

autoSHARP reference card	
set up (if not already done automatically for you)	
Set up for csh or tesh	<code>source /some/where/SHARP/installed/setup.csh</code>
Set up for bash, ksh, zsh, or sh	<code>./some/where/SHARP/installed/setup.sh</code>
Input file information	
Sequence file format (*.pir)	>1022 MGSDKIHMMMMRLMDILEILYYKKGKEFGILEKKMKEIFNETGVSLEPVNSEL IGRIFLKIISVLEEVEEVPVSFAIKALTPKENAVDLPLGDWTDLKNVFEVVEIDYLDLDS YGDMKILSEKNWYKIYVPYSSVKKKRNRELVEEFMKYFFESKGNPGEYTFVQEQE IDNLF *
Reflection file format	SCALEPACK (*.sca) or MTZ (*.mtz), e.g. from autoPROC
Known heavy-atom positions (fractional coordinates – use 'coordconv' for conversion from PDB)	ATOM Se 0.7050 -0.1857 -0.0639 ATOM Se 0.4613 0.4419 0.0687 ATOM Se 0.7190 0.1720 -0.2294 ATOM Se 0.7287 0.2058 -0.2216
autoSHARP: most useful options	
Brief help message	<code>run_autoSHARP.sh -h</code>
Describe (unique) content of asymmetric unit	<code>run_autoSHARP.sh -seq <file.pir></code> - or - <code>run_autoSHARP.sh -nres <# residues></code>
Give space group instead of reading it from reflection file(s)	<code>run_autoSHARP.sh -spgr <SG-name></code>
Define output directory	<code>run_autoSHARP.sh -id <output></code>
Skip automatic model building	<code>run_autoSHARP.sh -nobuild</code>
Examples (see also http://www.globalphasing.com/sharp/wiki/)	
SAD (Se-MET)	<code>run_autoSHARP.sh -seq 1o22.pir \ -ha "Se" \ -wvl 0.9778 peak -7 5 -sca 1o22_peak.sca</code>
MAD (2-wavelength Se-MET)	<code>run_autoSHARP.sh -seq 3isy.pir \ -ha Se \ -wvl 0.97934 infl -11 3.3 -sca aimless_0.97934A.sca \ -wvl 0.91162 hrem -1.8 3.3 -sca aimless_0.91162A.sca</code>
SIR(AS) (mercury derivative)	<code>run_autoSHARP.sh -seq 1GXT.pir \ -nat -mtz 1GXT_nat.mtz \ -ha Hg -nsit 2 \ -wvl 0.99970 peak -16 10 -mtz 1GXT_hg.mtz</code>
MIR(AS) (two derivatives)	<code>run_autoSHARP.sh -seq 3zft.pir \ -nat -mtz 3zft_nat.mtz \ -ha Hg -nsit 1 \ -wvl 1.54179 -mtz 3zfq_Hg.mtz \ -ha Ir -nsit 2 \ -wvl 1.54179 -mtz 3zfr_Ir.mtz</code>
Including partial model or initial MR solution (can be used for all situations)	<code>run_autoSHARP.sh -seq 3get.pir \ -ha Se \ -pdb 3ffh_ala_MR.pdb \ -wvl 0.9789 peak -8 4 -sca 3get.sca</code>
SAD with Ta₆Br₁₂ cluster at Ta edge	<code>run_autoSHARP.sh -seq 4cv5.pir \ -ha "Ta6Br12:Ta" -nsit 1 \ -wvl 1.25472 peak -mtz 4cv5.mtz</code>

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Analysing output	
Log file	Open <output>/LISTautoSHARP.html to browse through the different stages of data analysis, substructure solution, HA model refinement, phasing, density modification and automatic model building.
Coot scripts	Within the output directory there will be a “Results” subdirectory containing various scripts for running Coot (to display models and maps at different stages): see also standard output for details.
LLG residual maps (resid.mtz)	Columns for amplitude (* _F) and phase (* _P) are given. The naming conventions are: “* _HAT_* ” for the current heavy atom model and “* _RES_* ” for residual maps (to find new sites or adjust current model). The first 4 numbers correspond to the Compound-Crystal-Wavelength-Batch hierarchy of SHARP .
Initial experimental phases (eden.mtz)	Useful columns are: FP/SIGFP (unperturbed structure factor), HLA-D (Hendrickson-Lattmann coefficients), FB/PHIB or Fcent/PHIcent (purely experimental map, ie. before solvent flattening)
Solvent-flattened map (eden_flat_*pc.mtz)	Use columns FBshasol/PHIBshasol in Coot
Some useful commands	
Converting from PDB to fractional coordinates	coordconv xyzin some.pdb xyzout some.frc <<e INPU PDB OUTP FRAC e
Calculating difference Fourier maps	diff_fourier -h # from BUSTER package
Further information	
See also:	http://www.globalphasing.com/sharp/ http://www.globalphasing.com/sharp/wiki/
Global Phasing home page	http://www.globalphasing.com/