUG : Final Phi0: -0.08
2023-Oct-27 06:24:39 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:39 INFO : FWHM right ppm = 2.002278
2023-Oct-27 06:24:39 INFO : FWHM left ppm = 2.048126
2023-Oct-27 06:24:39 INFO : Metabolite FWHM (ppm) = 0.045848
2023-Oct-27 06:24:39 INFO : Spec noise = 0.000013
2023-Oct-27 06:24:39 INFO : sdev noise = 0.000671
2023-Oct-27 06:24:39 INFO : SNR residual = 19.551767
2023-Oct-27 06:24:39 INFO : SNR max = 44.783720
2023-Oct-27 06:24:39 INFO : Ymax = 0.026249
2023-Oct-27 06:24:39 INFO : Ymax metab = 0.026249
2023-Oct-27 06:24:39 INFO : Fit quality = 2.290520
2023-Oct-27 06:24:39 INFO : Baseline dev = 0.026990
2023-Oct-27 06:24:39 INFO : Ymax = 0.026249
2023-Oct-27 06:24:39 INFO : BSL = 0.030250
2023-Oct-27 06:24:39 INFO : Computing CRLBs.
2023-Oct-27 06:24:39 DEBUG : Sigma: 1.747828e-10
2023-Oct-27 06:24:39 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 3.19846
l2 norm of error at final p = 1.75738
l2 norm of J.*e at final p = 6.49779
l2 norm of D*p at final p = 7.79166e-14
number of iterations = 7
number of function evaluations = 2
number of Jacobian evaluations = 174
stopped by small D*p
```

```
2023-Oct-27 06:24:39 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:39 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:39 INFO : Loading data file : Temporary/cs/db5.raw
2023-Oct-27 06:24:39 INFO : nStart = 20
2023-Oct-27 06:24:39 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:39 INFO : Loading data file : W.raw
2023-Oct-27 06:24:39 INFO : nStart = 20
2023-Oct-27 06:24:39 INFO : nEnd = 500
```

Parameters Before Preprocessing

-----  
Input file: Temporary/cs/db5.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:39 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:39 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:39 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:39 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:39 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:39 INFO : Ref new = 4.676745 ppm  
2023-Oct-27 06:24:39 INFO : Residual water freq. (Hz) : 3.417969  
2023-Oct-27 06:24:39 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:39 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:39 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:39 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:39 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:39 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:39 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:39 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:39 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:39 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:39 DEBUG : Max Phi0 : 0.19  
2023-Oct-27 06:24:39 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:39 INFO : Ref new = 4.707310 ppm  
2023-Oct-27 06:24:39 DEBUG : Width pts : 19.72  
2023-Oct-27 06:24:39 DEBUG : Width Hz est : 6.42  
2023-Oct-27 06:24:39 DEBUG : Init beta est : 104.54  
2023-Oct-27 06:24:39 INFO : Ymax = 0.028919  
2023-Oct-27 06:24:39 INFO : sdev noise = 0.000278  
2023-Oct-27 06:24:39 INFO : SNR guess = 52.0192  
2023-Oct-27 06:24:39 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/cs/db5.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.70731 ppm

2023-Oct-27 06:24:39 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:39 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:39 INFO : Running optimiser  
2023-Oct-27 06:24:39 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:39 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:39 INFO : 31 group vectors in total  
2023-Oct-27 06:24:39 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:39 INFO : Final nStart = 20  
2023-Oct-27 06:24:39 INFO : Final nEnd = 500  
2023-Oct-27 06:24:39 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:39 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:39 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:39 INFO : Adjusting basis set to 4.707310 ppm  
2023-Oct-27 06:24:39 INFO : Time domain noise = 0.000014  
2023-Oct-27 06:24:39 DEBUG : Using init\_beta: 104.537936  
2023-Oct-27 06:24:39 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:39 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:40 INFO : done.  
2023-Oct-27 06:24:40 DEBUG : Final Beta: 129.52  
2023-Oct-27 06:24:40 DEBUG : Final Phi0: 0.20  
2023-Oct-27 06:24:40 DEBUG : Final Phi1: -0.00  
2023-Oct-27 06:24:40 INFO : FWHM right ppm = 1.994636  
2023-Oct-27 06:24:40 INFO : FWHM left ppm = 2.040484  
2023-Oct-27 06:24:40 INFO : Metabolite FWHM (ppm) = 0.045848  
2023-Oct-27 06:24:40 INFO : Spec noise = 0.000012  
2023-Oct-27 06:24:40 INFO : sdev noise = 0.000682  
2023-Oct-27 06:24:40 INFO : SNR residual = 19.448139  
2023-Oct-27 06:24:40 INFO : SNR max = 49.131869  
2023-Oct-27 06:24:40 INFO : Ymax = 0.026544

```
2023-Oct-27 06:24:40 INFO : Ymax metab = 0.026544
2023-Oct-27 06:24:40 INFO : Fit quality = 2.526302
2023-Oct-27 06:24:40 INFO : Baseline dev = 0.025474
2023-Oct-27 06:24:40 INFO : Ymax          = 0.026544
2023-Oct-27 06:24:40 INFO : BSL           = 0.015402
2023-Oct-27 06:24:40 INFO : Computing CRLBs.
2023-Oct-27 06:24:40 DEBUG : Sigma: 2.022562e-10
2023-Oct-27 06:24:40 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.82602
l2 norm of error at final p   = 1.79865
l2 norm of J.'*e at final p  = 217.694
l2 norm of D*p at final p    = 4.31352e-10
number of iterations         = 9
number of function evaluations = 2
number of Jacobian evaluations = 161
stopped by small D*p
```

```
2023-Oct-27 06:24:40 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:40 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:40 INFO : Loading data file : Temporary/cs/db6.raw
2023-Oct-27 06:24:40 INFO : nStart = 20
2023-Oct-27 06:24:40 INFO : nEnd   = 500
TARQUIN Version 4.3.11
```

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

```
2023-Oct-27 06:24:40 INFO : Loading data file : W.raw
2023-Oct-27 06:24:40 INFO : nStart = 20
2023-Oct-27 06:24:40 INFO : nEnd   = 500
Parameters Before Preprocessing
```

```
-----
Input file:           Temporary/cs/db6.raw
Water reference file: W.raw
Data points:         512
Rows:                1
Columns:             1
Slices:              1
Echo time:           0.03 s
Sampling frequency:  2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample:     20
Ending sample:       500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference:           4.65 ppm
```

```
2023-Oct-27 06:24:40 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:40 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:40 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:40 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:40 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:40 INFO : Ref new = 4.692027 ppm
2023-Oct-27 06:24:40 INFO : Residual water freq. (Hz) : 5.371094
2023-Oct-27 06:24:40 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:40 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:40 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:40 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:40 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:40 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:40 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:40 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:40 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:40 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:40 DEBUG : Max Phi0 : 0.31
2023-Oct-27 06:24:40 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:40 INFO : Ref new = 4.714951 ppm
2023-Oct-27 06:24:40 DEBUG : Width pts   : 13.49
2023-Oct-27 06:24:40 DEBUG : Width Hz est : 4.39
2023-Oct-27 06:24:40 DEBUG : Init beta est : 40.94
2023-Oct-27 06:24:40 INFO : Ymax        = 0.027552
2023-Oct-27 06:24:40 INFO : sdev noise = 0.000300
2023-Oct-27 06:24:40 INFO : SNR guess  = 45.8604
2023-Oct-27 06:24:40 INFO : Finished 'Preprocessing'
```

#### Parameters After Preprocessing

```
-----
Input file:           Temporary/cs/db6.raw
Water reference file: W.raw
Data points:         512
Rows:                1
Columns:             1
Slices:              1
Echo time:           0.03 s
Sampling frequency:  2000 Hz
Transmitter frequency: 1.278e+08 Hz
```

Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.71495 ppm

2023-Oct-27 06:24:40 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:40 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:40 INFO : Running optimiser  
2023-Oct-27 06:24:40 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:40 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:40 INFO : 31 group vectors in total  
2023-Oct-27 06:24:40 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:40 INFO : Final nStart = 20  
2023-Oct-27 06:24:40 INFO : Final nEnd = 500  
2023-Oct-27 06:24:40 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:40 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:40 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:40 INFO : Adjusting basis set to 4.714951 ppm  
2023-Oct-27 06:24:40 INFO : Time domain noise = 0.000014  
2023-Oct-27 06:24:40 DEBUG : Using init\_beta: 40.944639  
2023-Oct-27 06:24:40 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:40 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:40 INFO : done.  
2023-Oct-27 06:24:40 DEBUG : Final Beta: 122.44  
2023-Oct-27 06:24:40 DEBUG : Final Phi0: 0.28  
2023-Oct-27 06:24:40 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:40 INFO : FWHM right ppm = 1.994636  
2023-Oct-27 06:24:40 INFO : FWHM left ppm = 2.040484  
2023-Oct-27 06:24:40 INFO : Metabolite FWHM (ppm) = 0.045848  
2023-Oct-27 06:24:40 INFO : Spec noise = 0.000012  
2023-Oct-27 06:24:40 INFO : sdev noise = 0.000630  
2023-Oct-27 06:24:40 INFO : SNR residual = 20.316103  
2023-Oct-27 06:24:40 INFO : SNR max = 48.131631  
2023-Oct-27 06:24:40 INFO : Ymax = 0.025601  
2023-Oct-27 06:24:40 INFO : Ymax metab = 0.025601  
2023-Oct-27 06:24:40 INFO : Fit quality = 2.369137  
2023-Oct-27 06:24:40 INFO : Baseline dev = 0.025247  
2023-Oct-27 06:24:40 INFO : Ymax = 0.025601  
2023-Oct-27 06:24:40 INFO : BSL = 0.027545  
2023-Oct-27 06:24:40 INFO : Computing CRLBs.  
2023-Oct-27 06:24:40 DEBUG : Sigma: 2.074372e-10  
2023-Oct-27 06:24:40 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 4.2442  
l2 norm of error at final p = 1.83498  
l2 norm of J.\*e at final p = 229.761  
l2 norm of D\*p at final p = 2.19029e-13  
number of iterations = 7  
number of function evaluations = 2  
number of Jacobian evaluations = 191  
stopped by small D\*p

2023-Oct-27 06:24:40 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:40 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:40 INFO : Loading data file : Temporary/cs/db7.raw  
2023-Oct-27 06:24:40 INFO : nStart = 20  
2023-Oct-27 06:24:40 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:40 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:40 INFO : nStart = 20  
2023-Oct-27 06:24:40 INFO : nEnd = 500

#### Parameters Before Preprocessing

-----  
Input file: Temporary/cs/db7.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:40 INFO : Starting 'Preprocessing'

```

2023-Oct-27 06:24:40 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:40 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:40 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:40 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:40 INFO : Ref new = 4.703489 ppm
2023-Oct-27 06:24:40 INFO : Residual water freq. (Hz) : 6.835938
2023-Oct-27 06:24:40 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:40 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:40 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:40 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:40 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:40 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:40 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:40 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:40 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:40 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:40 DEBUG : Max Phi0 : 0.38
2023-Oct-27 06:24:40 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:41 INFO : Ref new = 4.730234 ppm
2023-Oct-27 06:24:41 DEBUG : Width pts : 19.45
2023-Oct-27 06:24:41 DEBUG : Width Hz est : 6.33
2023-Oct-27 06:24:41 DEBUG : Init beta est : 101.20
2023-Oct-27 06:24:41 INFO : Ymax = 0.028605
2023-Oct-27 06:24:41 INFO : sdev noise = 0.000292
2023-Oct-27 06:24:41 INFO : SNR guess = 48.9439
2023-Oct-27 06:24:41 INFO : Finished 'Preprocessing'

```

Parameters After Preprocessing

```

-----
Input file: Temporary/cs/db7.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.73023 ppm

```

```

2023-Oct-27 06:24:41 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:41 INFO : All simulation threads stopped.
2023-Oct-27 06:24:41 INFO : Running optimiser
2023-Oct-27 06:24:41 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:41 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:41 INFO : 31 group vectors in total
2023-Oct-27 06:24:41 INFO : 31 basis vectors in total
2023-Oct-27 06:24:41 INFO : Final nStart = 20
2023-Oct-27 06:24:41 INFO : Final nEnd = 500
2023-Oct-27 06:24:41 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:41 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:41 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:41 INFO : Adjusting basis set to 4.730234 ppm
2023-Oct-27 06:24:41 INFO : Time domain noise = 0.000013
2023-Oct-27 06:24:41 DEBUG : Using init_beta: 101.204475
2023-Oct-27 06:24:41 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:41 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:41 INFO : done.
2023-Oct-27 06:24:41 DEBUG : Final Beta: 132.86
2023-Oct-27 06:24:41 DEBUG : Final Phi0: 0.39
2023-Oct-27 06:24:41 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:41 INFO : FWHM right ppm = 1.994636
2023-Oct-27 06:24:41 INFO : FWHM left ppm = 2.048126
2023-Oct-27 06:24:41 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:41 INFO : Spec noise = 0.000013
2023-Oct-27 06:24:41 INFO : sdev noise = 0.000785
2023-Oct-27 06:24:41 INFO : SNR residual = 16.497524
2023-Oct-27 06:24:41 INFO : SNR max = 45.196675
2023-Oct-27 06:24:41 INFO : Ymax = 0.025911
2023-Oct-27 06:24:41 INFO : Ymax metab = 0.025911
2023-Oct-27 06:24:41 INFO : Fit quality = 2.739604
2023-Oct-27 06:24:41 INFO : Baseline dev = 0.024818
2023-Oct-27 06:24:41 INFO : Ymax = 0.025911
2023-Oct-27 06:24:41 INFO : BSL = 0.026364
2023-Oct-27 06:24:41 INFO : Computing CRLBs.
2023-Oct-27 06:24:41 DEBUG : Sigma: 1.774876e-10
2023-Oct-27 06:24:41 INFO : done.

```

Optimisation details

```

-----
l2 norm of error at initial p = 2.84859
l2 norm of error at final p = 1.80402
l2 norm of J.'*e at final p = 68.6908
l2 norm of D*p at final p = 1.735e-21
number of iterations = 10
number of function evaluations = 2
number of Jacobian evaluations = 309
stopped by small D*p

```

2023-Oct-27 06:24:41 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:41 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:41 INFO : Loading data file : Temporary/cs/db8.raw  
2023-Oct-27 06:24:41 INFO : nStart = 20  
2023-Oct-27 06:24:41 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:41 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:41 INFO : nStart = 20  
2023-Oct-27 06:24:41 INFO : nEnd = 500  
Parameters Before Preprocessing

-----  
Input file: Temporary/cs/db8.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:41 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:41 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:41 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:41 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:41 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:41 INFO : Ref new = 4.714951 ppm  
2023-Oct-27 06:24:41 INFO : Residual water freq. (Hz) : 8.300781  
2023-Oct-27 06:24:41 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:41 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:41 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:42 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:42 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:42 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:42 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:42 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:42 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:42 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:42 DEBUG : Max Phi0 : 0.06  
2023-Oct-27 06:24:42 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:42 INFO : Ref new = 4.737875 ppm  
2023-Oct-27 06:24:42 DEBUG : Width pts : 20.34  
2023-Oct-27 06:24:42 DEBUG : Width Hz est : 6.62  
2023-Oct-27 06:24:42 DEBUG : Init beta est : 112.45  
2023-Oct-27 06:24:42 INFO : Ymax = 0.028142  
2023-Oct-27 06:24:42 INFO : sdev noise = 0.000296  
2023-Oct-27 06:24:42 INFO : SNR guess = 47.5395  
2023-Oct-27 06:24:42 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/cs/db8.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.73788 ppm

2023-Oct-27 06:24:42 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:42 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:42 INFO : Running optimiser  
2023-Oct-27 06:24:42 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:42 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:42 INFO : 31 group vectors in total  
2023-Oct-27 06:24:42 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:42 INFO : Final nStart = 20  
2023-Oct-27 06:24:42 INFO : Final nEnd = 500  
2023-Oct-27 06:24:42 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:42 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:42 INFO : Fitting fid 1 of 1

```
2023-Oct-27 06:24:42 INFO : Adjusting basis set to 4.737875 ppm
2023-Oct-27 06:24:42 INFO : Time domain noise = 0.000015
2023-Oct-27 06:24:42 DEBUG : Using init_beta: 112.448948
2023-Oct-27 06:24:42 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:42 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:42 INFO : done.
2023-Oct-27 06:24:42 DEBUG : Final Beta: 139.86
2023-Oct-27 06:24:42 DEBUG : Final Phi0: -0.29
2023-Oct-27 06:24:42 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:42 INFO : FWHM right ppm = 1.986995
2023-Oct-27 06:24:42 INFO : FWHM left ppm = 2.040484
2023-Oct-27 06:24:42 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:42 INFO : Spec noise = 0.000013
2023-Oct-27 06:24:42 INFO : sdev noise = 0.000747
2023-Oct-27 06:24:42 INFO : SNR residual = 18.015934
2023-Oct-27 06:24:42 INFO : SNR max = 47.117845
2023-Oct-27 06:24:42 INFO : Ymax = 0.026916
2023-Oct-27 06:24:42 INFO : Ymax metab = 0.026916
2023-Oct-27 06:24:42 INFO : Fit quality = 2.615343
2023-Oct-27 06:24:42 INFO : Baseline dev = 0.023712
2023-Oct-27 06:24:42 INFO : Ymax = 0.026916
2023-Oct-27 06:24:42 INFO : BSL = 0.032566
2023-Oct-27 06:24:42 INFO : Computing CRLBs.
2023-Oct-27 06:24:42 DEBUG : Sigma: 2.157403e-10
2023-Oct-27 06:24:42 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 3.00073
l2 norm of error at final p = 1.83632
l2 norm of J.*e at final p = 185.918
l2 norm of D*p at final p = 1.74355e-14
number of iterations = 10
number of function evaluations = 2
number of Jacobian evaluations = 210
stopped by small D*p
```

```
2023-Oct-27 06:24:42 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:42 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:42 INFO : Loading data file : Temporary/cs/db9.raw
2023-Oct-27 06:24:42 INFO : nStart = 20
2023-Oct-27 06:24:42 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:42 INFO : Loading data file : W.raw
2023-Oct-27 06:24:42 INFO : nStart = 20
2023-Oct-27 06:24:42 INFO : nEnd = 500
```

#### Parameters Before Preprocessing

```
-----
Input file: Temporary/cs/db9.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:42 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:42 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:42 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:42 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:42 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:42 INFO : Ref new = 4.726413 ppm
2023-Oct-27 06:24:42 INFO : Residual water freq. (Hz) : 9.765625
2023-Oct-27 06:24:42 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:42 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:42 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:42 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:42 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:42 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:42 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:42 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:42 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:42 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:42 DEBUG : Max Phi0 : 0.13
2023-Oct-27 06:24:42 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:42 INFO : Ref new = 4.749337 ppm
2023-Oct-27 06:24:42 DEBUG : Width pts : 13.58
2023-Oct-27 06:24:42 DEBUG : Width Hz est : 4.42
```

```
2023-Oct-27 06:24:42 DEBUG : Init beta est : 41.64
2023-Oct-27 06:24:42 INFO : Ymax = 0.027654
2023-Oct-27 06:24:42 INFO : sdev noise = 0.000298
2023-Oct-27 06:24:42 INFO : SNR guess = 46.4055
2023-Oct-27 06:24:42 INFO : Finished 'Preprocessing'
```

Parameters After Preprocessing

```
-----
Input file: Temporary/cs/db9.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.74934 ppm
```

```
2023-Oct-27 06:24:42 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:43 INFO : All simulation threads stopped.
2023-Oct-27 06:24:43 INFO : Running optimiser
2023-Oct-27 06:24:43 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:43 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:43 INFO : 31 group vectors in total
2023-Oct-27 06:24:43 INFO : 31 basis vectors in total
2023-Oct-27 06:24:43 INFO : Final nStart = 20
2023-Oct-27 06:24:43 INFO : Final nEnd = 500
2023-Oct-27 06:24:43 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:43 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:43 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:43 INFO : Adjusting basis set to 4.749337 ppm
2023-Oct-27 06:24:43 INFO : Time domain noise = 0.000014
2023-Oct-27 06:24:43 DEBUG : Using init_beta: 41.635463
2023-Oct-27 06:24:43 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:43 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:43 INFO : done.
2023-Oct-27 06:24:43 DEBUG : Final Beta: 139.80
2023-Oct-27 06:24:43 DEBUG : Final Phi0: 0.14
2023-Oct-27 06:24:43 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:43 INFO : FWHM right ppm = 1.990816
2023-Oct-27 06:24:43 INFO : FWHM left ppm = 2.036664
2023-Oct-27 06:24:43 INFO : Metabolite FWHM (ppm) = 0.045848
2023-Oct-27 06:24:43 INFO : Spec noise = 0.000012
2023-Oct-27 06:24:43 INFO : sdev noise = 0.000740
2023-Oct-27 06:24:43 INFO : SNR residual = 17.216195
2023-Oct-27 06:24:43 INFO : SNR max = 48.794729
2023-Oct-27 06:24:43 INFO : Ymax = 0.025491
2023-Oct-27 06:24:43 INFO : Ymax metab = 0.025491
2023-Oct-27 06:24:43 INFO : Fit quality = 2.834234
2023-Oct-27 06:24:43 INFO : Baseline dev = 0.024765
2023-Oct-27 06:24:43 INFO : Ymax = 0.025491
2023-Oct-27 06:24:43 INFO : BSL = 0.020841
2023-Oct-27 06:24:43 INFO : Computing CRLBs.
2023-Oct-27 06:24:43 DEBUG : Sigma: 1.997975e-10
2023-Oct-27 06:24:43 INFO : done.
```

Optimisation details

```
-----
l2 norm of error at initial p = 4.55165
l2 norm of error at final p = 1.83766
l2 norm of J.'*e at final p = 466.273
l2 norm of D*p at final p = 9.91624e-11
number of iterations = 12
number of function evaluations = 2
number of Jacobian evaluations = 183
stopped by small D*p
```

```
2023-Oct-27 06:24:43 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:43 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:43 INFO : Loading data file : Temporary/cs/db10.raw
2023-Oct-27 06:24:43 INFO : nStart = 20
2023-Oct-27 06:24:43 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

```
2023-Oct-27 06:24:43 INFO : Loading data file : W.raw
2023-Oct-27 06:24:43 INFO : nStart = 20
2023-Oct-27 06:24:43 INFO : nEnd = 500
```

Parameters Before Preprocessing

```
-----
Input file: Temporary/cs/db10.raw
Water reference file: W.raw
```

Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:43 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:43 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:43 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:43 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:43 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:43 INFO : Ref new = 4.737875 ppm  
2023-Oct-27 06:24:43 INFO : Residual water freq. (Hz) : 11.230469  
2023-Oct-27 06:24:43 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:43 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:43 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:43 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:43 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:43 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:43 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:43 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:43 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:43 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:43 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:43 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:43 INFO : Ref new = 4.749337 ppm  
2023-Oct-27 06:24:43 DEBUG : Width pts : 15.35  
2023-Oct-27 06:24:43 DEBUG : Width Hz est : 5.00  
2023-Oct-27 06:24:43 DEBUG : Init beta est : 56.90  
2023-Oct-27 06:24:43 INFO : Ymax = 0.028785  
2023-Oct-27 06:24:43 INFO : sdev noise = 0.000286  
2023-Oct-27 06:24:43 INFO : SNR guess = 50.3160  
2023-Oct-27 06:24:43 INFO : Finished 'Preprocessing'

#### Parameters After Preprocessing

-----  
Input file: Temporary/cs/db10.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.74934 ppm

2023-Oct-27 06:24:43 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:43 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:43 INFO : Running optimiser  
2023-Oct-27 06:24:43 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:43 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:43 INFO : 31 group vectors in total  
2023-Oct-27 06:24:43 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:43 INFO : Final nStart = 20  
2023-Oct-27 06:24:43 INFO : Final nEnd = 500  
2023-Oct-27 06:24:43 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:43 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:43 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:43 INFO : Adjusting basis set to 4.749337 ppm  
2023-Oct-27 06:24:43 INFO : Time domain noise = 0.000013  
2023-Oct-27 06:24:43 DEBUG : Using init\_beta: 56.895857  
2023-Oct-27 06:24:43 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:43 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:44 INFO : done.  
2023-Oct-27 06:24:44 DEBUG : Final Beta: 103.78  
2023-Oct-27 06:24:44 DEBUG : Final Phi0: 0.29  
2023-Oct-27 06:24:44 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:44 INFO : FWHM right ppm = 1.975533  
2023-Oct-27 06:24:44 INFO : FWHM left ppm = 2.029022  
2023-Oct-27 06:24:44 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:44 INFO : Spec noise = 0.000012  
2023-Oct-27 06:24:44 INFO : sdev noise = 0.000823  
2023-Oct-27 06:24:44 INFO : SNR residual = 15.456925  
2023-Oct-27 06:24:44 INFO : SNR max = 45.148835  
2023-Oct-27 06:24:44 INFO : Ymax = 0.025455  
2023-Oct-27 06:24:44 INFO : Ymax metab = 0.025455  
2023-Oct-27 06:24:44 INFO : Fit quality = 2.920945  
2023-Oct-27 06:24:44 INFO : Baseline dev = 0.022476  
2023-Oct-27 06:24:44 INFO : Ymax = 0.025455

2023-Oct-27 06:24:44 INFO : BSL = 0.016124  
2023-Oct-27 06:24:44 INFO : Computing CRLBs.  
2023-Oct-27 06:24:44 DEBUG : Sigma: 1.614386e-10  
2023-Oct-27 06:24:44 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 4.16651  
l2 norm of error at final p = 1.88789  
l2 norm of J.\*e at final p = 279.761  
l2 norm of D\*p at final p = 2.75013e-12  
number of iterations = 6  
number of function evaluations = 2  
number of Jacobian evaluations = 178  
stopped by small D\*p

2023-Oct-27 06:24:44 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:44 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:44 INFO : Loading data file : Temporary/dd/filters1.raw  
2023-Oct-27 06:24:44 INFO : nStart = 20  
2023-Oct-27 06:24:44 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:44 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:44 INFO : nStart = 20  
2023-Oct-27 06:24:44 INFO : nEnd = 500

#### Parameters Before Preprocessing

-----  
Input file: Temporary/dd/filters1.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:44 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:44 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:44 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:44 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:44 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:44 INFO : Ref new = 4.627076 ppm  
2023-Oct-27 06:24:44 INFO : Residual water freq. (Hz) : -2.929688  
2023-Oct-27 06:24:44 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:44 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:44 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:44 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:44 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:44 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:44 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:44 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:44 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:44 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:44 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:44 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:44 INFO : Ref new = 4.646179 ppm  
2023-Oct-27 06:24:44 DEBUG : Width pts : 20.17  
2023-Oct-27 06:24:44 DEBUG : Width Hz est : 6.57  
2023-Oct-27 06:24:44 DEBUG : Init beta est : 110.32  
2023-Oct-27 06:24:44 INFO : Ymax = 0.027833  
2023-Oct-27 06:24:44 INFO : sdev noise = 0.000247  
2023-Oct-27 06:24:44 INFO : SNR guess = 56.4290  
2023-Oct-27 06:24:44 INFO : Finished 'Preprocessing'

#### Parameters After Preprocessing

-----  
Input file: Temporary/dd/filters1.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes

Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.64618 ppm

2023-Oct-27 06:24:44 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:44 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:44 INFO : Running optimiser  
2023-Oct-27 06:24:44 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:44 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:44 INFO : 31 group vectors in total  
2023-Oct-27 06:24:44 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:44 INFO : Final nStart = 20  
2023-Oct-27 06:24:44 INFO : Final nEnd = 500  
2023-Oct-27 06:24:44 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:44 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:44 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:44 INFO : Adjusting basis set to 4.646179 ppm  
2023-Oct-27 06:24:44 INFO : Time domain noise = 0.000012  
2023-Oct-27 06:24:44 DEBUG : Using init\_beta: 110.318297  
2023-Oct-27 06:24:44 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:44 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:44 INFO : done.  
2023-Oct-27 06:24:44 DEBUG : Final Beta: 164.65  
2023-Oct-27 06:24:44 DEBUG : Final Phi0: -0.32  
2023-Oct-27 06:24:44 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:44 INFO : FWHM right ppm = 1.994636  
2023-Oct-27 06:24:44 INFO : FWHM left ppm = 2.048126  
2023-Oct-27 06:24:44 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:44 INFO : Spec noise = 0.000011  
2023-Oct-27 06:24:44 INFO : sdev noise = 0.000609  
2023-Oct-27 06:24:44 INFO : SNR residual = 20.867550  
2023-Oct-27 06:24:44 INFO : SNR max = 50.090754  
2023-Oct-27 06:24:44 INFO : Ymax = 0.025396  
2023-Oct-27 06:24:44 INFO : Ymax metab = 0.025396  
2023-Oct-27 06:24:44 INFO : Fit quality = 2.400414  
2023-Oct-27 06:24:44 INFO : Baseline dev = 0.039073  
2023-Oct-27 06:24:44 INFO : Ymax = 0.025396  
2023-Oct-27 06:24:44 INFO : BSL = 0.071423  
2023-Oct-27 06:24:44 INFO : Computing CRLBs.  
2023-Oct-27 06:24:44 DEBUG : Sigma: 1.448069e-10  
2023-Oct-27 06:24:44 INFO : done.

Optimisation details

-----  
l2 norm of error at initial p = 2.2312  
l2 norm of error at final p = 1.42146  
l2 norm of J.'\*e at final p = 454.585  
l2 norm of D\*p at final p = 1.86571e-10  
number of iterations = 7  
number of function evaluations = 2  
number of Jacobian evaluations = 159  
stopped by small D\*p

2023-Oct-27 06:24:44 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:45 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:45 INFO : Loading data file : Temporary/dd/filters2.raw  
2023-Oct-27 06:24:45 INFO : nStart = 20  
2023-Oct-27 06:24:45 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:45 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:45 INFO : nStart = 20  
2023-Oct-27 06:24:45 INFO : nEnd = 500  
Parameters Before Preprocessing

-----  
Input file: Temporary/dd/filters2.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:45 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:45 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:45 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:45 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:45 INFO : Ref start = 4.650000 ppm

2023-Oct-27 06:24:45 INFO : Ref new = 4.619435 ppm  
2023-Oct-27 06:24:45 INFO : Residual water freq. (Hz) : -3.906250  
2023-Oct-27 06:24:45 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:45 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:45 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:45 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:45 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:45 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:45 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:45 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:45 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:45 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:45 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:45 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:45 INFO : Ref new = 4.646179 ppm  
2023-Oct-27 06:24:45 DEBUG : Width pts : 20.36  
2023-Oct-27 06:24:45 DEBUG : Width Hz est : 6.63  
2023-Oct-27 06:24:45 DEBUG : Init beta est : 112.75  
2023-Oct-27 06:24:45 INFO : Ymax = 0.027823  
2023-Oct-27 06:24:45 INFO : sdev noise = 0.000242  
2023-Oct-27 06:24:45 INFO : SNR guess = 57.4223  
2023-Oct-27 06:24:45 INFO : Finished 'Preprocessing'

#### Parameters After Preprocessing

-----  
Input file: Temporary/dd/filters2.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.64618 ppm

2023-Oct-27 06:24:45 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:45 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:45 INFO : Running optimiser  
2023-Oct-27 06:24:45 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:45 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:45 INFO : 31 group vectors in total  
2023-Oct-27 06:24:45 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:45 INFO : Final nStart = 20  
2023-Oct-27 06:24:45 INFO : Final nEnd = 500  
2023-Oct-27 06:24:45 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:45 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:45 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:45 INFO : Adjusting basis set to 4.646179 ppm  
2023-Oct-27 06:24:45 INFO : Time domain noise = 0.000012  
2023-Oct-27 06:24:45 DEBUG : Using init\_beta: 112.746734  
2023-Oct-27 06:24:45 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:45 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:45 INFO : done.  
2023-Oct-27 06:24:45 DEBUG : Final Beta: 168.60  
2023-Oct-27 06:24:45 DEBUG : Final Phi0: -0.21  
2023-Oct-27 06:24:45 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:45 INFO : FWHM right ppm = 1.994636  
2023-Oct-27 06:24:45 INFO : FWHM left ppm = 2.048126  
2023-Oct-27 06:24:45 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:45 INFO : Spec noise = 0.000011  
2023-Oct-27 06:24:45 INFO : sdev noise = 0.000637  
2023-Oct-27 06:24:45 INFO : SNR residual = 19.776332  
2023-Oct-27 06:24:45 INFO : SNR max = 52.926490  
2023-Oct-27 06:24:45 INFO : Ymax = 0.025200  
2023-Oct-27 06:24:45 INFO : Ymax metab = 0.025200  
2023-Oct-27 06:24:45 INFO : Fit quality = 2.676254  
2023-Oct-27 06:24:45 INFO : Baseline dev = 0.035193  
2023-Oct-27 06:24:45 INFO : Ymax = 0.025200  
2023-Oct-27 06:24:45 INFO : BSL = 0.059245  
2023-Oct-27 06:24:45 INFO : Computing CRLBs.  
2023-Oct-27 06:24:45 DEBUG : Sigma: 1.464524e-10  
2023-Oct-27 06:24:45 INFO : done.

#### Optimisation details

-----  
l2 norm of error at initial p = 2.34951  
l2 norm of error at final p = 1.44512  
l2 norm of J.\*e at final p = 248.511  
l2 norm of D\*p at final p = 4.25265e-11  
number of iterations = 7  
number of function evaluations = 2  
number of Jacobian evaluations = 166  
stopped by small D\*p

2023-Oct-27 06:24:45 INFO : TARQUIN Finished

Writing txt results file.

Done.

```
2023-Oct-27 06:24:45 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:45 INFO : Loading data file : Temporary/cplx/df1.raw
2023-Oct-27 06:24:45 INFO : nStart = 20
2023-Oct-27 06:24:45 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

```
2023-Oct-27 06:24:45 INFO : Loading data file : W.raw
2023-Oct-27 06:24:45 INFO : nStart = 20
2023-Oct-27 06:24:45 INFO : nEnd = 500
```

Parameters Before Preprocessing

```
-----
Input file: Temporary/cplx/df1.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:45 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:45 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:45 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:45 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:45 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:45 INFO : Ref new = 4.619435 ppm
2023-Oct-27 06:24:45 INFO : Residual water freq. (Hz) : -3.906250
2023-Oct-27 06:24:45 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:45 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:45 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:45 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:45 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:45 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:45 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:45 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:45 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:45 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:45 DEBUG : Max Phi0 : 0.25
2023-Oct-27 06:24:45 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:45 INFO : Ref new = 4.642359 ppm
2023-Oct-27 06:24:45 DEBUG : Width pts : 18.96
2023-Oct-27 06:24:45 DEBUG : Width Hz est : 6.17
2023-Oct-27 06:24:45 DEBUG : Init beta est : 95.21
2023-Oct-27 06:24:45 INFO : Ymax = 0.020662
2023-Oct-27 06:24:45 INFO : sdev noise = 0.000201
2023-Oct-27 06:24:45 INFO : SNR guess = 51.4178
2023-Oct-27 06:24:45 INFO : Finished 'Preprocessing'
```

Parameters After Preprocessing

```
-----
Input file: Temporary/cplx/df1.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.64236 ppm
```

```
2023-Oct-27 06:24:45 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:45 INFO : All simulation threads stopped.
2023-Oct-27 06:24:45 INFO : Running optimiser
2023-Oct-27 06:24:45 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:45 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:45 INFO : 31 group vectors in total
2023-Oct-27 06:24:45 INFO : 31 basis vectors in total
2023-Oct-27 06:24:45 INFO : Final nStart = 20
2023-Oct-27 06:24:45 INFO : Final nEnd = 500
2023-Oct-27 06:24:45 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:45 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:45 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:45 INFO : Adjusting basis set to 4.642359 ppm
2023-Oct-27 06:24:45 INFO : Time domain noise = 0.000011
2023-Oct-27 06:24:45 DEBUG : Using init_beta: 95.209341
2023-Oct-27 06:24:45 DEBUG : Doing a maximum of 75 iterations.
```

```
2023-Oct-27 06:24:46 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:46 INFO : done.
2023-Oct-27 06:24:46 DEBUG : Final Beta: 142.69
2023-Oct-27 06:24:46 DEBUG : Final Phi0: -0.21
2023-Oct-27 06:24:46 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:46 INFO : FWHM right ppm = 1.990816
2023-Oct-27 06:24:46 INFO : FWHM left ppm = 2.044305
2023-Oct-27 06:24:46 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:46 INFO : Spec noise = 0.000009
2023-Oct-27 06:24:46 INFO : sdev noise = 0.000502
2023-Oct-27 06:24:46 INFO : SNR residual = 18.624059
2023-Oct-27 06:24:46 INFO : SNR max = 48.080079
2023-Oct-27 06:24:46 INFO : Ymax = 0.018715
2023-Oct-27 06:24:46 INFO : Ymax metab = 0.018715
2023-Oct-27 06:24:46 INFO : Fit quality = 2.581611
2023-Oct-27 06:24:46 INFO : Baseline dev = 0.032590
2023-Oct-27 06:24:46 INFO : Ymax = 0.018715
2023-Oct-27 06:24:46 INFO : BSL = 0.055240
2023-Oct-27 06:24:46 INFO : Computing CRLBs.
2023-Oct-27 06:24:46 DEBUG : Sigma: 1.121573e-10
2023-Oct-27 06:24:46 INFO : done.
```

Optimisation details

```
-----
l2 norm of error at initial p = 2.62613
l2 norm of error at final p = 1.71616
l2 norm of J.'*e at final p = 240.998
l2 norm of D*p at final p = 7.15706e-32
number of iterations = 8
number of function evaluations = 2
number of Jacobian evaluations = 396
stopped by small D*p
```

2023-Oct-27 06:24:46 INFO : TARQUIN Finished

Writing txt results file.  
Done.

```
2023-Oct-27 06:24:46 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:46 INFO : Loading data file : Temporary/cplx/df2.raw
2023-Oct-27 06:24:46 INFO : nStart = 20
2023-Oct-27 06:24:46 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

```
2023-Oct-27 06:24:46 INFO : Loading data file : W.raw
2023-Oct-27 06:24:46 INFO : nStart = 20
2023-Oct-27 06:24:46 INFO : nEnd = 500
Parameters Before Preprocessing
```

```
-----
Input file: Temporary/cplx/df2.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:46 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:46 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:46 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:46 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:46 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:46 INFO : Ref new = 4.619435 ppm
2023-Oct-27 06:24:46 INFO : Residual water freq. (Hz) : -3.906250
2023-Oct-27 06:24:46 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:46 INFO : Finished 'building Hankel LP matrix'
2023-Oct-27 06:24:46 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:47 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:47 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:47 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:47 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:47 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:47 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:47 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:47 DEBUG : Max Phi0 : 0.25
2023-Oct-27 06:24:47 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:47 INFO : Ref new = 4.642359 ppm
2023-Oct-27 06:24:47 DEBUG : Width pts : 18.96
2023-Oct-27 06:24:47 DEBUG : Width Hz est : 6.17
2023-Oct-27 06:24:47 DEBUG : Init beta est : 95.21
2023-Oct-27 06:24:47 INFO : Ymax = 0.020662
2023-Oct-27 06:24:47 INFO : sdev noise = 0.000201
2023-Oct-27 06:24:47 INFO : SNR guess = 51.4178
```

2023-Oct-27 06:24:47 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/cplx/df2.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.64236 ppm

2023-Oct-27 06:24:47 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:47 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:47 INFO : Running optimiser  
2023-Oct-27 06:24:47 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:47 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:47 INFO : 31 group vectors in total  
2023-Oct-27 06:24:47 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:47 INFO : Final nStart = 20  
2023-Oct-27 06:24:47 INFO : Final nEnd = 500  
2023-Oct-27 06:24:47 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:47 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:47 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:47 INFO : Adjusting basis set to 4.642359 ppm  
2023-Oct-27 06:24:47 INFO : Time domain noise = 0.000011  
2023-Oct-27 06:24:47 DEBUG : Using init\_beta: 95.209341  
2023-Oct-27 06:24:47 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:47 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:48 INFO : done.  
2023-Oct-27 06:24:48 DEBUG : Final Beta: 142.69  
2023-Oct-27 06:24:48 DEBUG : Final Phi0: -0.21  
2023-Oct-27 06:24:48 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:48 INFO : FWHM right ppm = 1.990816  
2023-Oct-27 06:24:48 INFO : FWHM left ppm = 2.044305  
2023-Oct-27 06:24:48 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:48 INFO : Spec noise = 0.000009  
2023-Oct-27 06:24:48 INFO : sdev noise = 0.000502  
2023-Oct-27 06:24:48 INFO : SNR residual = 18.624059  
2023-Oct-27 06:24:48 INFO : SNR max = 48.080079  
2023-Oct-27 06:24:48 INFO : Ymax = 0.018715  
2023-Oct-27 06:24:48 INFO : Ymax metab = 0.018715  
2023-Oct-27 06:24:48 INFO : Fit quality = 2.581611  
2023-Oct-27 06:24:48 INFO : Baseline dev = 0.032590  
2023-Oct-27 06:24:48 INFO : Ymax = 0.018715  
2023-Oct-27 06:24:48 INFO : BSL = 0.055240  
2023-Oct-27 06:24:48 INFO : Computing CRLBs.  
2023-Oct-27 06:24:48 DEBUG : Sigma: 1.121573e-10  
2023-Oct-27 06:24:48 INFO : done.

Optimisation details

-----  
l2 norm of error at initial p = 2.62613  
l2 norm of error at final p = 1.71616  
l2 norm of J.\*e at final p = 240.998  
l2 norm of D\*p at final p = 7.15706e-32  
number of iterations = 8  
number of function evaluations = 2  
number of Jacobian evaluations = 396  
stopped by small D\*p

2023-Oct-27 06:24:48 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:48 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:48 INFO : Loading data file : Temporary/cplx/df3.raw  
2023-Oct-27 06:24:48 INFO : nStart = 20  
2023-Oct-27 06:24:48 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:48 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:48 INFO : nStart = 20  
2023-Oct-27 06:24:48 INFO : nEnd = 500  
Parameters Before Preprocessing

-----  
Input file: Temporary/cplx/df3.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1

Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:48 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:48 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:48 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:48 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:48 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:48 INFO : Ref new = 4.619435 ppm  
2023-Oct-27 06:24:48 INFO : Residual water freq. (Hz) : -3.906250  
2023-Oct-27 06:24:48 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:48 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:48 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:48 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:48 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:48 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:48 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:48 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:48 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:48 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:48 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:48 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:48 INFO : Ref new = 4.642359 ppm  
2023-Oct-27 06:24:48 DEBUG : Width pts : 18.96  
2023-Oct-27 06:24:48 DEBUG : Width Hz est : 6.17  
2023-Oct-27 06:24:48 DEBUG : Init beta est : 95.21  
2023-Oct-27 06:24:48 INFO : Ymax = 0.020662  
2023-Oct-27 06:24:48 INFO : sdev noise = 0.000201  
2023-Oct-27 06:24:48 INFO : SNR guess = 51.4178  
2023-Oct-27 06:24:48 INFO : Finished 'Preprocessing'

#### Parameters After Preprocessing

-----  
Input file: Temporary/cplx/dtf3.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.64236 ppm

2023-Oct-27 06:24:48 INFO : Simulating using 6 threads.  
2023-Oct-27 06:24:48 INFO : All simulation threads stopped.  
2023-Oct-27 06:24:48 INFO : Running optimiser  
2023-Oct-27 06:24:48 INFO : Setting metab shift limit to 0.030000 ppm  
2023-Oct-27 06:24:48 INFO : Setting broad shift limit to 0.100000 ppm  
2023-Oct-27 06:24:48 INFO : 31 group vectors in total  
2023-Oct-27 06:24:48 INFO : 31 basis vectors in total  
2023-Oct-27 06:24:48 INFO : Final nStart = 20  
2023-Oct-27 06:24:48 INFO : Final nEnd = 500  
2023-Oct-27 06:24:48 INFO : 1 voxel(s) to be fitted  
2023-Oct-27 06:24:48 DEBUG : Overlapping signals found: 16  
2023-Oct-27 06:24:48 INFO : Fitting fid 1 of 1  
2023-Oct-27 06:24:48 INFO : Adjusting basis set to 4.642359 ppm  
2023-Oct-27 06:24:48 INFO : Time domain noise = 0.000011  
2023-Oct-27 06:24:48 DEBUG : Using init\_beta: 95.209341  
2023-Oct-27 06:24:48 DEBUG : Doing a maximum of 75 iterations.  
2023-Oct-27 06:24:48 DEBUG : Initial phase fit completed.....  
2023-Oct-27 06:24:49 INFO : done.  
2023-Oct-27 06:24:49 DEBUG : Final Beta: 142.69  
2023-Oct-27 06:24:49 DEBUG : Final Phi0: -0.21  
2023-Oct-27 06:24:49 DEBUG : Final Phi1: 0.00  
2023-Oct-27 06:24:49 INFO : FWHM right ppm = 1.990816  
2023-Oct-27 06:24:49 INFO : FWHM left ppm = 2.044305  
2023-Oct-27 06:24:49 INFO : Metabolite FWHM (ppm) = 0.053489  
2023-Oct-27 06:24:49 INFO : Spec noise = 0.000009  
2023-Oct-27 06:24:49 INFO : sdev noise = 0.000502  
2023-Oct-27 06:24:49 INFO : SNR residual = 18.624059  
2023-Oct-27 06:24:49 INFO : SNR max = 48.080079  
2023-Oct-27 06:24:49 INFO : Ymax = 0.018715  
2023-Oct-27 06:24:49 INFO : Ymax metab = 0.018715  
2023-Oct-27 06:24:49 INFO : Fit quality = 2.581611  
2023-Oct-27 06:24:49 INFO : Baseline dev = 0.032590  
2023-Oct-27 06:24:49 INFO : Ymax = 0.018715  
2023-Oct-27 06:24:49 INFO : BSL = 0.055240  
2023-Oct-27 06:24:49 INFO : Computing CRLBs.  
2023-Oct-27 06:24:49 DEBUG : Sigma: 1.121573e-10  
2023-Oct-27 06:24:49 INFO : done.

Optimisation details

-----  
l2 norm of error at initial p = 2.62613  
l2 norm of error at final p = 1.71616  
l2 norm of J.\*e at final p = 240.998  
l2 norm of D\*p at final p = 7.15706e-32  
number of iterations = 8  
number of function evaluations = 2  
number of Jacobian evaluations = 396  
stopped by small D\*p

2023-Oct-27 06:24:49 INFO : TARQUIN Finished

Writing txt results file.  
Done.

2023-Oct-27 06:24:49 INFO : TARQUIN 4.3.11 Started  
2023-Oct-27 06:24:49 INFO : Loading data file : Temporary/cplx/df4.raw  
2023-Oct-27 06:24:49 INFO : nStart = 20  
2023-Oct-27 06:24:49 INFO : nEnd = 500  
TARQUIN Version 4.3.11

\*\*\*\* TARQUIN is a research tool and is NOT for clinical use. \*\*\*\*

2023-Oct-27 06:24:49 INFO : Loading data file : W.raw  
2023-Oct-27 06:24:49 INFO : nStart = 20  
2023-Oct-27 06:24:49 INFO : nEnd = 500  
Parameters Before Preprocessing

-----  
Input file: Temporary/cplx/df4.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.65 ppm

2023-Oct-27 06:24:49 INFO : Starting 'Preprocessing'  
2023-Oct-27 06:24:49 INFO : Preprocessing fid 1 of 1  
2023-Oct-27 06:24:49 INFO : Starting 'autophasing mag method water'  
2023-Oct-27 06:24:49 INFO : Finished 'autophasing mag method water'  
2023-Oct-27 06:24:49 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:49 INFO : Ref new = 4.619435 ppm  
2023-Oct-27 06:24:49 INFO : Residual water freq. (Hz) : -3.906250  
2023-Oct-27 06:24:49 INFO : Starting 'building Hankel LP matrix'  
2023-Oct-27 06:24:49 INFO : Finished 'building Hankel LP matrix'  
2023-Oct-27 06:24:49 INFO : Starting 'SVD of LP matrix'  
2023-Oct-27 06:24:49 INFO : Finished 'SVD of LP matrix'  
2023-Oct-27 06:24:49 INFO : Starting 'estimating LP parameters'  
2023-Oct-27 06:24:49 INFO : Finished 'estimating LP parameters'  
2023-Oct-27 06:24:49 INFO : Starting 'estimating LP amplitudes'  
2023-Oct-27 06:24:49 INFO : Finished 'estimating LP amplitudes'  
2023-Oct-27 06:24:49 INFO : Starting 'autophasing (new)'  
2023-Oct-27 06:24:49 INFO : Finished 'autophasing (new)'  
2023-Oct-27 06:24:49 DEBUG : Max Phi0 : 0.25  
2023-Oct-27 06:24:49 INFO : Ref start = 4.650000 ppm  
2023-Oct-27 06:24:49 INFO : Ref new = 4.642359 ppm  
2023-Oct-27 06:24:49 DEBUG : Width pts : 18.96  
2023-Oct-27 06:24:49 DEBUG : Width Hz est : 6.17  
2023-Oct-27 06:24:49 DEBUG : Init beta est : 95.21  
2023-Oct-27 06:24:49 INFO : Ymax = 0.020662  
2023-Oct-27 06:24:49 INFO : sdev noise = 0.000201  
2023-Oct-27 06:24:49 INFO : SNR guess = 51.4178  
2023-Oct-27 06:24:49 INFO : Finished 'Preprocessing'

Parameters After Preprocessing

-----  
Input file: Temporary/cplx/df4.raw  
Water reference file: W.raw  
Data points: 512  
Rows: 1  
Columns: 1  
Slices: 1  
Echo time: 0.03 s  
Sampling frequency: 2000 Hz  
Transmitter frequency: 1.278e+08 Hz  
Starting sample: 20  
Ending sample: 500  
Removing signals in: [-45,+45] Hz  
Autophasing yes/no?: yes  
Water eddy correction?: no  
Autoreferencing yes/no?: yes  
Reference: 4.64236 ppm

```
2023-Oct-27 06:24:49 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:49 INFO : All simulation threads stopped.
2023-Oct-27 06:24:49 INFO : Running optimiser
2023-Oct-27 06:24:49 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:49 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:49 INFO : 31 group vectors in total
2023-Oct-27 06:24:49 INFO : 31 basis vectors in total
2023-Oct-27 06:24:49 INFO : Final nStart = 20
2023-Oct-27 06:24:49 INFO : Final nEnd = 500
2023-Oct-27 06:24:49 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:49 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:49 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:49 INFO : Adjusting basis set to 4.642359 ppm
2023-Oct-27 06:24:49 INFO : Time domain noise = 0.000011
2023-Oct-27 06:24:49 DEBUG : Using init_beta: 95.209341
2023-Oct-27 06:24:49 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:49 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:50 INFO : done.
2023-Oct-27 06:24:50 DEBUG : Final Beta: 142.69
2023-Oct-27 06:24:50 DEBUG : Final Phi0: -0.21
2023-Oct-27 06:24:50 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:50 INFO : FWHM right ppm = 1.990816
2023-Oct-27 06:24:50 INFO : FWHM left ppm = 2.044305
2023-Oct-27 06:24:50 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:50 INFO : Spec noise = 0.000009
2023-Oct-27 06:24:50 INFO : sdev noise = 0.000502
2023-Oct-27 06:24:50 INFO : SNR residual = 18.624059
2023-Oct-27 06:24:50 INFO : SNR max = 48.080079
2023-Oct-27 06:24:50 INFO : Ymax = 0.018715
2023-Oct-27 06:24:50 INFO : Ymax metab = 0.018715
2023-Oct-27 06:24:50 INFO : Fit quality = 2.581611
2023-Oct-27 06:24:50 INFO : Baseline dev = 0.032590
2023-Oct-27 06:24:50 INFO : Ymax = 0.018715
2023-Oct-27 06:24:50 INFO : BSL = 0.055240
2023-Oct-27 06:24:50 INFO : Computing CRLBs.
2023-Oct-27 06:24:50 DEBUG : Sigma: 1.121573e-10
2023-Oct-27 06:24:50 INFO : done.
```

#### Optimisation details

```
-----
l2 norm of error at initial p = 2.62613
l2 norm of error at final p = 1.71616
l2 norm of J.*e at final p = 240.998
l2 norm of D*p at final p = 7.15706e-32
number of iterations = 8
number of function evaluations = 2
number of Jacobian evaluations = 396
stopped by small D*p
```

```
2023-Oct-27 06:24:50 INFO : TARQUIN Finished
```

```
Writing txt results file.
Done.
```

```
2023-Oct-27 06:24:50 INFO : TARQUIN 4.3.11 Started
2023-Oct-27 06:24:50 INFO : Loading data file : Temporary/ddd/dddtf1.raw
2023-Oct-27 06:24:50 INFO : nStart = 20
2023-Oct-27 06:24:50 INFO : nEnd = 500
TARQUIN Version 4.3.11
```

```
**** TARQUIN is a research tool and is NOT for clinical use. ****
```

```
2023-Oct-27 06:24:50 INFO : Loading data file : W.raw
2023-Oct-27 06:24:50 INFO : nStart = 20
2023-Oct-27 06:24:50 INFO : nEnd = 500
Parameters Before Preprocessing
```

```
-----
Input file: Temporary/ddd/dddtf1.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.65 ppm
```

```
2023-Oct-27 06:24:50 INFO : Starting 'Preprocessing'
2023-Oct-27 06:24:50 INFO : Preprocessing fid 1 of 1
2023-Oct-27 06:24:50 INFO : Starting 'autophasing mag method water'
2023-Oct-27 06:24:50 INFO : Finished 'autophasing mag method water'
2023-Oct-27 06:24:50 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:50 INFO : Ref new = 4.619435 ppm
2023-Oct-27 06:24:50 INFO : Residual water freq. (Hz) : -3.906250
2023-Oct-27 06:24:50 INFO : Starting 'building Hankel LP matrix'
2023-Oct-27 06:24:50 INFO : Finished 'building Hankel LP matrix'
```

```
2023-Oct-27 06:24:50 INFO : Starting 'SVD of LP matrix'
2023-Oct-27 06:24:50 INFO : Finished 'SVD of LP matrix'
2023-Oct-27 06:24:50 INFO : Starting 'estimating LP parameters'
2023-Oct-27 06:24:50 INFO : Finished 'estimating LP parameters'
2023-Oct-27 06:24:50 INFO : Starting 'estimating LP amplitudes'
2023-Oct-27 06:24:50 INFO : Finished 'estimating LP amplitudes'
2023-Oct-27 06:24:50 INFO : Starting 'autophasing (new)'
2023-Oct-27 06:24:50 INFO : Finished 'autophasing (new)'
2023-Oct-27 06:24:50 DEBUG : Max Phi0 : 0.25
2023-Oct-27 06:24:50 INFO : Ref start = 4.650000 ppm
2023-Oct-27 06:24:50 INFO : Ref new = 4.646179 ppm
2023-Oct-27 06:24:50 DEBUG : Width pts : 20.36
2023-Oct-27 06:24:50 DEBUG : Width Hz est : 6.63
2023-Oct-27 06:24:50 DEBUG : Init beta est : 112.75
2023-Oct-27 06:24:50 INFO : Ymax = 0.019673
2023-Oct-27 06:24:50 INFO : sdev noise = 0.000171
2023-Oct-27 06:24:50 INFO : SNR guess = 57.4222
2023-Oct-27 06:24:50 INFO : Finished 'Preprocessing'
```

Parameters After Preprocessing

```
-----
Input file: Temporary/ddd/dddtf1.raw
Water reference file: W.raw
Data points: 512
Rows: 1
Columns: 1
Slices: 1
Echo time: 0.03 s
Sampling frequency: 2000 Hz
Transmitter frequency: 1.278e+08 Hz
Starting sample: 20
Ending sample: 500
Removing signals in: [-45,+45] Hz
Autophasing yes/no?: yes
Water eddy correction?: no
Autoreferencing yes/no?: yes
Reference: 4.64618 ppm
```

```
2023-Oct-27 06:24:50 INFO : Simulating using 6 threads.
2023-Oct-27 06:24:50 INFO : All simulation threads stopped.
2023-Oct-27 06:24:50 INFO : Running optimiser
2023-Oct-27 06:24:50 INFO : Setting metab shift limit to 0.030000 ppm
2023-Oct-27 06:24:50 INFO : Setting broad shift limit to 0.100000 ppm
2023-Oct-27 06:24:50 INFO : 31 group vectors in total
2023-Oct-27 06:24:50 INFO : 31 basis vectors in total
2023-Oct-27 06:24:50 INFO : Final nStart = 20
2023-Oct-27 06:24:50 INFO : Final nEnd = 500
2023-Oct-27 06:24:50 INFO : 1 voxel(s) to be fitted
2023-Oct-27 06:24:50 DEBUG : Overlapping signals found: 16
2023-Oct-27 06:24:50 INFO : Fitting fid 1 of 1
2023-Oct-27 06:24:50 INFO : Adjusting basis set to 4.646179 ppm
2023-Oct-27 06:24:50 INFO : Time domain noise = 0.000009
2023-Oct-27 06:24:50 DEBUG : Using init_beta: 112.746734
2023-Oct-27 06:24:50 DEBUG : Doing a maximum of 75 iterations.
2023-Oct-27 06:24:50 DEBUG : Initial phase fit completed.....
2023-Oct-27 06:24:51 INFO : done.
2023-Oct-27 06:24:51 DEBUG : Final Beta: 168.60
2023-Oct-27 06:24:51 DEBUG : Final Phi0: -0.21
2023-Oct-27 06:24:51 DEBUG : Final Phi1: 0.00
2023-Oct-27 06:24:51 INFO : FWHM right ppm = 1.994636
2023-Oct-27 06:24:51 INFO : FWHM left ppm = 2.048126
2023-Oct-27 06:24:51 INFO : Metabolite FWHM (ppm) = 0.053489
2023-Oct-27 06:24:51 INFO : Spec noise = 0.000007
2023-Oct-27 06:24:51 INFO : sdev noise = 0.000451
2023-Oct-27 06:24:51 INFO : SNR residual = 19.776331
2023-Oct-27 06:24:51 INFO : SNR max = 52.926567
2023-Oct-27 06:24:51 INFO : Ymax = 0.017819
2023-Oct-27 06:24:51 INFO : Ymax metab = 0.017819
2023-Oct-27 06:24:51 INFO : Fit quality = 2.676258
2023-Oct-27 06:24:51 INFO : Baseline dev = 0.035193
2023-Oct-27 06:24:51 INFO : Ymax = 0.017819
2023-Oct-27 06:24:51 INFO : BSL = 0.059244
2023-Oct-27 06:24:51 INFO : Computing CRLBs.
2023-Oct-27 06:24:51 DEBUG : Sigma: 7.322611e-11
2023-Oct-27 06:24:51 INFO : done.
```

Optimisation details

```
-----
l2 norm of error at initial p = 2.34951
l2 norm of error at final p = 1.44512
l2 norm of J.*e at final p = 248.509
l2 norm of D*p at final p = 4.25265e-11
number of iterations = 7
number of function evaluations = 2
number of Jacobian evaluations = 166
stopped by small D*p
```

2023-Oct-27 06:24:51 INFO : TARQUIN Finished

Writing txt results file.
Done.

ans =

