autoSHARP reference card

set up (if not already done automatically for you)

Set up for csh or tcsh	**source /some/where/SHARP/installed/setup.csh**
Set up for bash, ksh, zsh, or sh	**. /some/where/SHARP/installed/setup.sh**

Input file information

Sequence file format (*.pir)	>1O22 MGSDKIHHHHHHMRLMDILEILYYKKGKEFGILEKKMKEIFNETGVSLEPVNSEL IGRIFLKISVLEEGEEVPSFAIKALTPKENAVDLPLGDWTDLKNVFVEEIDYLDS YGDMKILSEKNWYKIYVPYSSVKKKNRNELVEEFMKYFFESKGWNPGEYTFSVQE 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	**run_autoSHARP.sh -h**
Describe (unique) content of asymmetric unit	**run_autoSHARP.sh -seq <file.pir>** - or - **run_autoSHARP.sh -nres <# residues>**
Give space group instead of reading it from reflection file(s)	**run_autoSHARP.sh -spgr <SG-name>**
Define output directory	**run_autoSHARP.sh -id <output>**
Skip automatic model building	**run_autoSHARP.sh -nobuild**

Examples (see also http://www.globalphasing.com/sharp/wiki/)

SAD (Se-MET)	**run_autoSHARP.sh** -seq **1o22.pir** \ -ha **"Se"** \ -wvl **0.9778 peak -7 5** -sca **1o22_peak.sca**
MAD (2-wavelength Se-MET)	**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
SIR(AS) (mercury derivative)	**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
MIR(AS) (two derivatives)	**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
Including **partial model** or **initial MR solution** (can be used for all situations)	**run_autoSHARP.sh** -seq 3get.pir \ -ha Se \ **-pdb 3ffh_ala_MR.pdb** \ -wvl 0.9789 peak -8 4 -sca 3get.sca
SAD with **Ta_6Br_{12} cluster at Ta edge**	**run_autoSHARP.sh** -seq 4cv5**.pir** \ **-ha "Ta6Br12:Ta" -nsit 1** \ -wvl **1.25472 peak** -mtz **4cv5.mtz**

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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`
See also:	**http://www.globalphasing.com/sharp/** **http://www.globalphasing.com/sharp/wiki/**