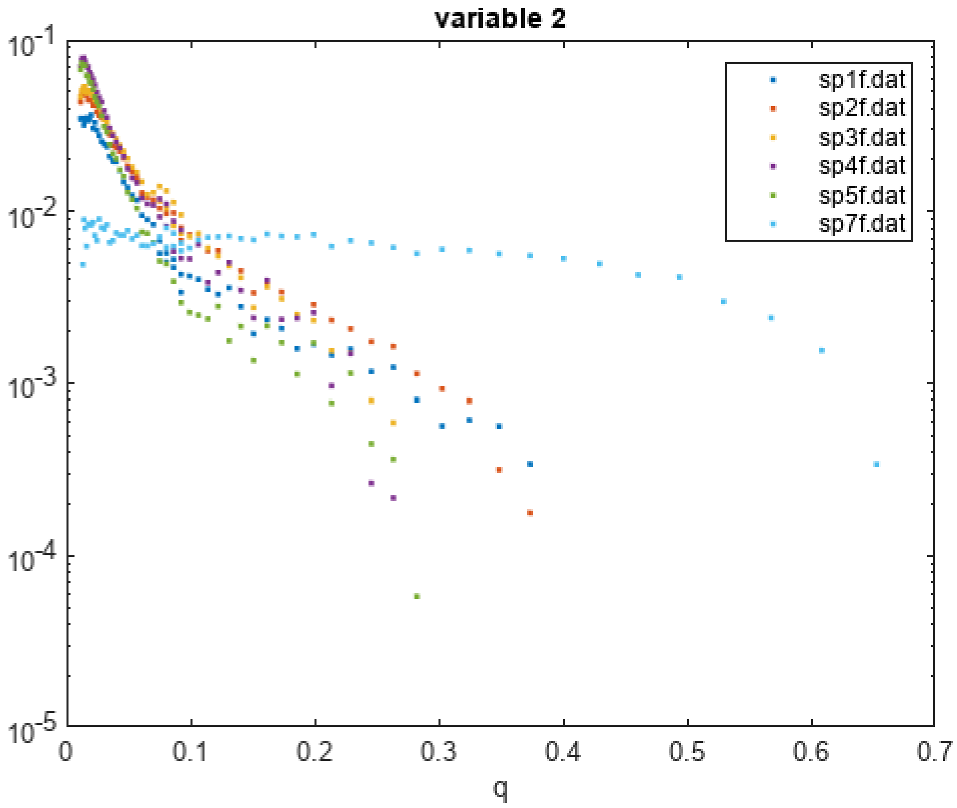
script for reduction of dat files DC 2/23,3/23

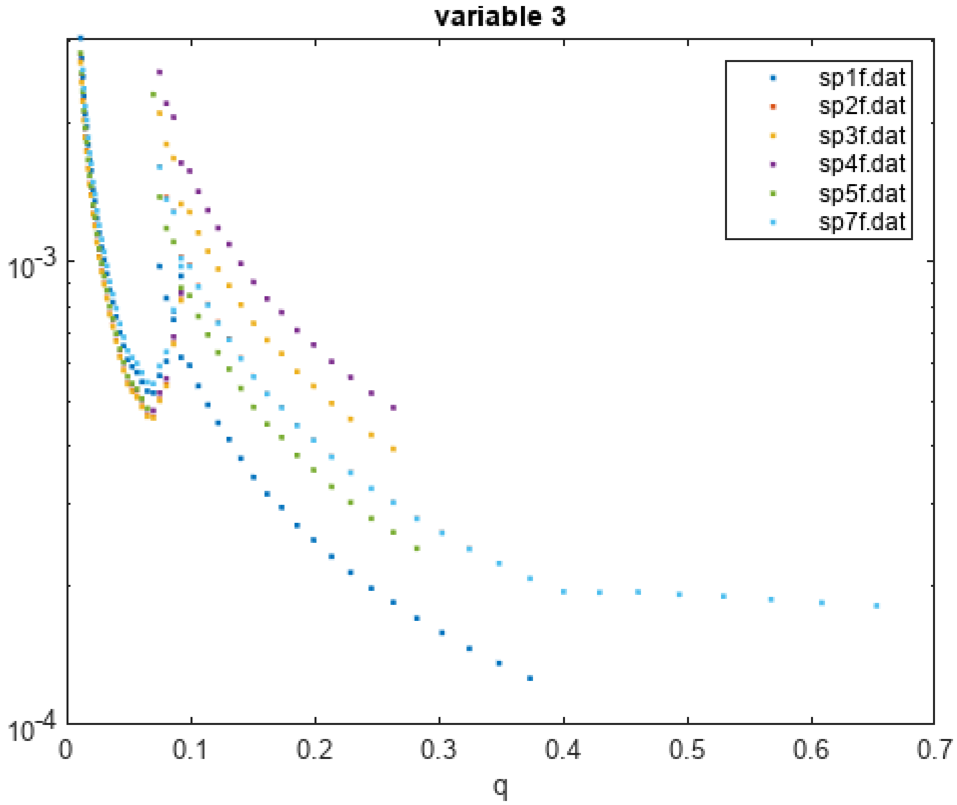
```
cd  'C:\Users\cowburn\My Drive\Nups\Neutrons\IPTS29023.1\2002Nov BioSANS'
clear ;
f=dir(pwd);
%fdat=strfind({f.name},'.dat');
fdat=regexp({f.name},'.dat$');
mask=cellfun(@numel,fdat);
fmask=find(mask);
yy=struct([]    );
```

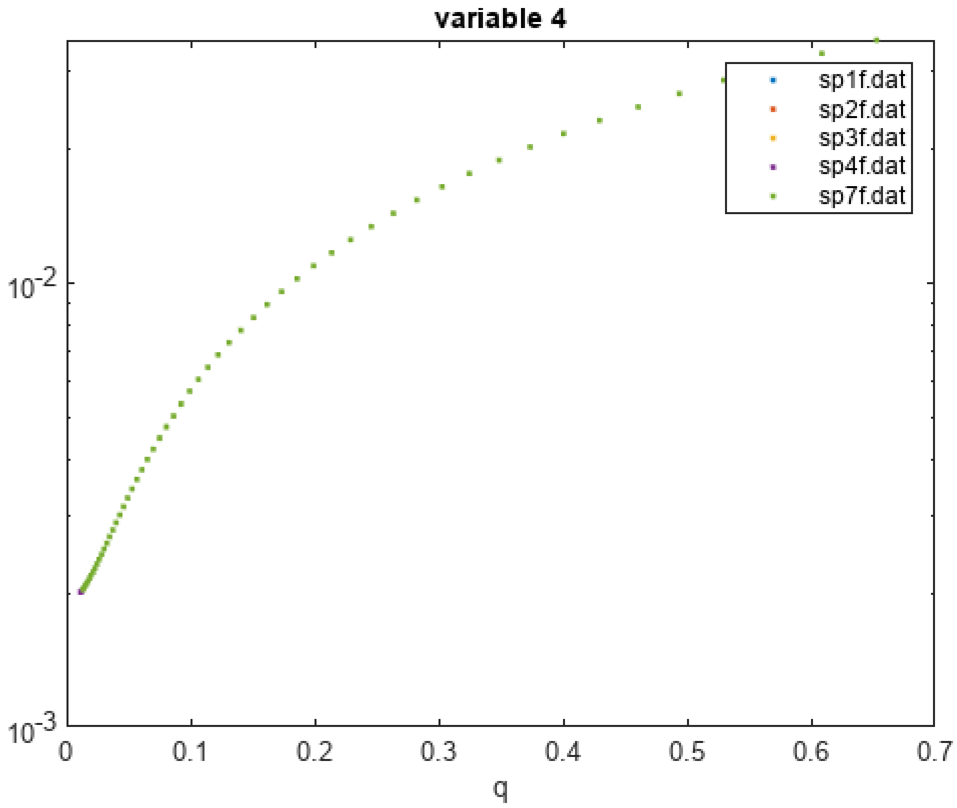
```
for ii=1:numel(fmask)  % remove comment lines
    jj=fmask(ii);
    s=readlines(f(jj).name);
 try   O(ii)=xmlstr(f(jj).name); %#ok<*SAGROW>
 catch
 end

    disp(f(jj).name);
        s2=s;
    p=strfind(s,'  Q  ');
    q=cellfun(@numel,p);
    r=find(q,1);
    s2(1:r)=[];
        % look through lines
    mask2=false(size(s2));
    tmax=0;
    for kk=1:numel(s2)
        t=sscanf(s2(kk),'%f');
        mask2(kk)=numel(t)>=3;
        tmax=max(tmax,numel(t));
    end
    s3=s2(mask2);
    x=zeros(numel(s3),tmax,'single');
    for kk=1:numel(s3)
        x(kk,:)=sscanf(s3(kk),'%f')';
    end
    yy(ii).f=f(jj);
    x=x(x(:,2)>0,:);
    yy(ii).x=x;
    % sum duplicate q's
    mask3=(-x(1:end-1,1)+x(2:end,1) < eps("single"));
    lm=find(mask3);
    for im=lm'
        x(im,:)=(x(im,:)+x(im+1,:))/2;
        x(im+1,:)=0;
    end
    disp('merging');
    disp(lm');
    x=x(x(:,2)>0,:);
    writematrix(x,[f(jj).name 'R.csv']);

end
```

```
sp1f.dat
merging
    28    30    32    34
sp2f.dat
merging
    28    30    32    34
sp3f.dat
merging
    28    30    32    34
sp4f.dat
merging
    28    30    32    34
sp5f.dat
merging
sp7f.dat
merging
    26    28    30    32
```

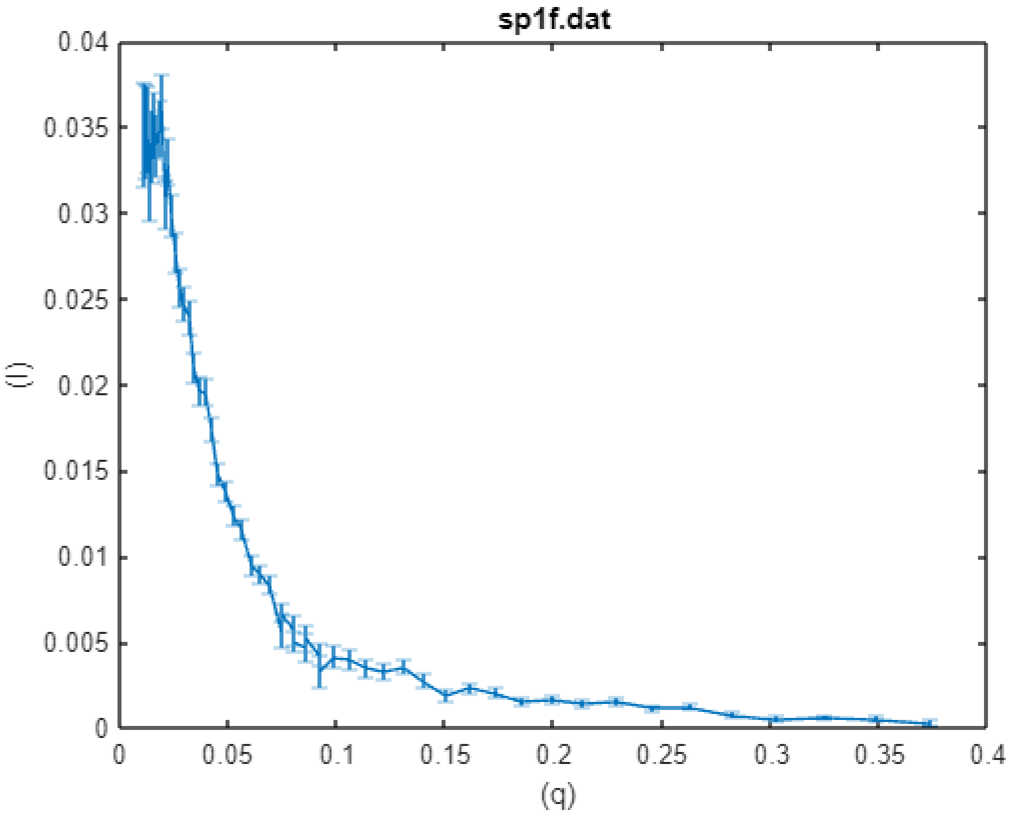
```

  P=struct2table(O);
    writetable(P,'P.csv');
close all
%tiledlayout(2,2);
for kk=2:4
    figure
    %nexttile;
    leg=string([]);
    for ii=1:numel(yy)
        y=yy(ii).x;
        if ~ isempty(y)  && kk <= size(y,2)
            maskk=y(:,kk)>0;
            if any(maskk), semilogy(y(maskk,1),y(maskk,kk),'.'); end
            hold on;
            leg(end+1)=(yy(ii).f.name); %#ok<SAGROW>
        end
    end
    xlabel('q'); legend(leg);
    title (['variable ' num2str(kk)]);
end
```

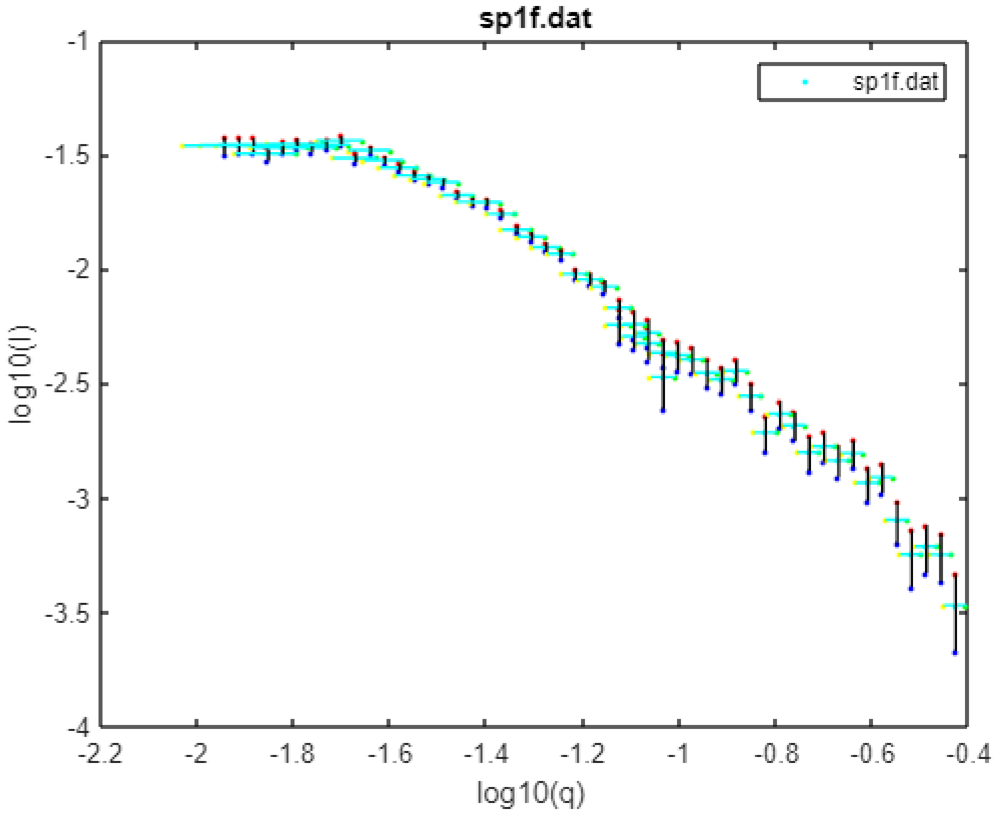

variable 2
10^-1
10^-2
10^-3
10^-4
10^-5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
q
sp1f.dat
sp2f.dat
sp3f.dat
sp4f.dat
sp5f.dat
sp7f.dat

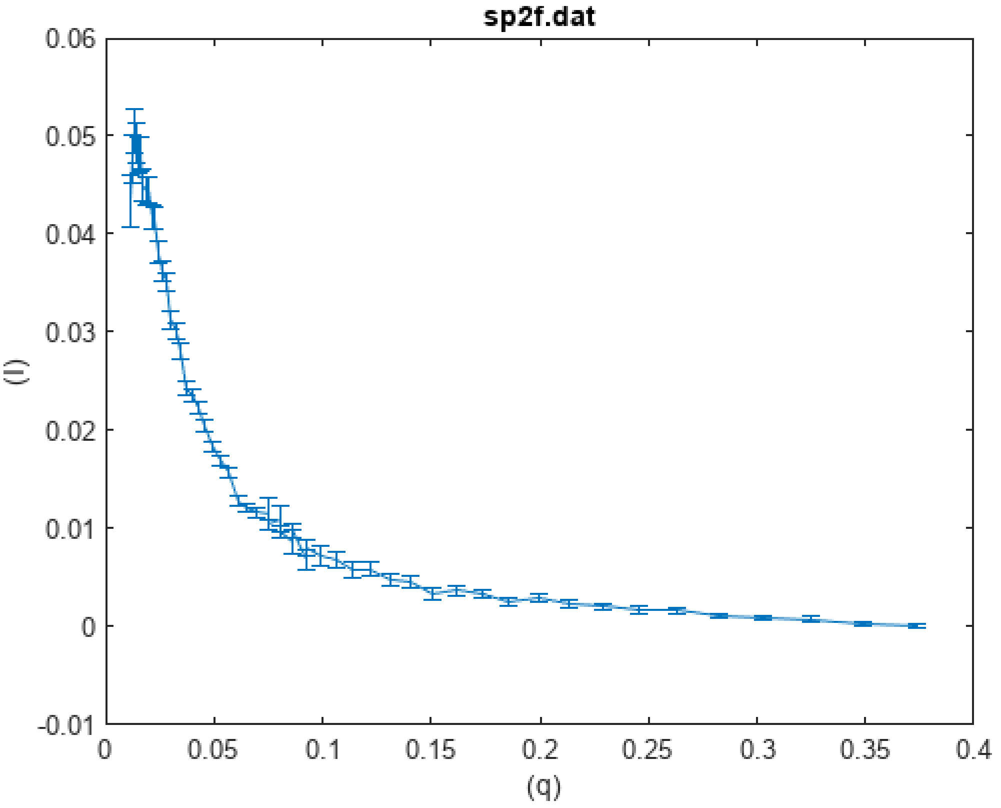

variable 3
10^-3
10^-4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
q
sp1f.dat
sp2f.dat
sp3f.dat
sp4f.dat
sp5f.dat
sp7f.dat

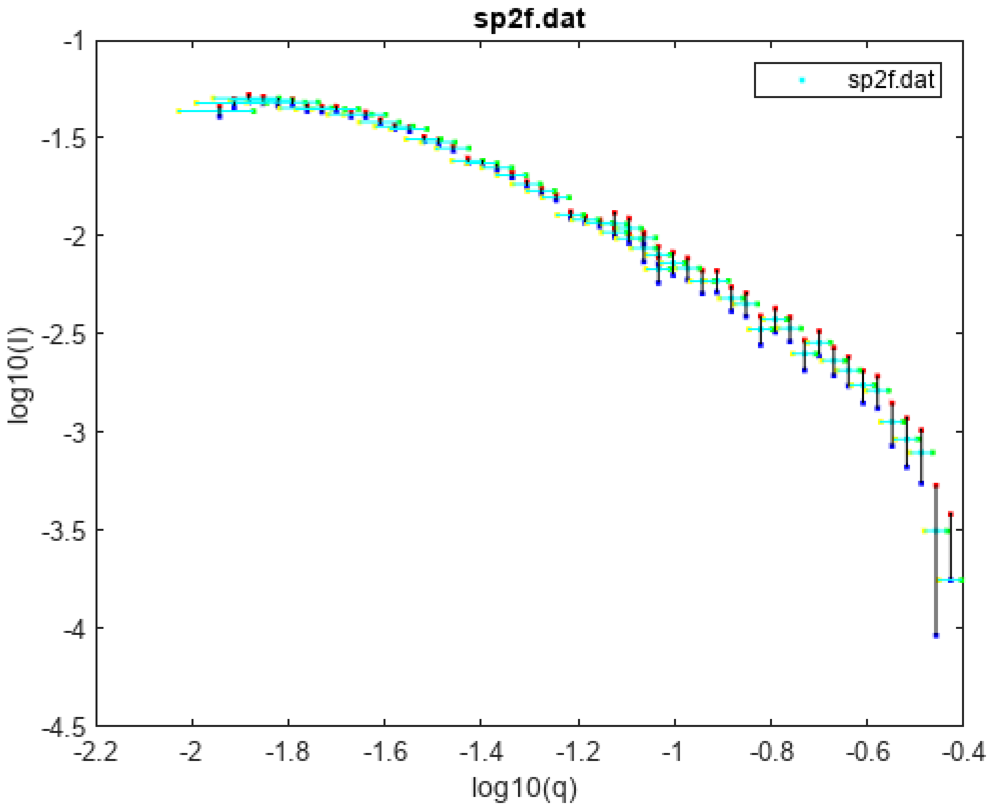


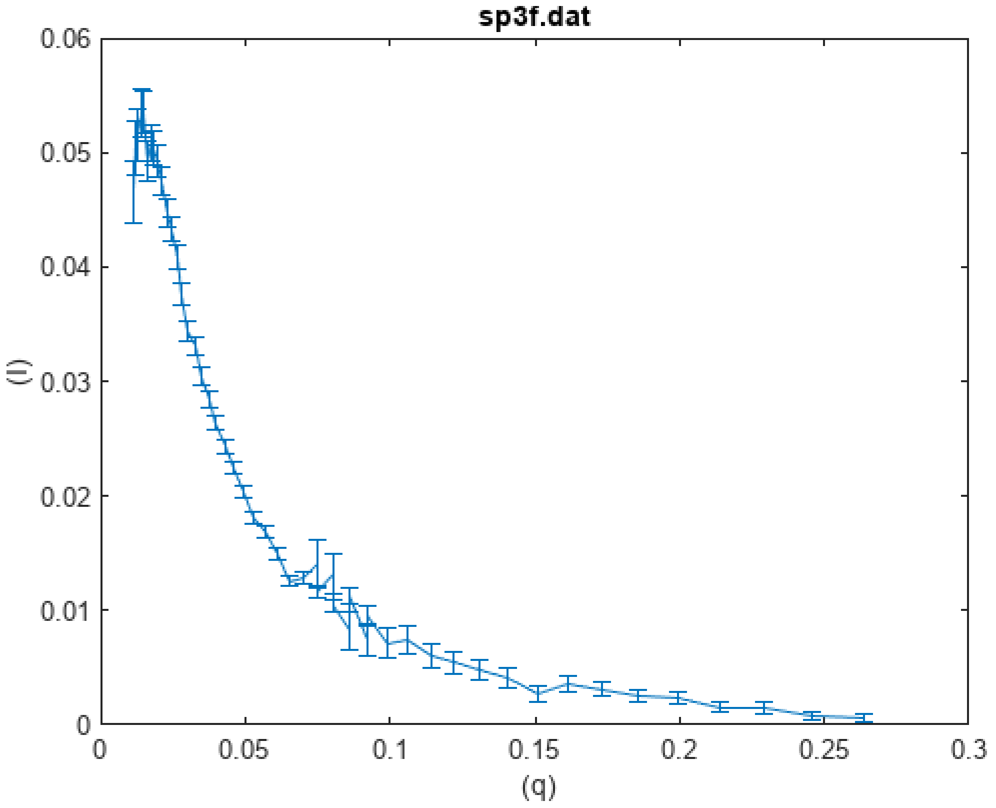
```
for kk=1:numel(fmask)
    figure;
    y=yy(kk).x;        if isempty(y), continue; end
    if size(y,2) == 3
        y= [y  yy(1).x(1:size(y,1),4)]; %#ok<AGROW> % approx fix
         disp(' set extended for q delta ');
         disp(kk);
    end

    leg=(yy(kk).f.name);
    %sc=sum(y(:,3));     % normalize errors
    xx=y(:,1);
    v=y(:,2);
    mask=v>eps;
    v=v(mask);
    xx=xx(mask);
    ve=y(:,3);
    vp=v+ve;
    vn=v-ve;
    mask=vn < eps;
    vn(mask)=v(mask);
    errorbar(y(:,1),v,ve);
    xlabel('  (q) ');    ylabel('  (I)');
    title (leg);
    figure;
    x=log10(xx);
    plot(x,log10(v),'.c',x,log10(vn),'.b',x,log10(vp),'.r'); hold on;
    qv=y(:,4);
    qs=sum(q);
    qe=qv.*qs;
    plot(log10(xx+qe),log10(v),'.g',log10(xx-qe),log10(v),'.y');
    for jj=1:numel(xx)
        plot([log10(xx(jj)-qe(jj)), log10(xx(jj)+qe(jj))], ...
            [log10(v(jj)), log10(v(jj))],'c'   );
        plot([x(jj), x(jj)],[log10(vp(jj)), log10(vn(jj))],'k');
    end
    xlabel('log10(q) ');    ylabel('  log10(I)');
    legend (leg);
    title (leg);

    % R values
end
```

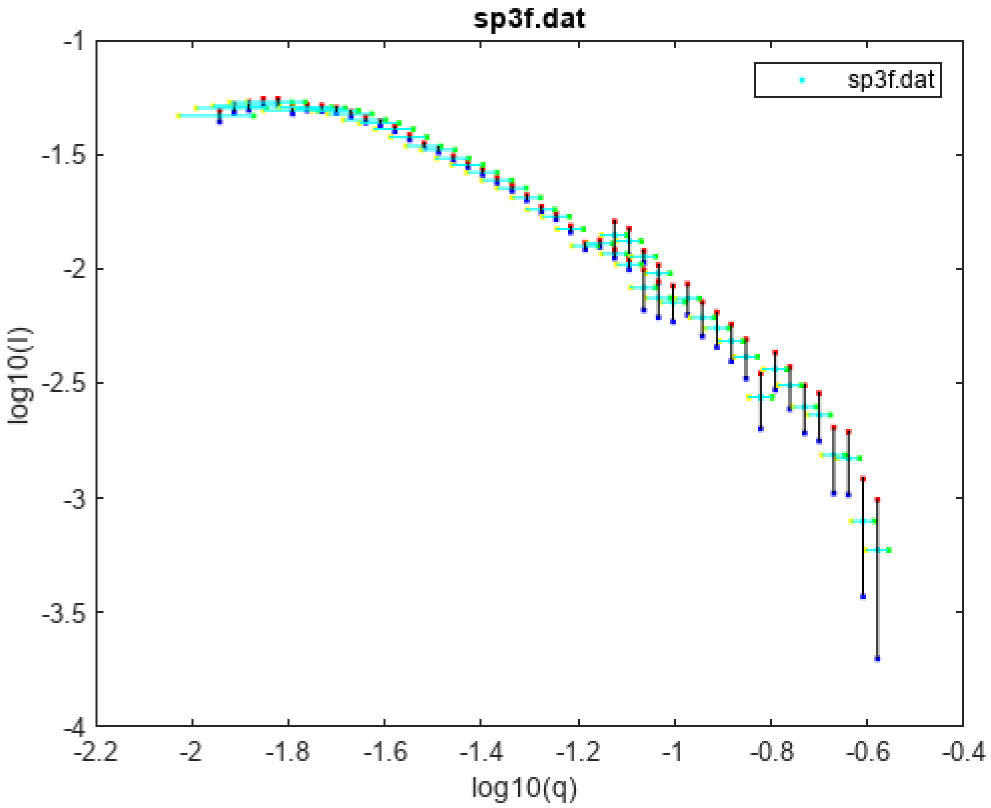


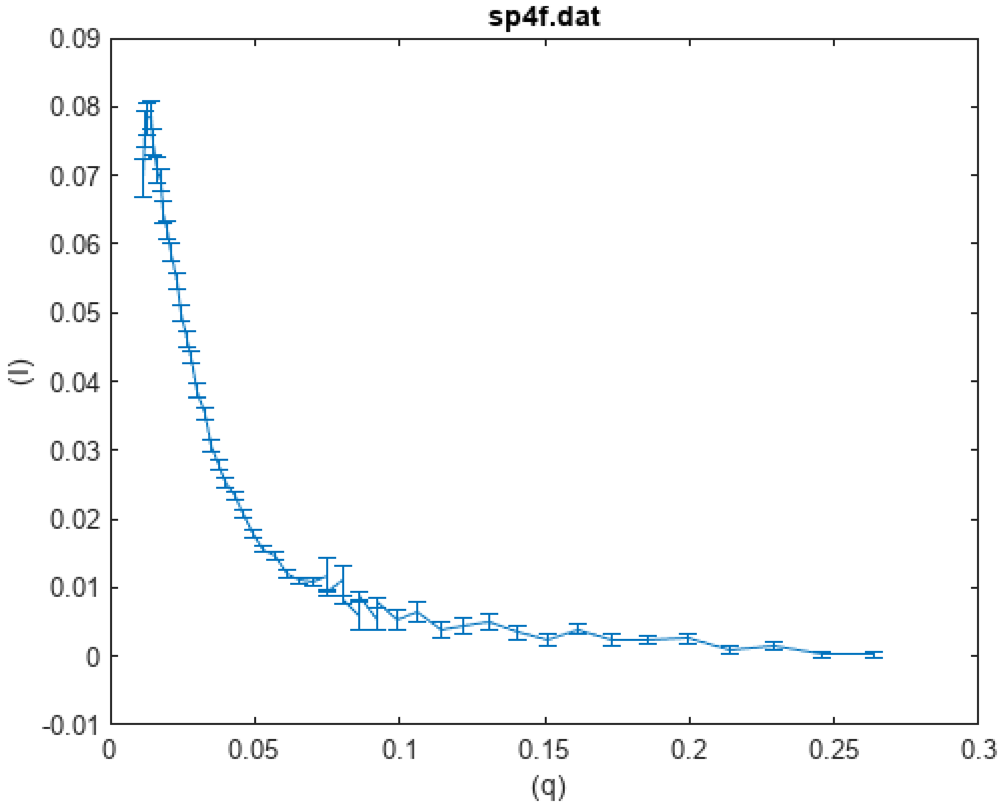

sp1f.dat
sp1f.dat
log10(I)
-1
-1.5
-2
-2.5
-3
-3.5
-4
-2.2
-2
-1.8
-1.6
-1.4
-1.2
-1
-0.8
-0.6
-0.4
log10(q)

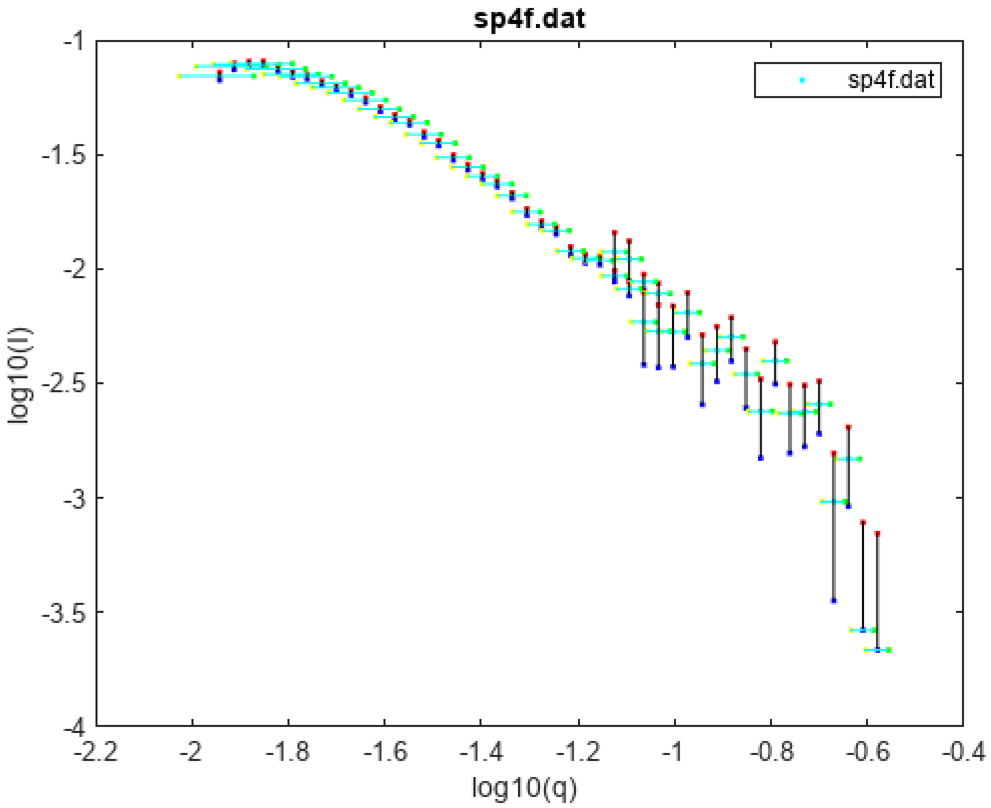

sp2f.dat
(I)
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
(q)


sp2f.dat
sp2f.dat
log10(I)
log10(q)
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-2.2
-2
-1.8
-1.6
-1.4
-1.2
-1
-0.8
-0.6
-0.4

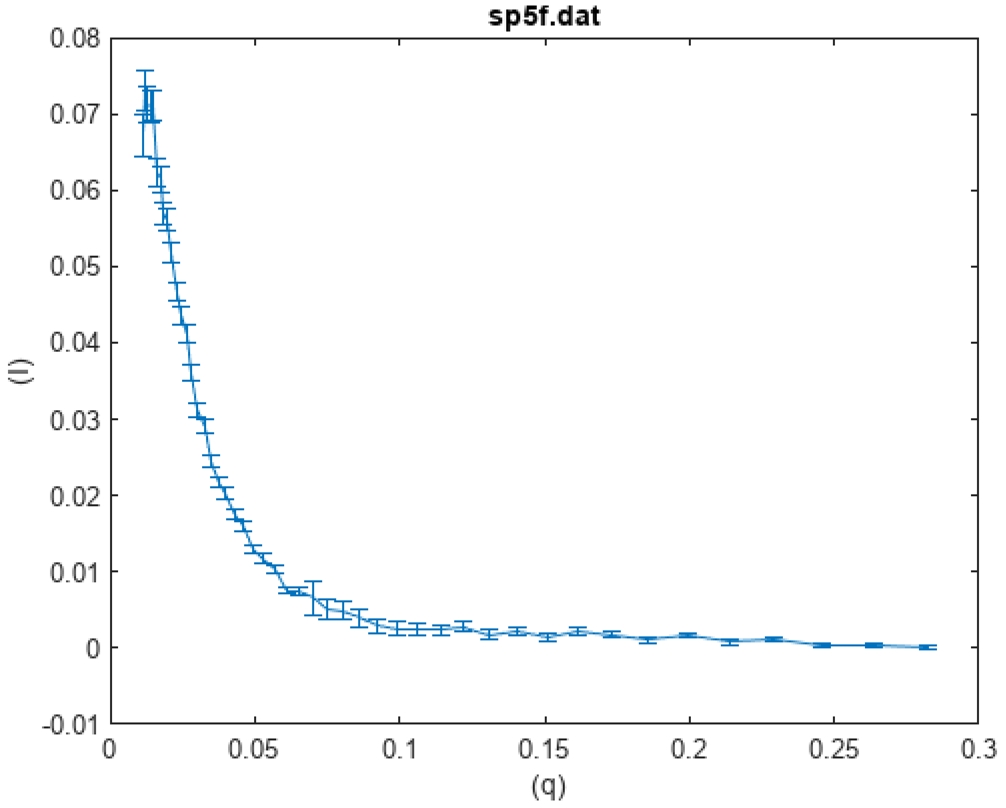

sp3f.dat
(I)
(q)
0.06
0.05
0.04
0.03
0.02
0.01
0
0
0.05
0.1
0.15
0.2
0.25
0.3

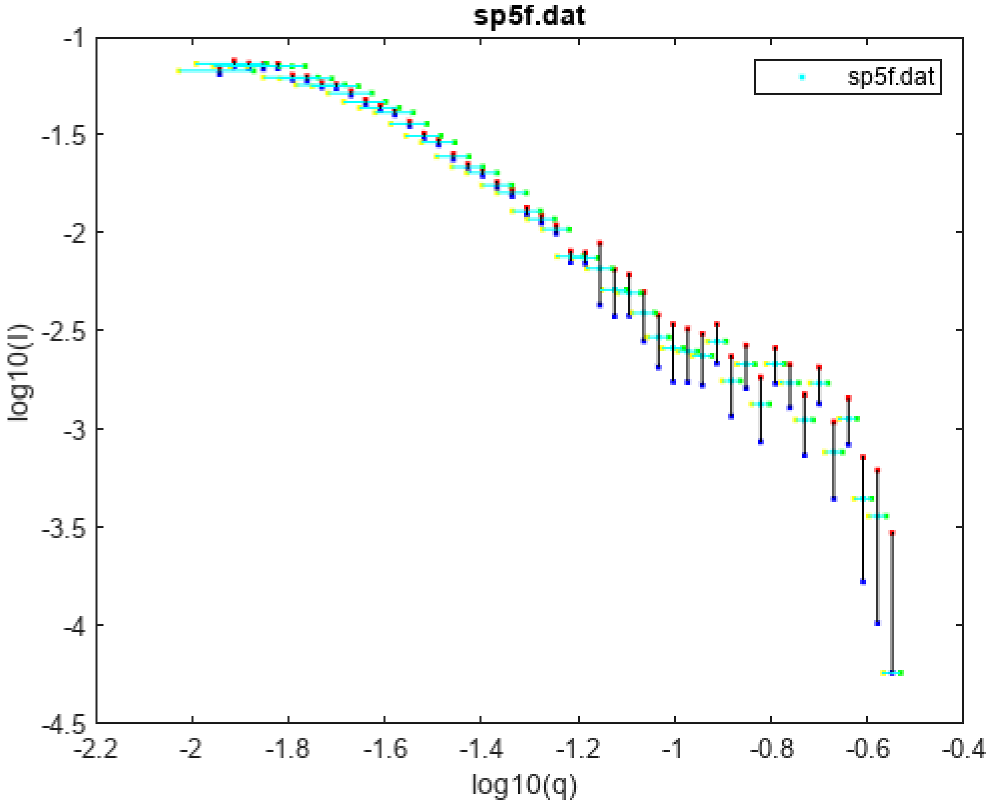

sp3f.dat
sp3f.dat
log10(I)
log10(q)
-1
-1.5
-2
-2.5
-3
-3.5
-4
-2.2
-2
-1.8
-1.6
-1.4
-1.2
-1
-0.8
-0.6
-0.4

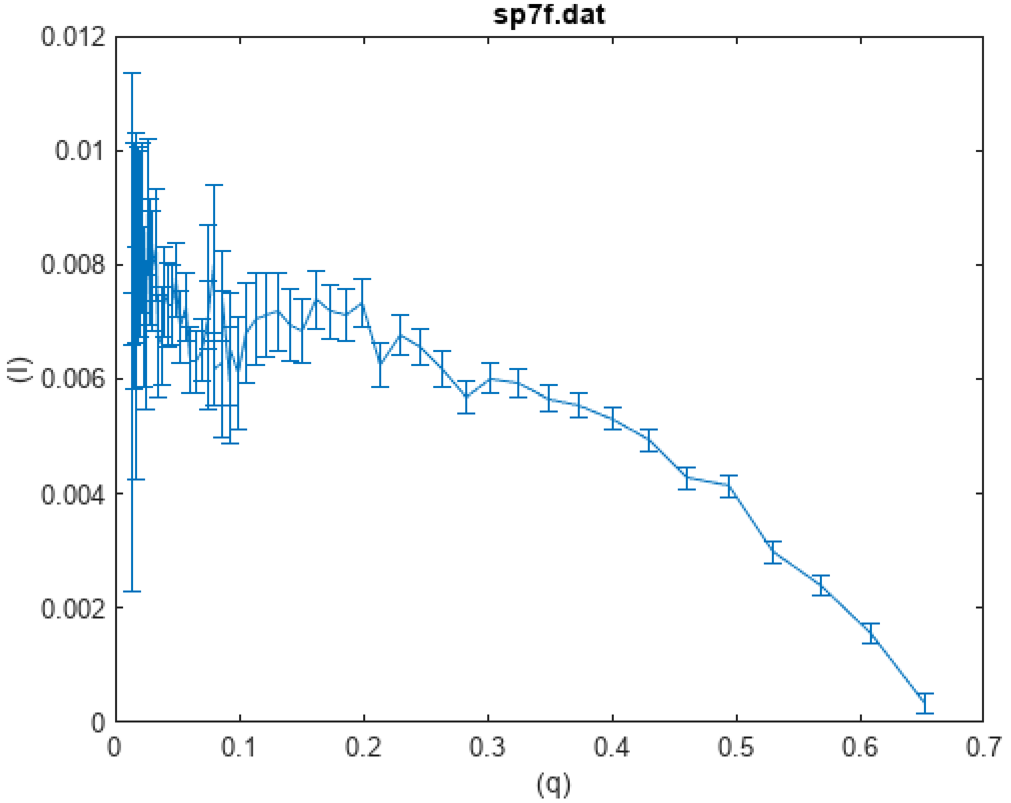

sp4f.dat
(I)
(q)
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
0.05
0.1
0.15
0.2
0.25
0.3

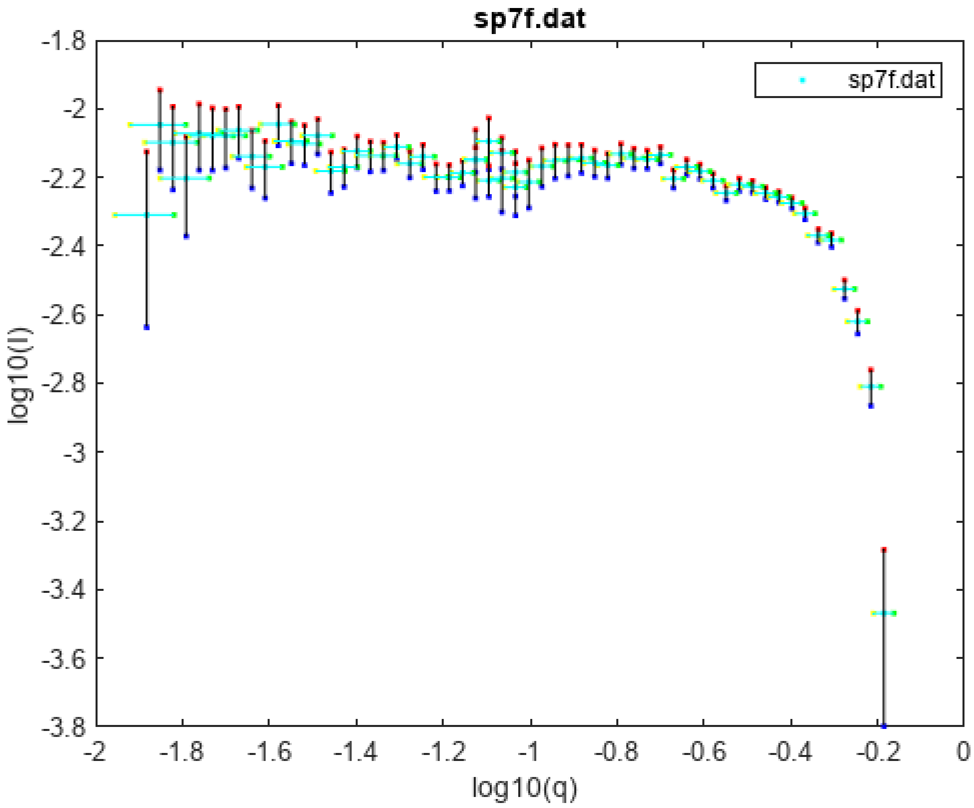


```
set extended for q delta
     5
```




sp5f.dat
sp5f.dat
log10(I)
log10(q)
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-2.2
-2
-1.8
-1.6
-1.4
-1.2
-1
-0.8
-0.6
-0.4


sp7f.dat
(I)
(q)
0.012
0.01
0.008
0.006
0.004
0.002
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

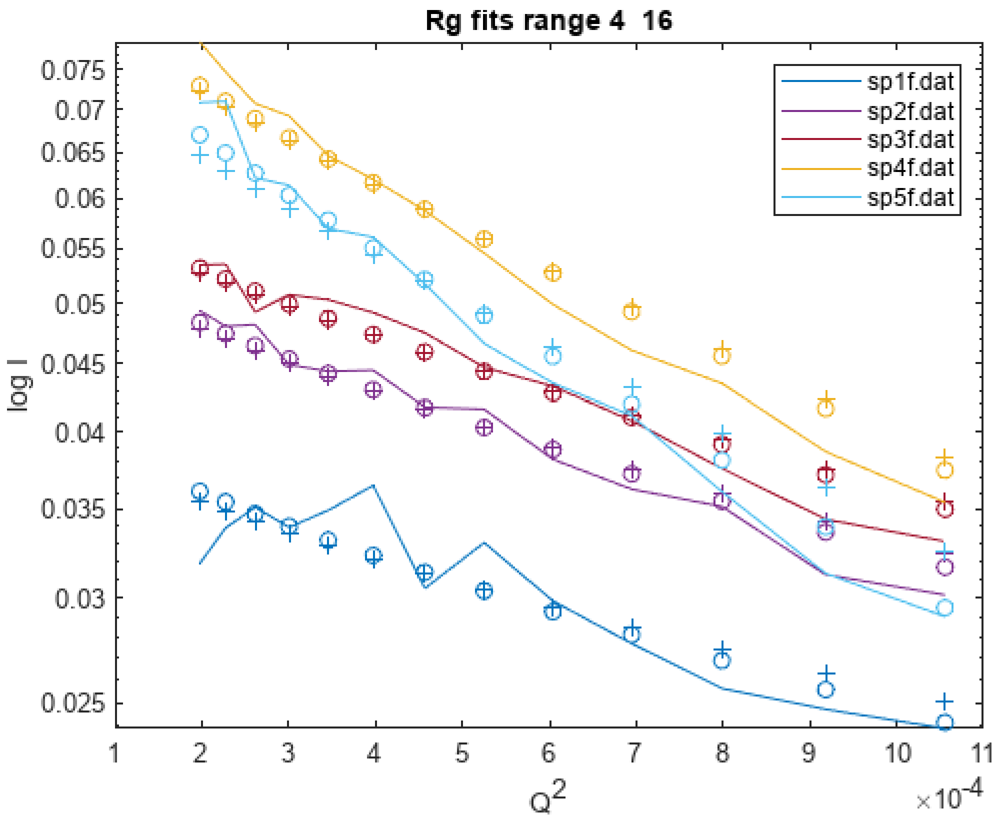


Rg plots

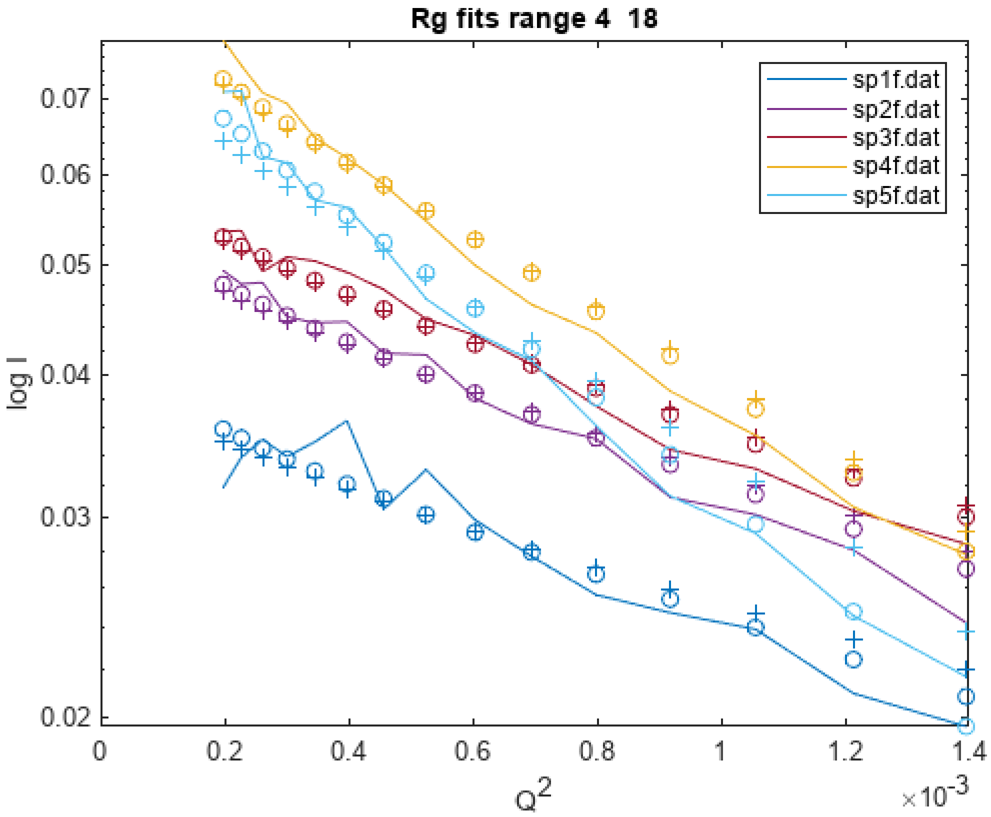
```
snapnow;
close all;

for ra2=16:2:24
ra=[4:ra2]; figure;
```

```
f_R= @(x,y) (exp((-(x*y).^2)/3));
ileg=3;
legs= cell(16,1);
for ii=1:numel(legs), legs{ii}=''; end
for ii=1:numel(yy)-1
    x=yy(ii).x;
    zz=semilogy(x(ra,1).^2,x(ra,2),'-' );  hold on;
    tmp=P{ii,"GNOMReal_Space_I0"} * (1-P{ii,"GNOMReal_Space_Rg"}./3.*x(ra,1));
    slra2=sum( (x(ra,2)));
    legs{1+(ii-1)*ileg}=yy(ii).f.name;
    lcolor(ii,:)=zz.Color;
zz2=semilogy(x(ra,1).^2, tmp*slra2./sum( (tmp)),'O') ;
zz2.Color=zz.Color;
tmp2=P{ii,"guinierI0"} * (1-P{ii,"guinierRg"}./3.*x(ra,1));
zz3=semilogy(x(ra,1).^2, tmp2*(slra2/sum(tmp2)) ,'+') ;
zz3.Color=zz.Color;
end
xlabel('Q^2'); ylabel ('log I'); legend(legs); title(['Rg fits range ' num2str([ra(1) ra(end)]

end
```

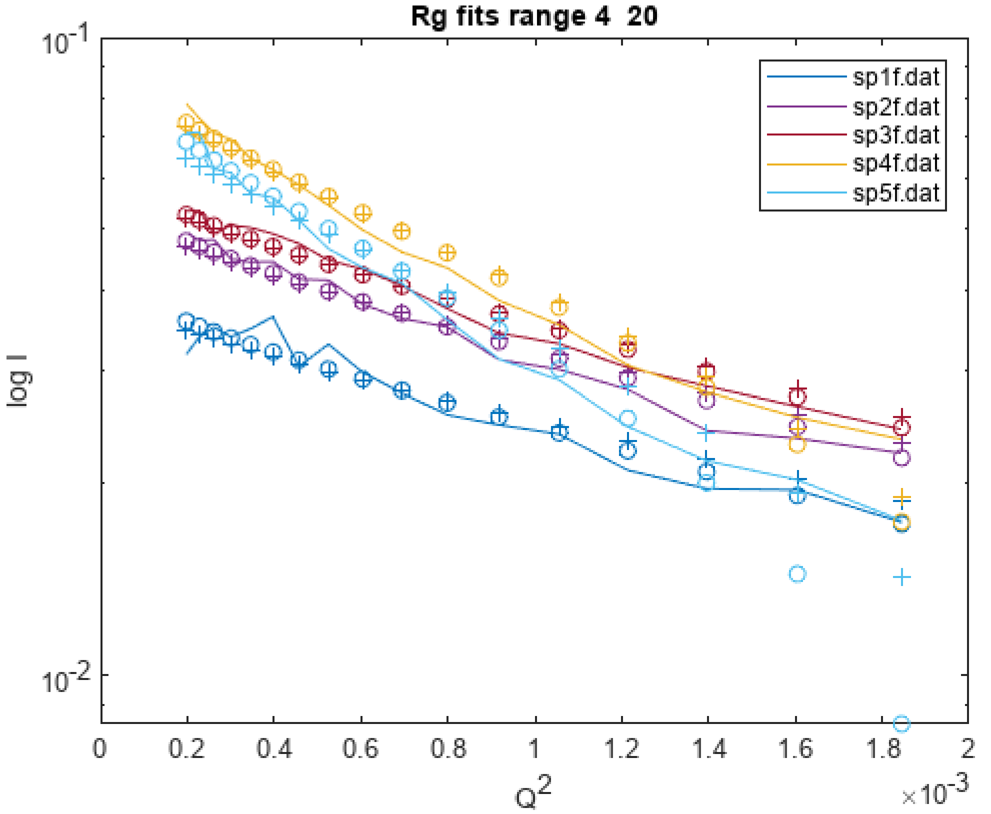
```
Warning: Ignoring extra legend entries.
```



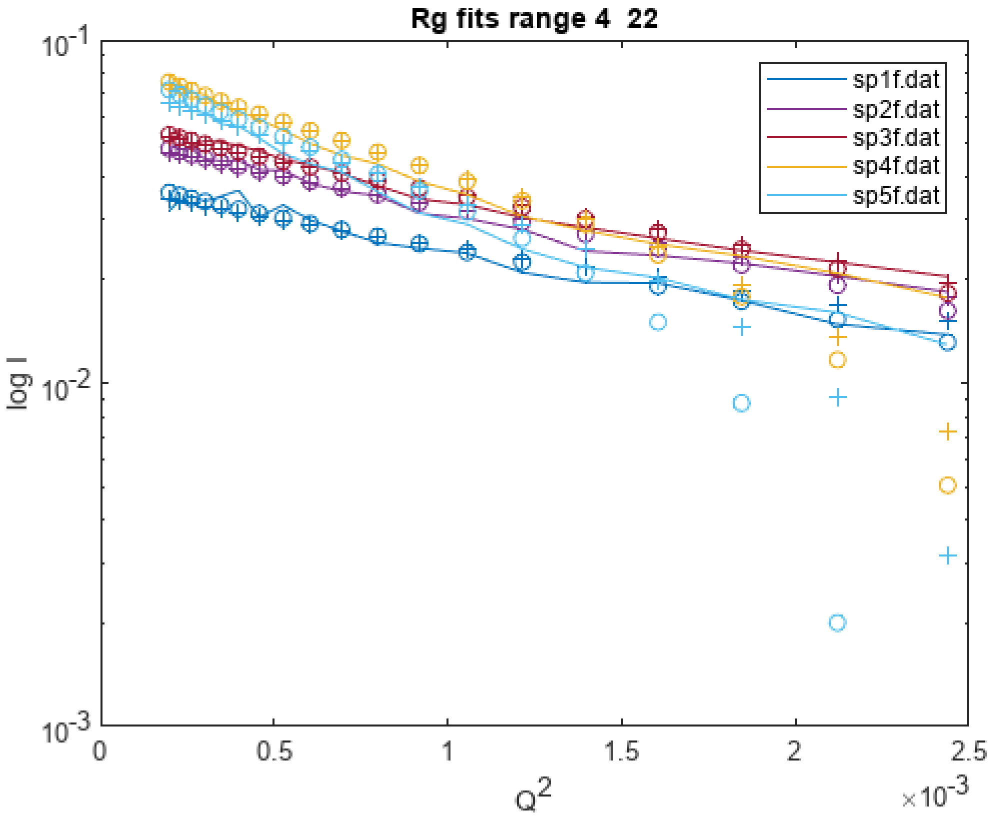
```
Warning: Ignoring extra legend entries.
```



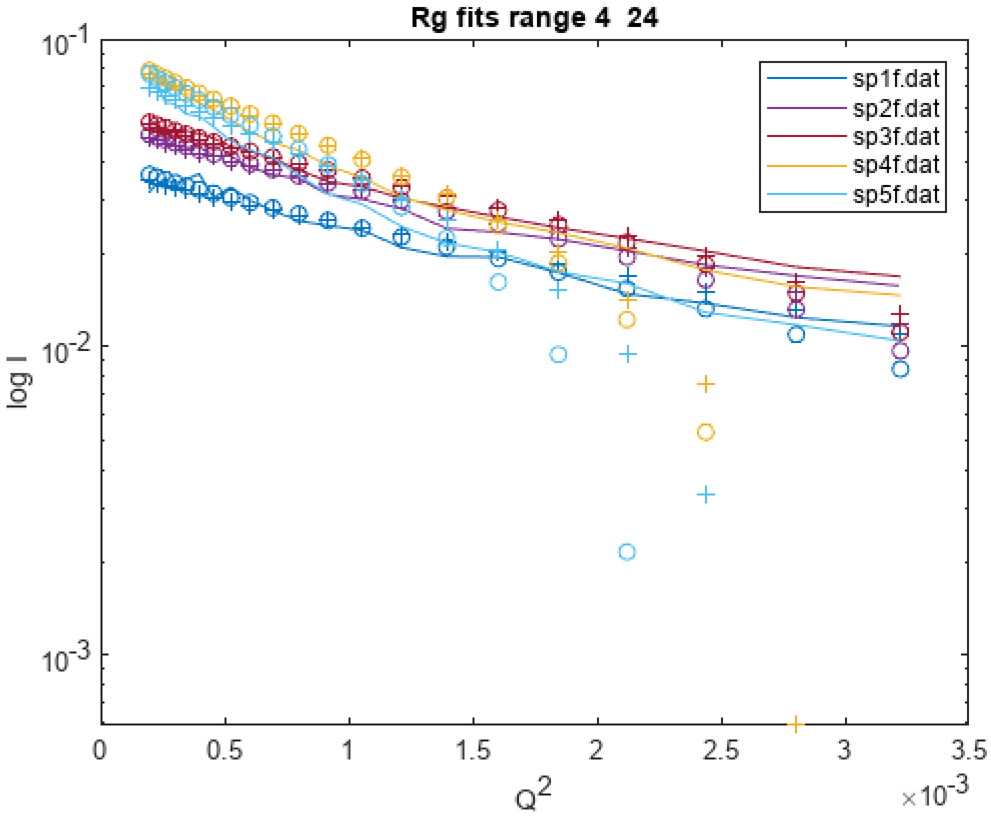
```
Warning: Ignoring extra legend entries.
```



```
Warning: Negative data ignored
Warning: Ignoring extra legend entries.
```



```
Warning: Negative data ignored
Warning: Ignoring extra legend entries.
```

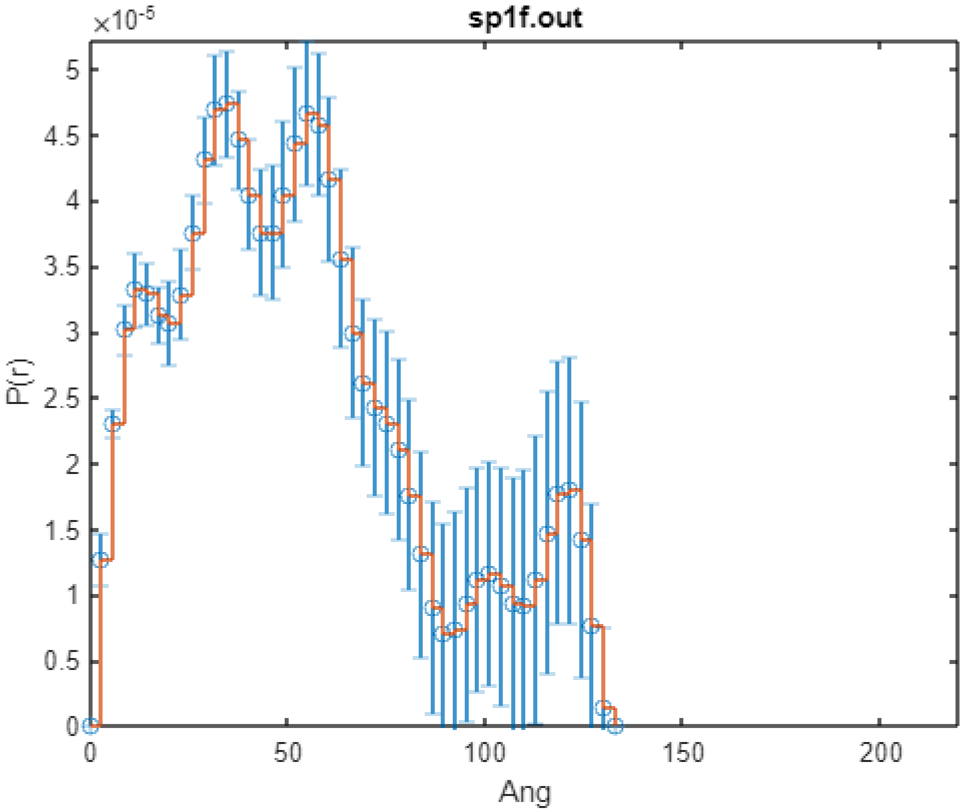


```
fdat=regexp({f.name},'.out$');
```

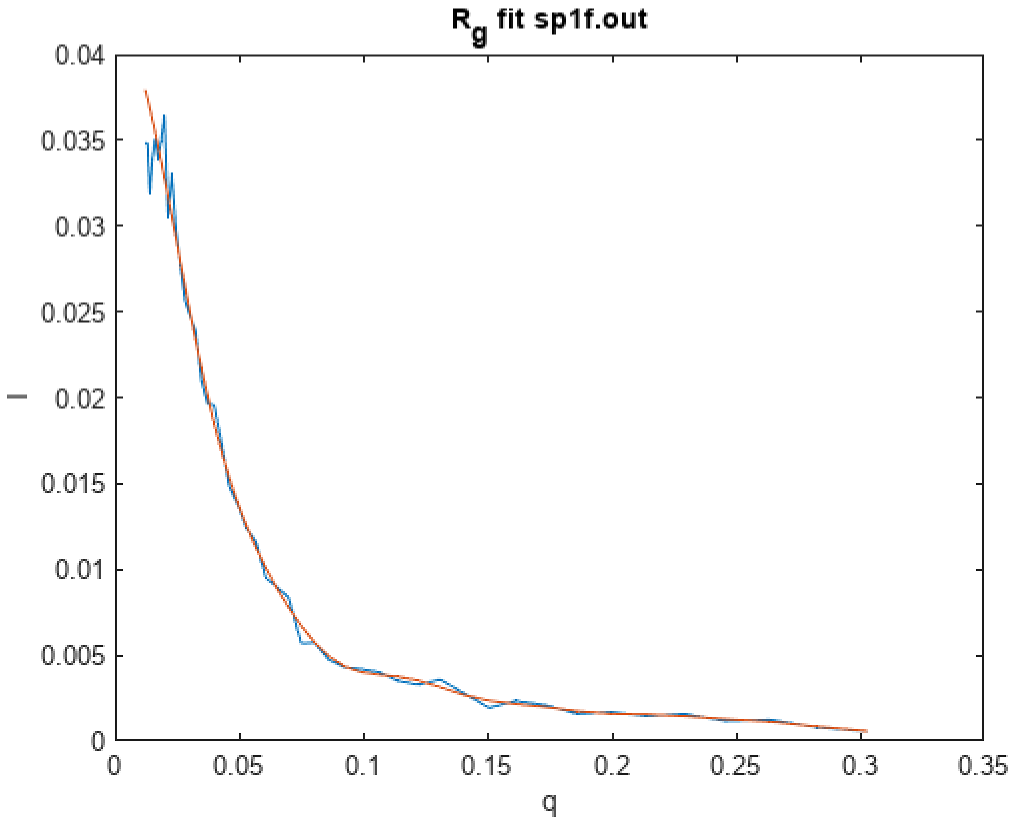
```
Warning: Negative data ignored
```

```
mask = cellfun(@numel,fdat);
fmask=find(mask);
yyyR=struct([]    );
Rg=[];
for ii=1:numel(fmask)  % remove comment lines
    jj=fmask(ii);
    s=readlines(f(jj).name);
    s2=s;
    p=strfind(s,'  R  ');
    q=cellfun(@numel,p);
    r=find(q,1);
    s2(1:r)=[];
    s2=s2(logical(strlength(s2)));
    x=zeros(numel(s2),3);
    for ll=1:numel(s2); x(ll,1:3)=sscanf(s2(ll),'%f');  end
    figure

    errorbar(x(:,1),x(:,2),x(:,3),"both","o"); hold on;
     stairs(x(:,1),x(:,2));
    title (f(jj).name);
    xlabel('Ang');
    ylabel('P(r)');
    axis([0   220 0 Inf]);
    yyR(ii).f=f(jj); %#ok<SAGROW>

    yyR(ii).x=x; %#ok<SAGROW>
    % now Rf fit
    p=contains(s, 'J EXP');
    r=find(p,1);
    ip=1;
    fr=[];
    for ijj=r+1:numel(s)
        tmp=sscanf(s(ijj),'%g');
        if numel(tmp)==5
            fr(ip,:)=tmp; %#ok<SAGROW>
            ip=ip+1;
        elseif numel(tmp)==0
            continue
        end
    end
    figure ;
    mask=fr(2:end,1)> fr(1:end-1,1);
    if any (~mask)
```

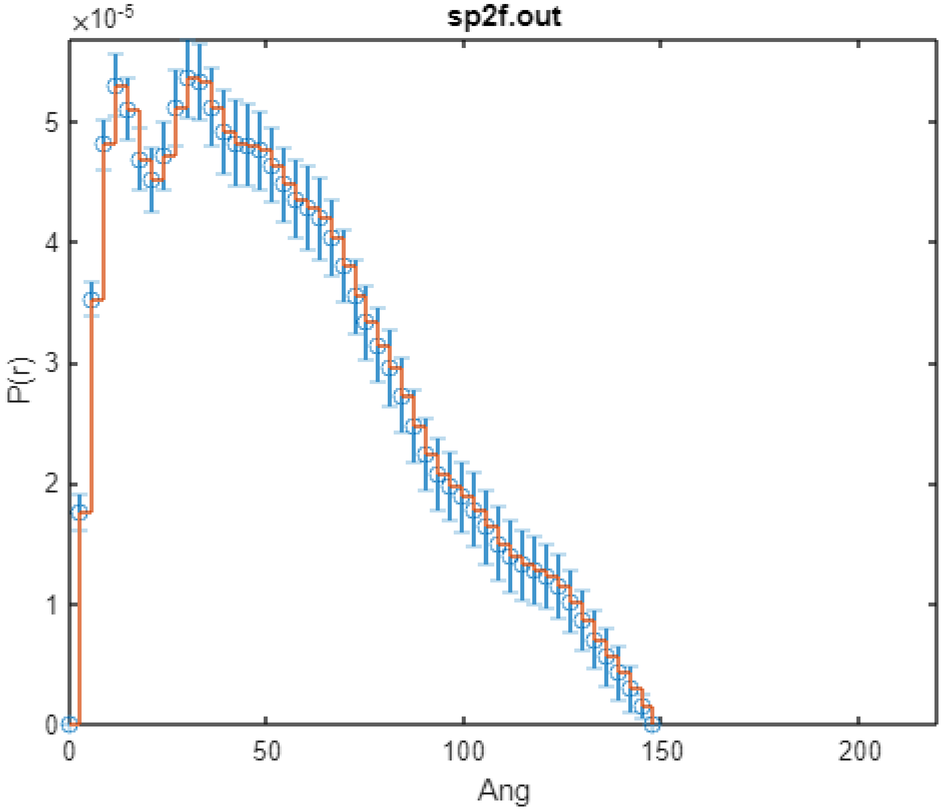
```
        warning('qorder')
        disp(fr(~mask,:));
       disp('removed');
       fr(~mask,:)=[]; %#ok<SAGROW>
    end
    plot(fr(:,1),fr(:,[2 4]));
    xlabel ('q'); ylabel('I'); title(['R_g fit ' f(jj).name] );
 p=contains(s,'Real space Rg:');
 r=find(p,1);
 disp(s(r));
 tmp=regexprep(s(r),'Real space Rg:','');
 tmp=regexprep(tmp, '+-','');
 Rg(ii,:)=sscanf(tmp,'%g'); %#ok<SAGROW>

end
```

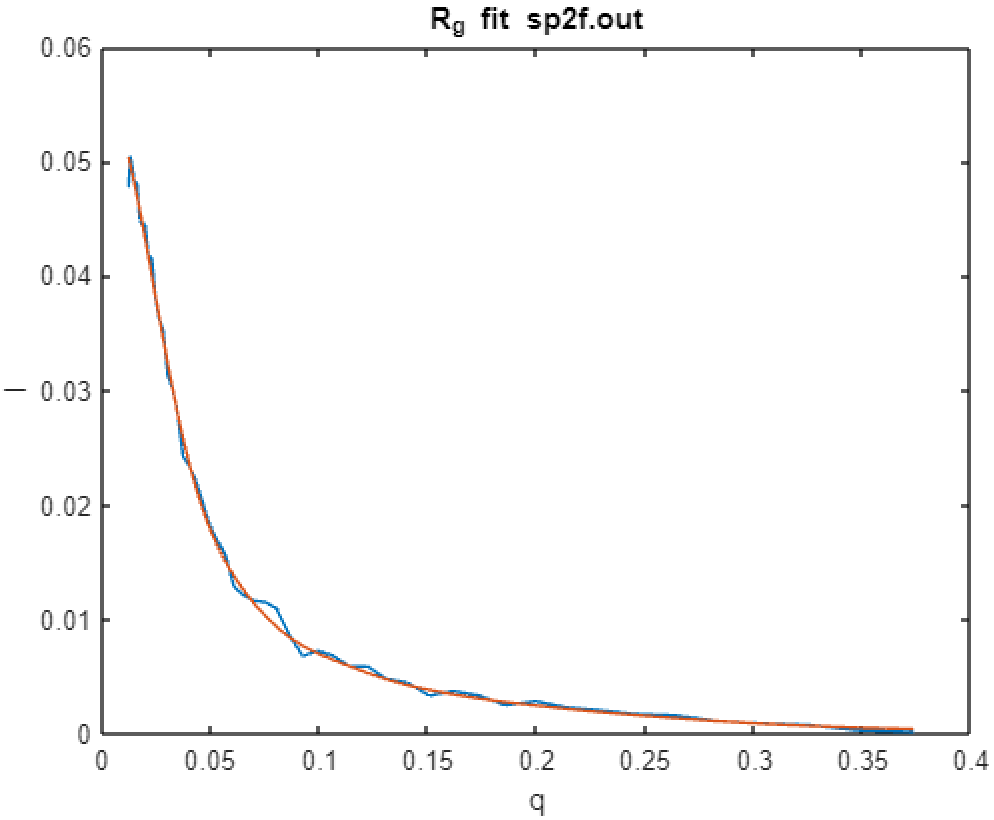


```
Warning: Negative data ignored
```

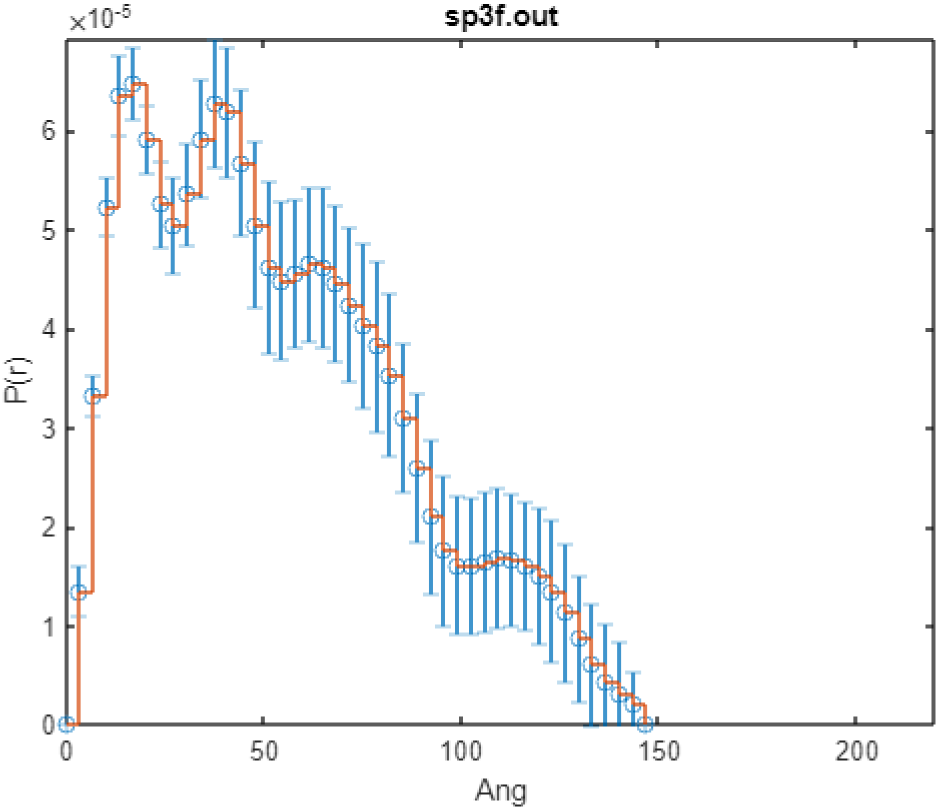


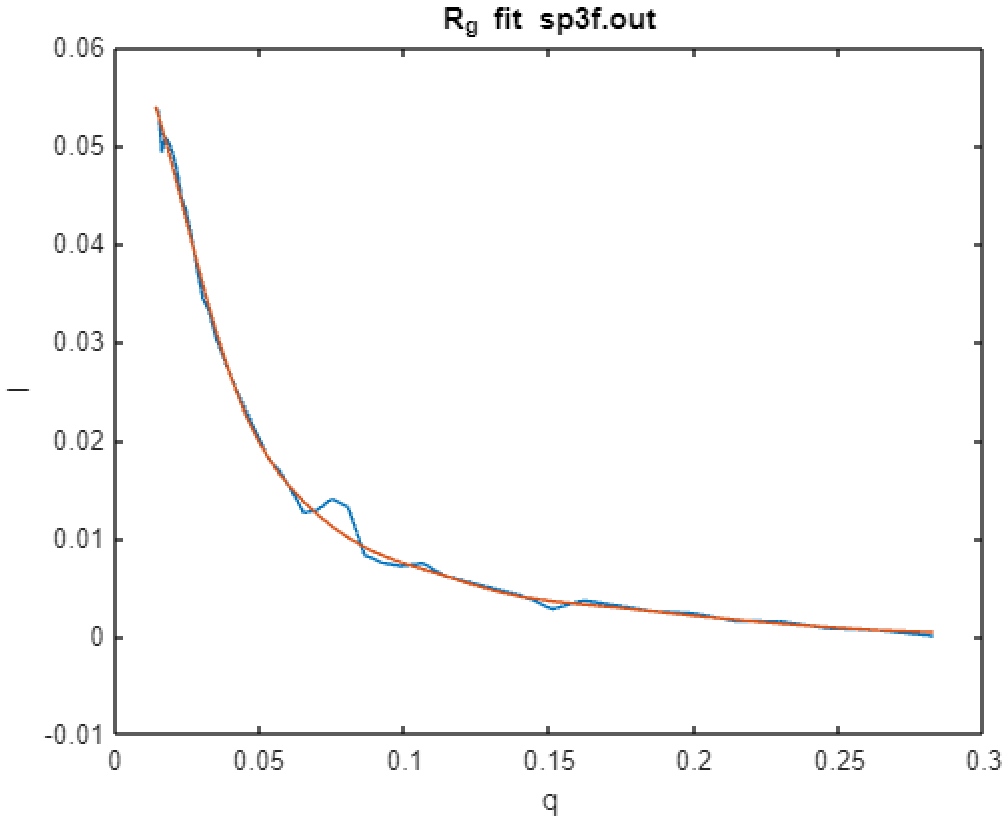
```
Real space Rg:                    0.4299E+02 +-   0.1979E+01
```



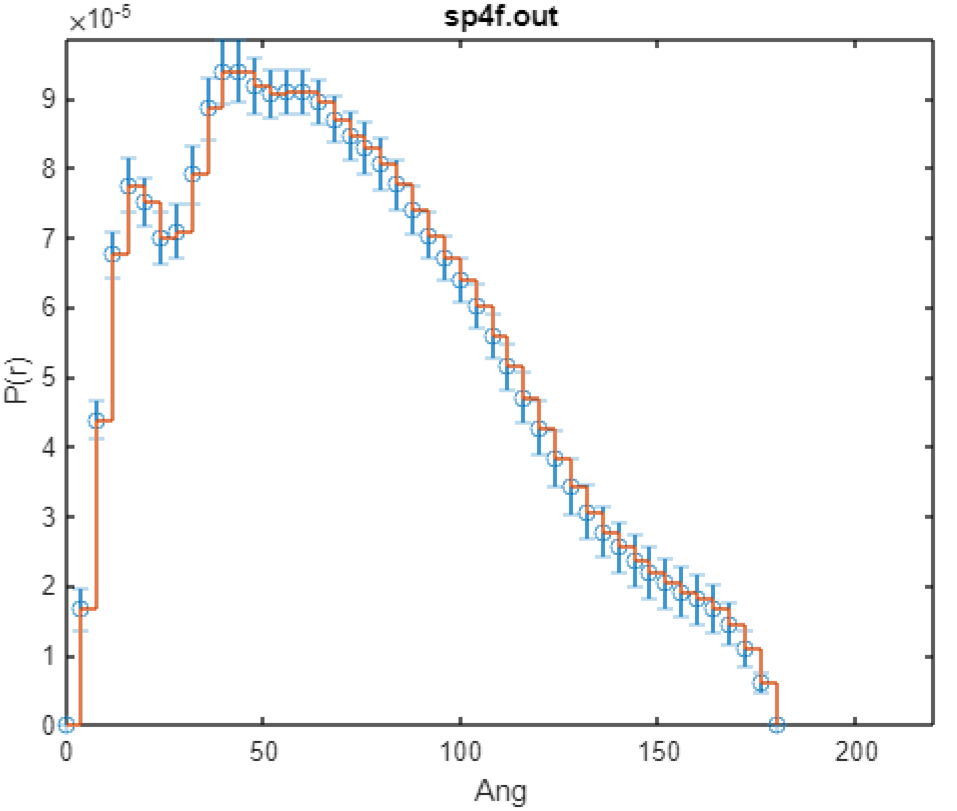


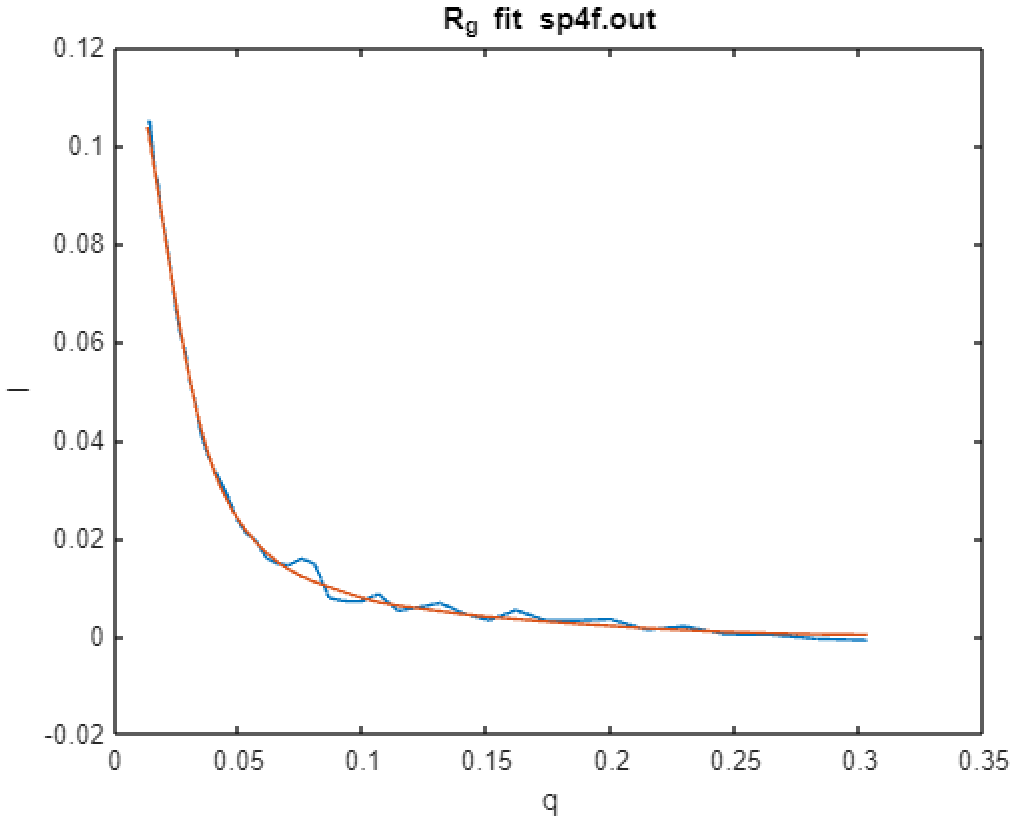
```
Real space Rg:                   0.4455E+02 +-   0.1050E+01
```



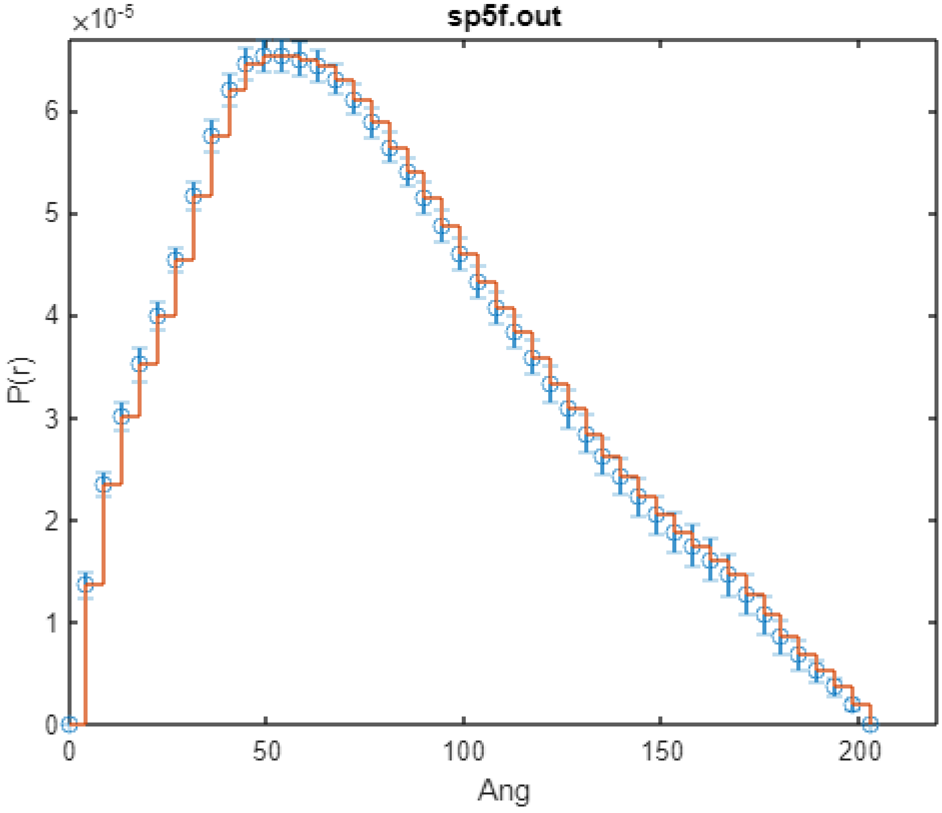


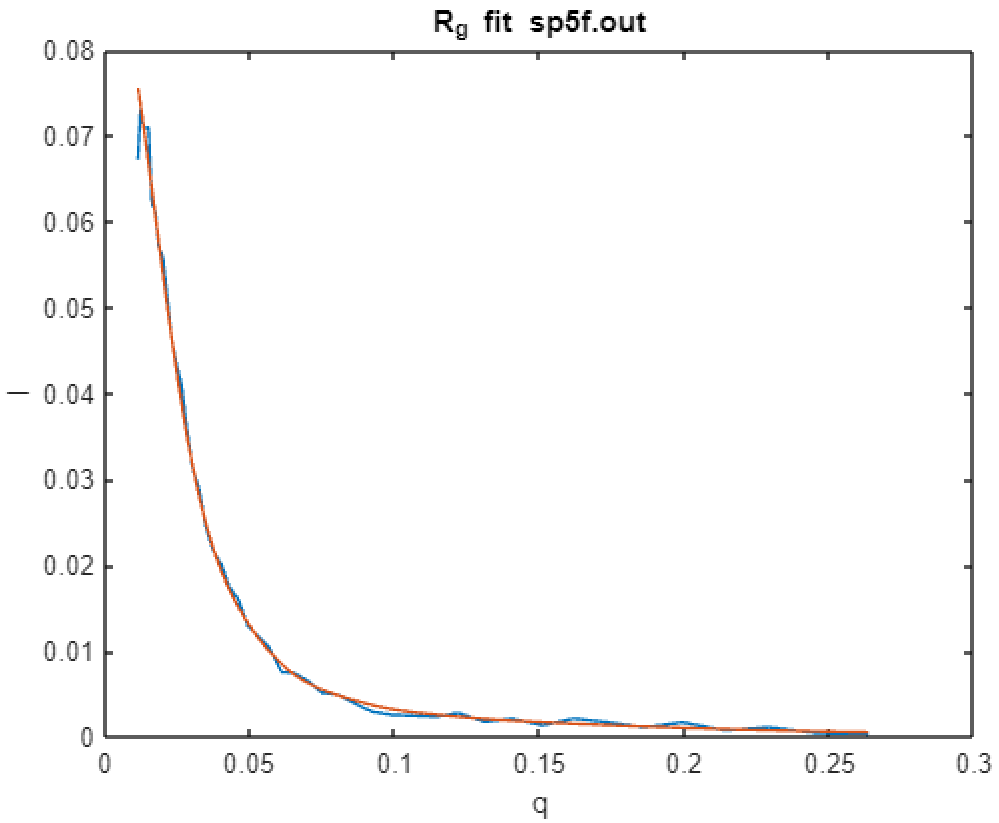
```
Real space Rg:                    0.4413E+02 +-    0.1528E+01
```





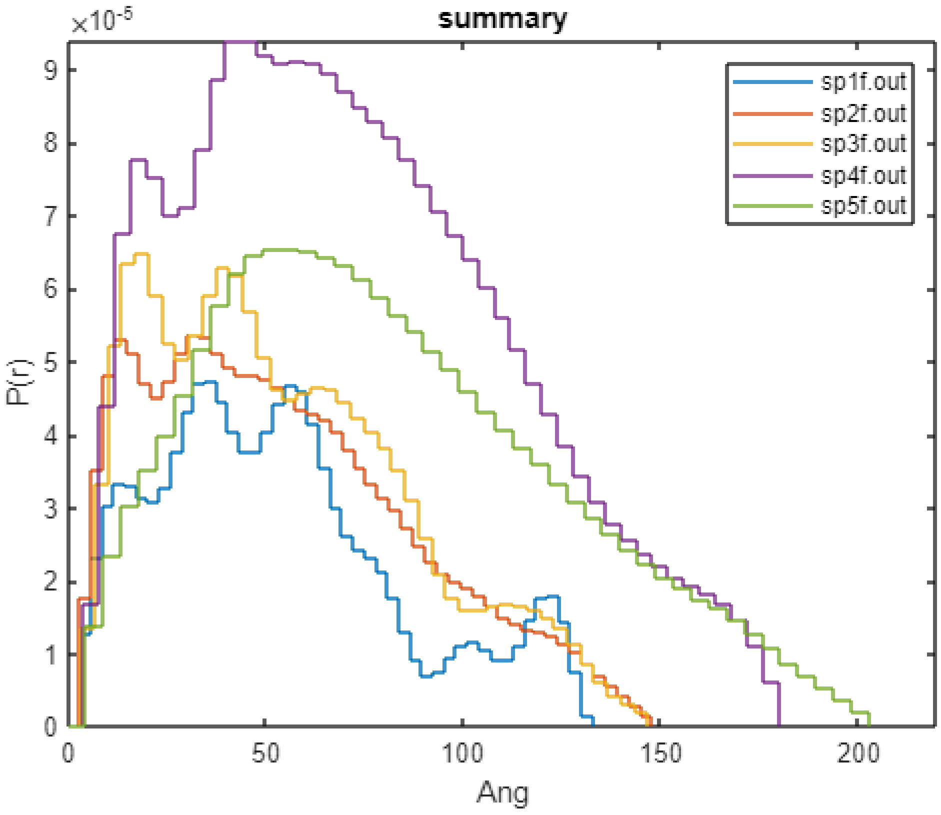
```
Real space Rg:                    0.5778E+02 +-   0.9809E+00
```





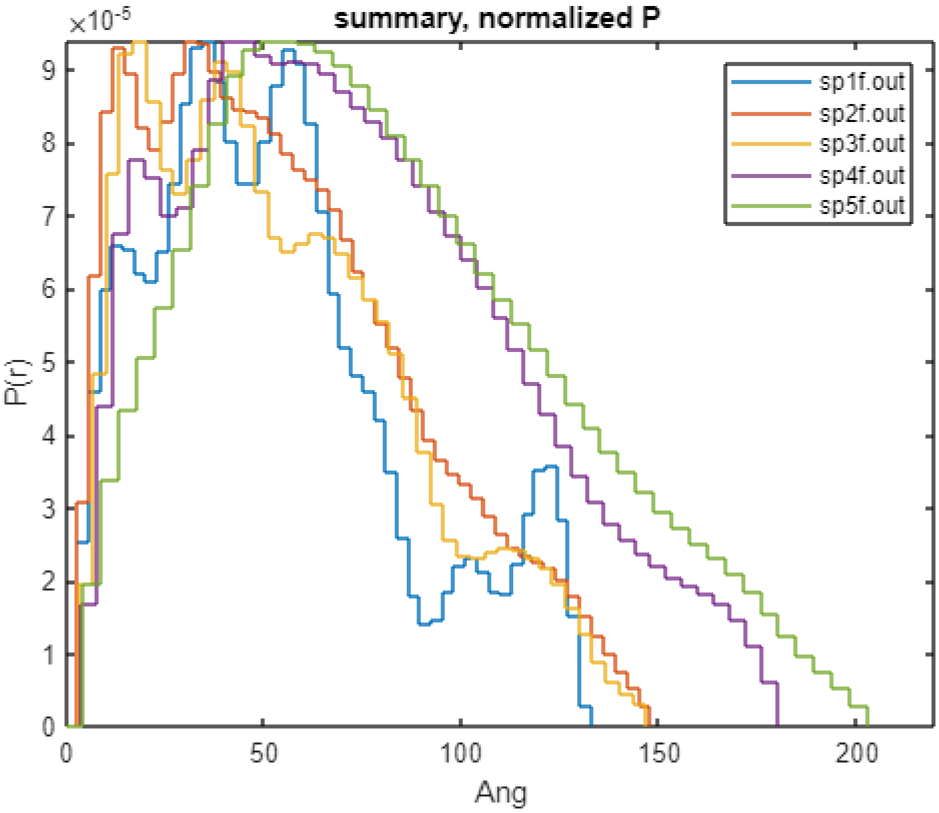
```
Real space Rg:                    0.6386E+02 +-   0.1079E+01
```

```
save Rg Rg
figure; leg=string(0); xm=0;
for ll=1:numel(yyR)
    x=yyR(ll).x;
    xm(ll)=max(x(:,2)); %#ok<SAGROW>
    stairs(x(:,1),x(:,2)); hold on
    leg(ll)=yyR(ll).f.name;
end
title ('summary')
xlabel('Ang')
ylabel('P(r)')
    axis([0   220 0 Inf]);
legend(leg)
```



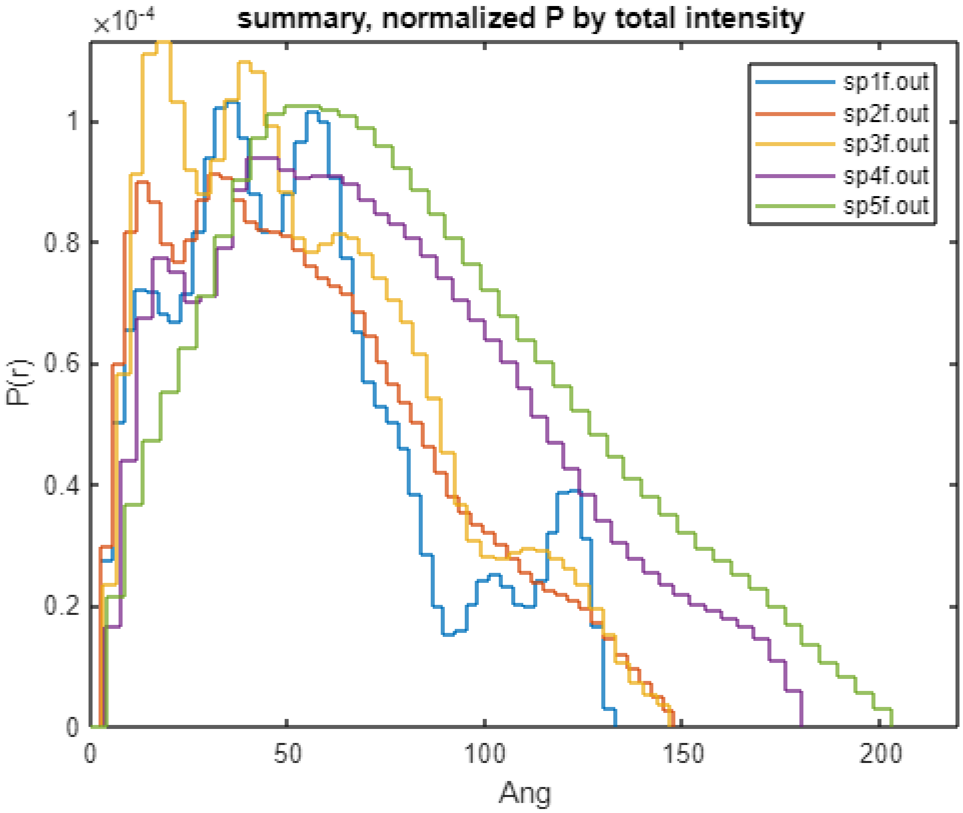
normalized to height

```
figure; xm=xm./max(xm);
for ll=1:numel(yyR)
    x=yyR(ll).x;

    stairs(x(:,1),x(:,2)./xm(ll)); hold on

end
title ('summary, normalized P ')
xlabel('Ang')
ylabel('P(r)')
legend(leg);     axis([0   220 0 Inf]);
```



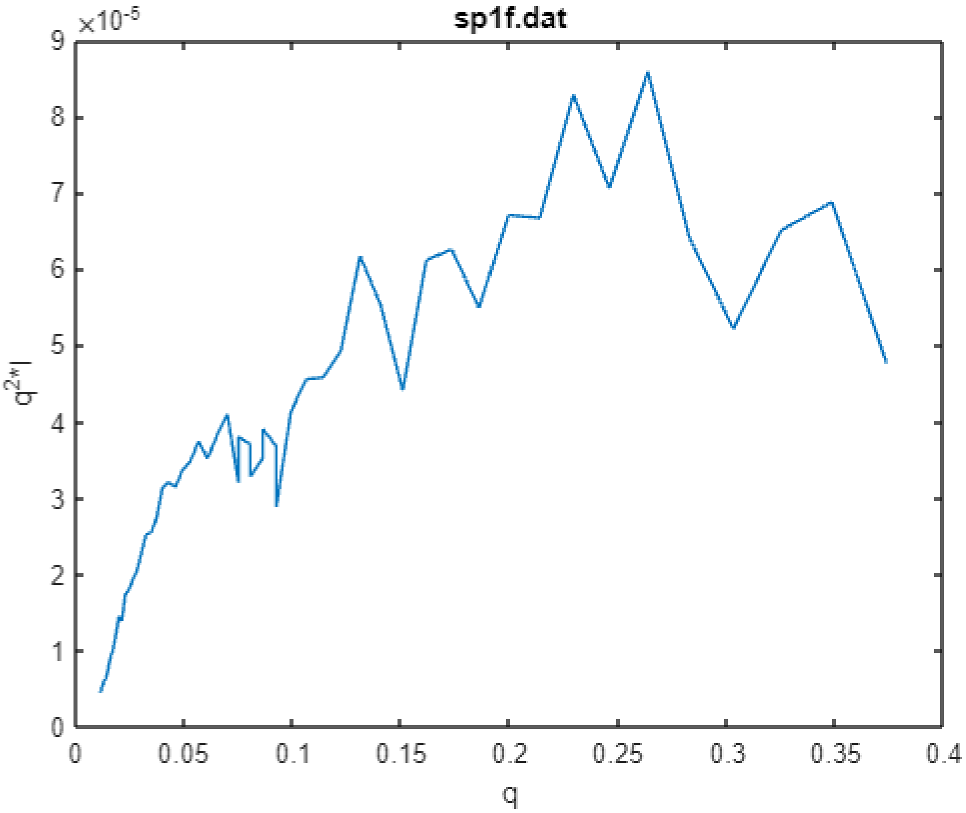
normalized to total intensity

```
figure; xm=xm./max(xm);
sms=zeros(1,numel(yyR));
for ii=1:numel(yyR)
    sms(ii)=sum(yyR(ii).x(:,2));
end
msms=max(sms);
for ll=1:numel(yyR)
    x=yyR(ll).x;

    stairs(x(:,1),x(:,2).*(msms./sms(ll))); hold on

end
title ('summary, normalized P by total intensity ')
xlabel('Ang')
ylabel('P(r)')
legend(leg);     axis([0   220 0 Inf]);
```

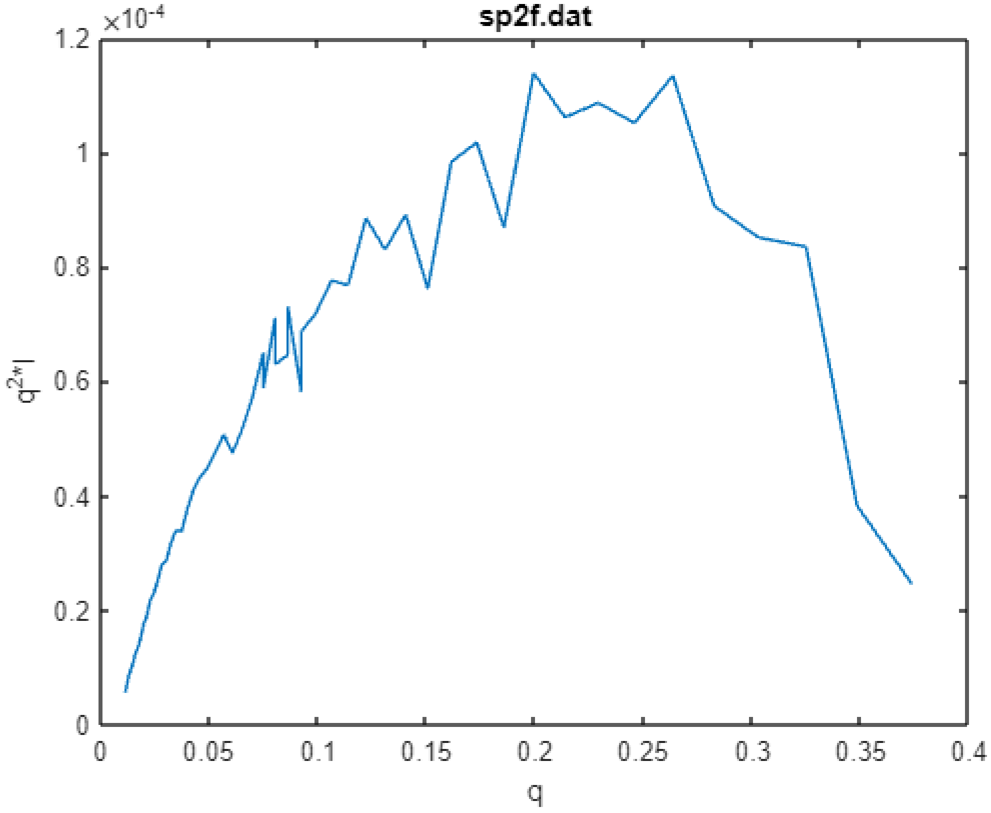


Kratky

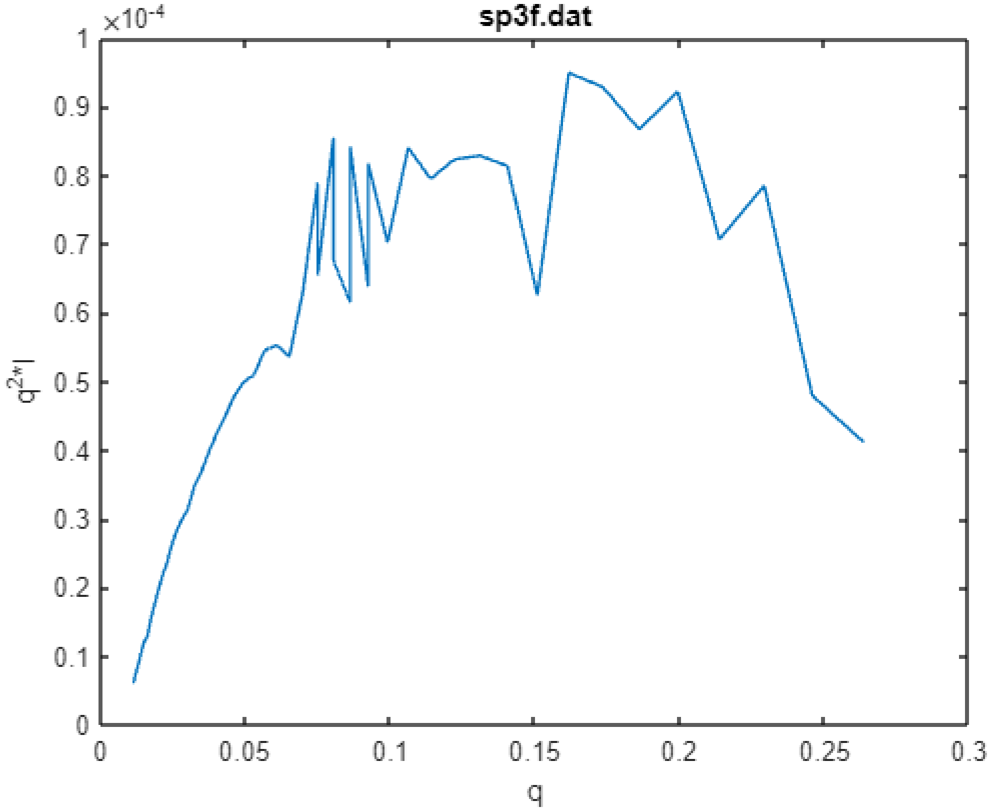
```
for ii=1:numel(yy)
    x=yy(ii).x;
    if isempty(x), continue; end
    figure;
    plot (x(:,1),x(:,1).^2.*x(:,2));
    title (yy(ii).f.name);
    xlabel('q');
    ylabel('q^2*I')
end
```

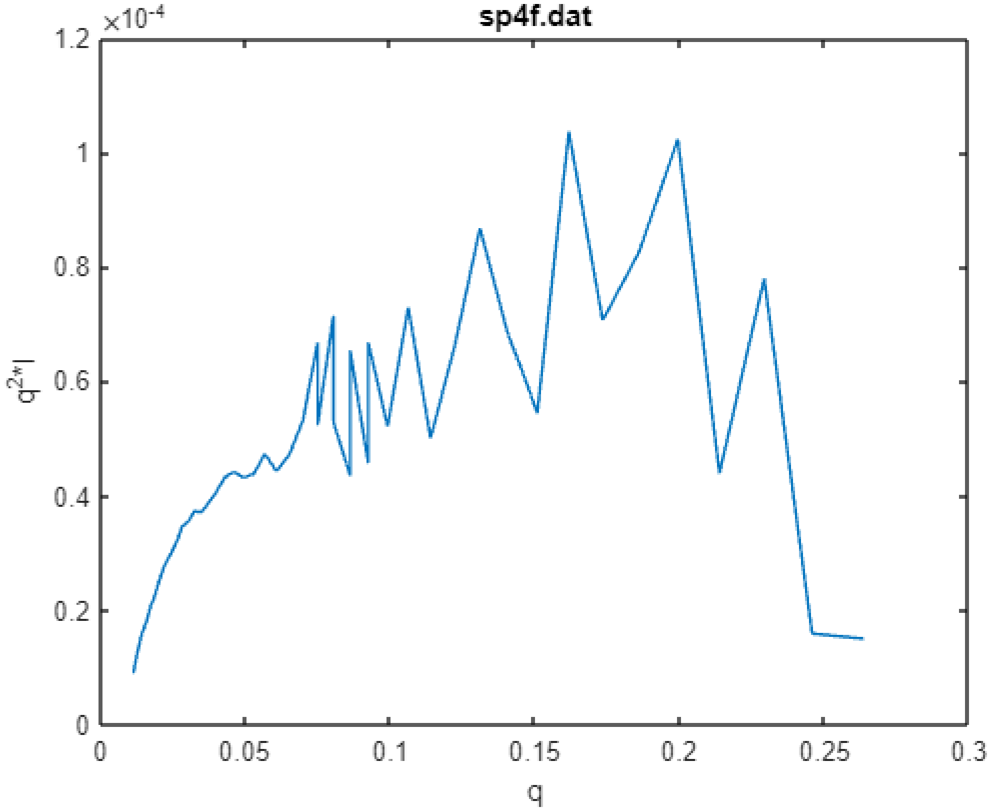


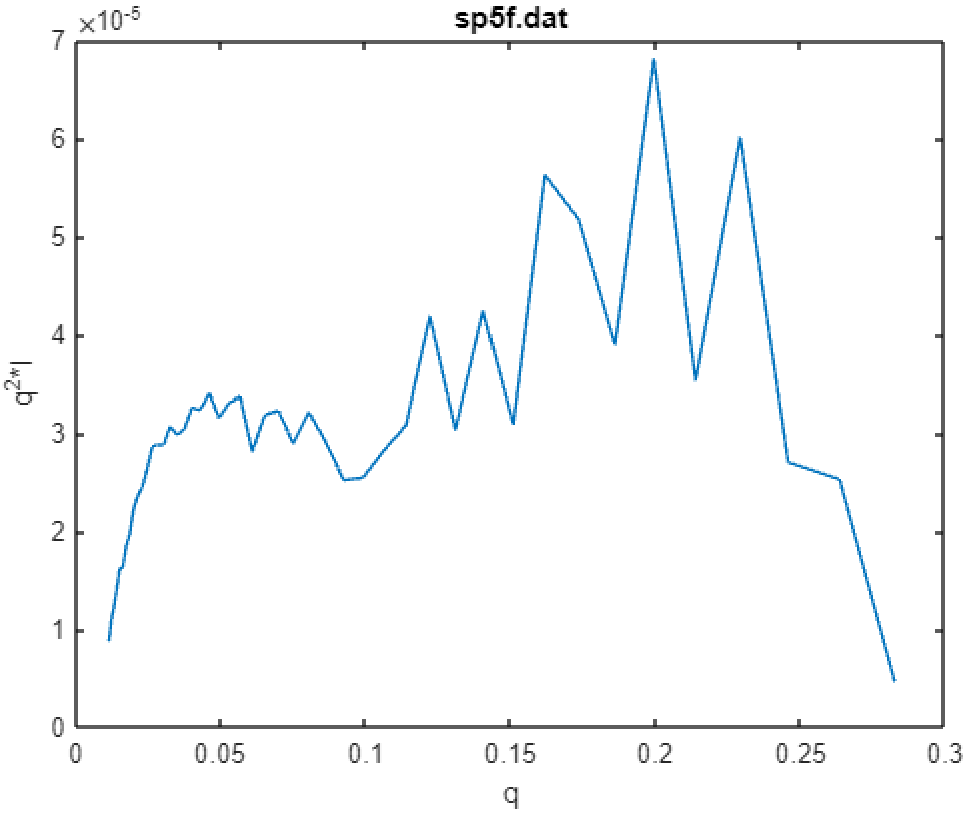
sp1f.dat
×10-5
9
8
7
6
5
4
3
2
1
0
q2*I
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
q

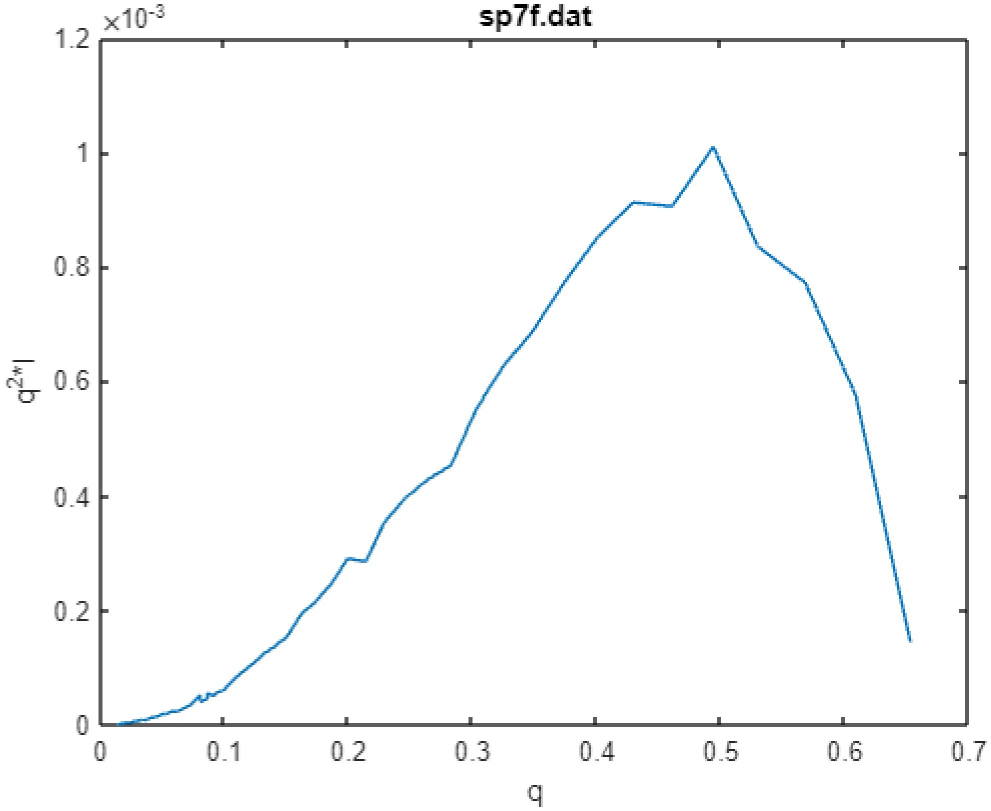


sp2f.dat
×10-4
1.2
1
0.8
0.6
0.4
0.2
0
q2*I
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
q


sp3f.dat
×10^-4
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
q^2*I
0
0.05
0.1
0.15
0.2
0.25
0.3
q


sp4f.dat
×10^-4
1.2
1
0.8
0.6
0.4
0.2
0
q^2*I
0
0.05
0.1
0.15
0.2
0.25
0.3
q


sp5f.dat


sp7f.dat