**HSPiP Version Information**

V6.0.04

* One bug sneaked into 6.0.03 – the HSPs calculated in the QSAR were correct then accidentally overwritten by the 5.4 versions. That’s been fixed.

V6.0.03 January 2024

* Those updating from versions earlier than 5.4 will find a significant face-lift which had been done in preparation for 6.0.
* Core HSP parameters are now calculated using the Y-MB24 algorithm. As always with a new Y-MB on *average* the values are better, but you might find examples where a specific estimate is worse. We have installed the 6th edition into a new folder so you can swap between versions.
* The good news is that the previous Y-MB that we have been using for years was impressively good, so the improved version doesn’t give huge changes to “normal” molecules. The bigger improvement is to large, multi-functional molecules where the previous Y-MB had problems.
* Some non-core parameters are, for deep technical reasons, calculated using the previous Y-MB. As we’ve always stressed, these are provided “as is” for those who find them helpful. The HSP@T option, which was little used, has been removed. Of course the standard T calculations are available throughout the program.
* Loading 3D files (molfiles etc.) into Y-MB has been streamlined. This has lost the ability to load some obscure file formats but is more reliable for the common ones. If necessary you can use OpenBabel to pre-convert to the .mol, .sdf or .pdf formats used.
* The P = Polymers form has always been used for storing other data such as pharma APIs or nanoparticles. But calling it P has discouraged some users from using it. We’ve now changed it to M = Materials & Polymers. The functionality is the same – though some controls have been renamed and the “Further Comments” column has been renamed to “Source” to encourage users to store a link showing where they got their data from.
* The Data Points fit, unless Fit to Exponential was selected, did not have graphics to show the results. These have been added. The results can look strange but that’s because the focus of the fitting is on the good values, rather than the whole set.
* There is an S+ option for when you click the S button to see your chosen solvents. You now get some metrics indicating how good your solvent selection might be, and a way to change one or two solvents to give you a better chance of a good measured value for your solute. Search for S+ in Help to find how to use this new capability.
* For those with data values, the S button shows the solvents colour coded by their distance from the maximum value
* An annoying feature of 3DO wire-frame that did not let your mouse identify solvents inside has been fixed.
* In DIY there is now an option to add your molecule to the main solvent table as well as to the Solvent Optimizer.
* Grids that used the same solvent in the first column would have redundant entries for 100%:0% entries for solvents beyond the first. These entries have been removed.
* We had decided not to increase HSPiP prices until the release of the 6th Edition. This means they have not changed since 2015! We’re happy that so many users got a good deal with the non-inflated prices, but it’s time to be fair to ourselves and catch up with the large $ inflation over that period. And, of course, all current users get their free update to new versions, plus free access to Steven’s tech support. HSPiP remains a very attractive package.
* And for this release we have a message from Hiroshi.

**Message from Dr YAMAMOTO Hiroshi**

Welcome to Y-MB24. For its launch I want to make some important points.

HSPiP is not a database software. Sometimes some users have a wrong understanding.

When dealing with solvents, users sometimes need not only HSP values but also experimental boiling points, Antoine constants, and RER.

It would be easy for us to leave them blank and let the user be responsible for collecting the experimental values. But if we do this, many of the functions will not work.

Therefore, the blanks are filled in using Y-MB’s property estimation functions. Since these are estimates, the answers will change in this new version. We provide the estimates as a convenience for users and do not guarantee the accuracy for each individual solvent.

Some users will see that the estimation accuracy of a given individual solvent has deteriorated. As we always say, if you already know the real values, why are you using Y-MB ones!

An AI company that analyzed the Y-MB results said, "We have created a model that predicts HSP with R = 0.98 from the molecular structure". This is clearly a mistake. The model they created is a model that predicts the estimated value of Y-MB.

This is what happens when they misinterpret HSPiP as a database software.

There have been case of people cracking Y-MB and claiming it as their own HSP estimation formula. As AI technology advances, it will become increasingly easy to do this. Users should think carefully about what that means. You can always choose to go with an AI Y-MB, but in the long run you will lose out on the continued, patient development of a better, smarter HSPiP where we care about the long term.

It is possible that this version will change the results described in patents or papers.

Of course, the patent or paper should clearly state which version was used and which option was adopted, so the conclusion itself will not change. As mentioned above, the new version installs into a fresh folder so you can run the 5th and 6th editions to compare results.

Because the HSPiP QSAR uses only the Y-MB estimates calculated from SMILES the new results will also be different. Maybe not very different, but you still have to check.

Let me explain the significance of QSARs in HSPiP. They are mainly to find the key players in determining the quantitative values based on molecular structure. If all quantitative values were solely dependent on HSP, there would be no need for a QSAR. Some solubility phenomena can be better explained by taking into account, say, the MVol or Ovality of the molecule in addition to HSP. Sometimes other parameters are important. QSAR is a tool to find such players.

Once the players are known, the exact QSAR equation should be made from *experimental* values, not Y-MB estimates. But before that, let's gain insights by looking at the positive and negative coefficients. And use FindMols to identify molecules that might be better. We can slowly collect the experimental values while actually experimenting with those predicted compound.

Some FindMols results will be different in the new version, especially for the high-functionality molecules that were a problem in previous versions. The new version is likely to identify better molecules.

If you have used Y-MB and FindMols to create, say, your own GreenSolvent.sofx, it will be a good idea to re-run your process, keeping your old version and creating a new GreenSolvent24.sofx.

I am proud of the old version of Y-MB that has worked well for HSPiP for so many years. I’m pleased that after a lot of work, Y-MB24 is improving on an already good model. No prediction scheme can be 100% reliable. Over the years the HSPiP community has fed back issues that have helped identify bugs and issues which we fixed to make things better for the whole community. I look forward to your feedback on Y-MB24 so I can continue to improve.

V5.4.09 April 2023

* The 3DO sometimes failed to update the solvents. The behaviour has been improved
* There was a wrong labelling of Wrong In and Wrong Out counts when showing In only and Out only plots. The fit itself was unaffected. Those wrong counts have been removed.

V5.4.08 February 2023

* Thanks to expert help from Dr Nicholas Tito, the SFB-FE user interface has been made much cleaner, some subtle calculation glitches were fixed, and the van der Waals attraction between particles has been added to the Interparticle calculations.
* A bug in the MolFile code created an error for molecules with more than 99 atoms. That has been fixed.

V5.4.07 November 2022

* If you click the S (Show) button with MVol Correction option clicked, you see your molecules in their 1-6 colour codes with different sized spheres. The sizes can be relative to the real MVols or you can enter dummy values to highlight differences. Hiroshi used this to highlight how large pharma molecules can be split into, say, 3 sub-components.

V5.4.06 August 2022

* An obscure problem loading a .hsdx file was traced to non-standard text line endings. The code has been updated to work with such endings.
* In the Diffusion model, mouse readout now shows the time as well as position and concentration.
* The “Fit” graphs from data rather than 0/1 scores were not reset when a new file was loaded. Fixed!
* A large number of glitches in Help and the eBook were spotted by an amazing HSPiP user so this release contains those updates.

V5.4.05 July 2022

* The S button always showed each of the solvents in blue. This has now been updated to be colour coded. For example, 0 & 1 solvents are shown as red and blue, while 1 to 6 scoring is shown as a gradation from blue to red. Values outside 0-6 are shown as a blue-ish colour.

V5.4.04 May 2022

* The Wt/Density addition from Dec 2021 introduced a bug into the =>SO button in DIY so that some values got pasted into wrong SO columns. Fixed.

V5.4.03 April 2022

* Because there are always lots of questions about the best way to fit the good/bad solvent data, we’ve added the Fit Explorer which systematically alters the status of borderline solvents to see whether a decision on 1 solvent has a big effect on the fitted result. You can also explore the balance between penalising Wrong Out and Wrong in solvents.
* The OB fit procedure has been made faster and a Help button added.

V5.4.02 February 2022

* You can now open .sofx files into the main form, allowing you to access all the SO-style data.
* Open with Autocheck is a powerful way to ensure that any HSP values in your .hsdx file match those in the Master Dataset. The comparison is based on CAS#. This has not been changed. Instead, the change is to the Help file which had the old information where Name and Number were used for comparison.
* Surfactant values in the DIY form could not be copy/pasted via Ctrl-D, Ctrl-P. They now can. The surfactant tab has been tidied up.
* A few minor layout issues on the main form have been fixed.

V5.4.01 January 2022

* This is a significant shift to the user interface in preparation for V6
* The first time HSPiP is used it now loads a Default Set rather than the overwhelming Master Dataset
* The 3 2D plots, which have been there from the start and were now only of historical interest have been removed.
* This gives room for the “Fitting” area where everything about fitting is contained in one place: the Classic Hansen along with the Genetic Algorithms and Data fitting, fitting options and the calculate button
* Mouse readout of the solvents in the 3D plots has been improved
* Other historical relics have been removed from the interface. “Hide unused” and the ability to load/save as .hsd and .sof files. Those old file formats were replaced in 2018 so users will have had plenty of time to convert them.
* The space freed up has also allowed us to increase the size of the 3D plot and the Master Dataset
* Help buttons have been added to SO, DIY and Polymer forms for easier access to the relevant Help text.
* In the SO an option to Open with Append allows you to add solvents from another .sofx file. No attempt is made to remove duplicates – this is deliberate so you can choose how to handle potential conflicts between data sources.
* In the SO the option to “Only use bad solvents beyond R” has moved to the more logical position next to the Radius value
* The separate Van Krevelen, Hoy and Numbers tabs in DIY have been condensed into one VK-H-F-N tab where the F is the Fedors method for calculating δTot that some users wanted to be added for historical reasons.
* The 3DO is now bigger and better with some items rearranged to give more space for the 3D view and better readouts of the Mixture data.

V5.3.09 December 2021

* This is the first version generated in Win11, VS2022 and DotNet 4.8 as we continue to develop for the long-term future. In our tests it works well on older Win10 machines
* The Help screen has an improved layout
* There is a Wt% option in the Solvent Optimizer. When this is selected, Wt% and ρ (density) columns appear and any Vol% entry is converted (via ρ) into Wt%. This will help users who want to formulate via weight rather than volume. The calculation is one way Vol🡪Wt, the other way is not supported.

V5.3.08 September 2021

* This is a fix for those using the CLI version. A subtle bug was spotted with some Y-MBF SMILES strings and has been fixed.
* A collection of Rhodiasolve Green Solvents has been added to the Solvent Optimizer

V5.3.07 July 2021

* For those who want to process a lot of SMILES molecules via File Convert in Y-MB there is now a File Check button that scans them all for being Good, Bad or Caution, where Caution means that it was converted from an unusable dotted SMILES or where the molecule contravenes a Lipinski Rule of 5 so might be too large or complex for a reliable estimation.
* Two popular greener solvents, Cyrene and γ-Valerolactone have been added to the standard database, with as many experimentally available properties as possible.

V5.3.06 December 2020

* Some users wanted DIY to calculate Number of Rotatable Bonds. Because intellectually this is linked to Molecular Connectivity Index, the results are shown together as MCI/NRB
* Some minor bug fixes to the DIY File Convert make it more robust to glitches in the input file and also keeps an exact match with the original file for when you need to copy paste the additional information

V5.3.05 October 2020

* Some users who have solvents working at super-high pressures as well as different temperatures asked for P effects to be added to the °C box. Those who work under less than, say, 50 bar pressure can ignore the change of HSP values!
* The **Genetic Algorithms** checkbox name has been changed to the more useful **Advanced Fitting**. There are no changes to the options when the Advanced box opens, though the accuracy of the Low/Med/Hi GA fit options has been increased because we all have more processing power than we used to.
* Some errors had crept in to the Antoine Coefficients in the standard Solvent Optimizer dataset. They are now, where applicable, identical to the master dataset.

V5.3.04 July 2020

* The polymers and di-blocks SFBox-P functionality has increased to provide a lot of information about micelles and about micelle solubilizers (host/guest systems). This is another major advance for HSPiP
* In FindMols an option to search via chemical fingerprint similarity has been added, using Tanimoto, Dice, Cosine etc.

V5.3.03 June 2020

* There was a glitch in the planar brush calculations. They are now correct
* A preliminary version of SFBox-P for handling polymers and di-blocks has been added. The current functionality is very limited but more will be added over time.

V5.3.02 June 2020

* We have now added the capability to do what are called SF (Scheutjens-Fleer) or SCF (Self-Consistent Field) theory calculations. This is a science of particle-polymer-solvent interactions developed/validated since the 1970s but unknown to most of us. Even if we had heard of it, it was too complex to implement. Fortunately, thanks to the generosity of Prof Frans Leermakers of Wageningen U in the Netherlands we have added his “SFBox” engine to do the calculations accessing it via a user-friendly front end within HSPiP. A new chapter in the eBook describes what users can achieve with SFBox.
* For IGC users, Cyclooctane has been moved from the 10K set to the standard set and the IGC Data set updated. And superglue, polyethylcyanoacrylate has been added to the Examples files and to the default polymer database.

V5.2.07 May 2020

* A couple of bugs importing into the SO, with conversion from old .hsd files were fixed
* The row headers could be accidentally resized. This has been fixed
* Doing a Ctrl-P paste into boxes gave an annoying “Ding” sound. This has been eliminated.
* Adding polymers to the Polymer Blends form can now be done via a Right Click on a polymer where at least one cell has been selected.
* Entering a dotted SMILES caused problems for EACNs. That’s been fixed.
* In preparation for v5.3.x the DC Radius has been moved to lower down the form.
* A SubCheck option was added to Y-MB File Convert. If selected, and if there is a valid sub-structure SMILES then an output file is created containing Name, SMILES and True or False depending on whether the sub-structure is present. This uses the powerful RDKit HasSubstructMatch capability.
* Similarly, FindMols can search for any given SMILES sub-structure.
* For those wanting more sophisticated sub-string searches, a SMARTS option can be chosen – but it’s up to you to teach yourself SMARTS from, e.g. <https://www.daylight.com/dayhtml/doc/theory/theory.smarts.html>.

V5.2.06 January 2020

* There has always been a blank row at the bottom of the Master Dataset, which implied that things could be added. Following an error when someone tried to do this, that blank row no longer exists. It’s also now not possible to accidentally delete rows.
* At the request of Lambiotte, a new Acetals Lambiotte.sofx file was added as these are an interesting class of solvents. We welcome other companies who would like us to add their list of solvents or other chemicals.
* A bug was found in the Evaporation Optimizer, making it difficult to use. This has been fixed.
* Some minor aesthetics were updated in the DIY Y-MB and Polymers tabs

V5.2.05 October 2019

* On some systems the 3D graphics could crash when showing large numbers of molecules. This is an obscure systems bug. A small change to the code has now stopped the crash on a few test systems, but it is always recommended to keep graphics drivers updated when there have been updates to Win10.

V5.2.04 October 2019

* Users found 2 bugs in the .hsdx creation from File Convert in DIY. The first placed δD values in all δP and δH, the second meant failure to recover from a bad entry in the file. Apologies for both bugs which are now fixed.

V5.2.03 October 2019

* Minor bug fixes

V5.2.02 August 2019

* We now have the Y-PB (Yamamoto Polymer Breaking) method for better predicting polymer HSP values and a range of other properties. It is anticipated that this first release is the start of a set of upgrades to Y-PB as we gain more experience with it.
* The polymer database linked to Y-PB now contains over 1400 polymers with a large number of experimental details selected by Hiroshi from a number of different datasets, plus the Y-PB estimates of HSP values
* Thanks to the amazing RDKit, an open source chemistry capability which we acknowledge with warmest thanks, we can now convert a Y-MB SMILES into a 3D structure for you to view.
* From this 3D structure we can calculate the charges on each atom via the famous Goddard QEq approach, using Hiroshi’s special implementation. Users might find this of interest in thinking about how the molecule might interact with others.
* RDKit comes with its own InChI-to-SMILES converter so the InChI handling is now more robust
* A little-used feature to view a polymer SMILES via a set of mol files has been removed because any Y-PB molecule can be viewed by clicking the Y-MB tab where the polymer molecule is shown with distinctive chain bonds
* The 3D views now all have Mouse-Wheel zoom in and out as well as Shift-Drag
* Ctrl-D/Ctrl-P between relevant tables now copies the name as well as the HSP and MVol values
* Showing names/numbers from the Solvent Match option in Polymers was unreliable. This has been fixed.
* A new estimator for Diffusion Coefficients has been added to Diffusion using the sophisticated Brandsch model that uses the Tg of the polymer and the Tm of the diffusing molecule. Brandsch has worked extensively with the issues of diffusion through food packaging and this is a further refinement of the estimation schemes associated with the names of Pirringer and Brandsch.
* A Help button has been added to Diffusion

V5.1.08 May 2019

* Minor bug fixes and inclusion of the Chem21 dataset in the Solvent Optimizer – a solvent set recommended by Pharma as being a good balance of safety and utility

V5.1.07 April 2019

* A new procedure for numerical data, the Optimal Binary (OB) Fit has been added. The technique was devised by Prof Dietmar Lerche of LUM GmbH and Prof Doris Segets at U. Duisberg-Essen and provides an automatic, objective way to find an optimal splitting point between Good and Bad solvents

V5.1.06 April 2019

* The export from QSAR to the main form was still in .hsd format; this has been upgraded to .hsdx format
* An important new NMP-replacement solvent has been added to the default Solvent Optimizer – dimethyl lactamide.

V5.1.05 March 2019

* Copying from the main form failed to include CAS and SMILES. Fixed
* The XO (Extra Optimization) option in the SO had not been updated to the new CAS format so was failing. The old .sof file with CAS numbers in the Names column will now no longer work.

V5.1.04 February 2019

* A bug in Sphere Radius Check from the 5.1.02 release was not spotted till now. The bug meant that it never found any useful solvents! It has been fixed.
* A user requested the ability to estimate the HSP at a chosen temperature within the Y-MB. This has been added. The estimate uses a more sophisticated approach (the same one used in the QSAR form) and so will differ from the simple expansion coefficient approach used on the main form.

V5.1.03 December 2018

* A bug in FindMols meant that the results were not placed on the Clipboard. This has been fixed

V5.1.02 November 2018

* The new XML-based .hsdx and .sofx file formats have been introduced as the future of HSPiP’s file system. These are far better for internal use within the program, but importantly, allow CAS and SMILES to be an integral part of the file formats, making it much easier to process data internally or externally. Note that you can always use your older files and if you want to save in the old format you simply choose the Save as .hsd and Save as .sof options in the main form and the Optimizer
* The PowerTools have been removed. They have been replaced by the SMILES drawing system and by the QSAR. Japanese users can still access similar tools via Hiroshi Yamamoto’s Pirika site.
* The Print and Screen Capture utilities have had problems for some years thanks to the complexities of screen resolutions so have been removed. Printing is less common these days and can be done via clicking the table icons to paste into Excel; and everyone now has good screen capture tools. Removing the capture buttons has freed up space to move some controls around to be more logical – you should have no trouble finding them.
* The NoChk option from 5.0.13 has been removed because the CAS-based checking does not cause the problems that the NoChk option was able to avoid.
* The transition from 32x to 64x caused some problems for users in the early days. But the vast majority of users are now on 64x systems so support for 32x (which was always a problem!) has been removed and users on super-old systems will need to continue using the classic 4.1.07 version.
* The small spheres of good solvents were not smooth, to save computational time in early versions. With modern PCs this limitation has been removed so spheres are smoother.
* The 3DO dataset did not auto-update if a fresh solvent set was added or if a solvent parameter was changed. This has been fixed.
* Following a user’s request, the Solvent Optimizer now estimates the density of the chosen blend., within the limits of simple approximations and the MVol and MWt entries (if they each exist) in the table.

V5.0.13 July 2018

* A NoChk option in the SO lets one do a Conversion import without automatically checking for the existence of the chemical in the master database.
* The OtherNames column in SO was unsortable. It is now sortable by user request
* An SO file with a Header row caused an error. Although the Header row is not used, if one exists, it is ignored.
* To make it easier to copy to Excel from the SO, create new files then re-load them with their headers, the format of the copy has been extended to include columns such as Other Names and Active which had previously been excluded as being unnecessary.
* A Params button has been added to the main form which becomes visible when the master data table is shown. Clicking on it tells you all the parameters in the dataset.
* A glitch in the IGC text file import made it fail to recognise 1,4-Dioxane. This has been fixed.

V5.0.12 July 2018

* A set of “improvements” to SO🡪Sphere and the Polymer Show Solvents caused multiple read-out problems in the 3D view. These have been thoroughly sorted out.
* The IGC fitting has been improved, and as a result, the interface has been simplified to remove two fitting options.

V5.0.11 June 2018

* There was another bug in the SO🡪Sphere button. This has been fixed and a few tweaks added to make it easier to select, for example, In Only.
* There was a bug with the Flash Point option in XO which has been fixed.
* From this version, the XO dataset is supplied as DefaultSolventData.txt so that a user’s SolventData.txt is not automatically overwritten during an upgrade.

V5.0.10 May 2018

* The last solvent in the SO was not included in the PW count. This has been fixed
* The File Convert in Y-MB now outputs a file containing all the Y-MB predicted data such as BPt.
* The δD/δP 2D plot sometimes showed an ellipse rather than circle. This has been fixed.

V5.0.09 March 2018

* When multiple spheres were plotted from Polymer Solv. Match, only the first had a dot in the middle. Now they each have a dot matching their own colour.
* The mouse readout now includes the names of those multiple spheres
* When a Polymer SMILES was entered in Y-MB the Formula said, e.g. C2H4OX2. This has been fixed to show (C2H4O)n to emphasise that it’s a polymer
* InChI had stopped working owing to some confusion within the InChI code dll about 32x and 64x. It now works fine on 64x
* There were some reports that the printing function was causing problems. This is old code and have not been looked at for many years. Some minor tweaks seem to have it working OK. But in future versions we might remove the print option – it is better to copy into Excel and print from there.
* The 3D-Optimizer has been added to allow exploration of complex formulations. This is similar to the Solv. Match from the Polymers form, but more convenient and general as it uses “Components” and “Ingredients” rather than “Polymers” and “Solvents”.
* In both the 3DO and the Solv. Match, the graphics of the non-wireframe spheres have been changed to make it clearer what is inside and what happens at intersections. The graphics can seem a bit odd (which is why they had previously been opaque spheres) but on balance it seems to be an improvement to understanding.

V5.0.08 Jan 2018

* This is a CLI-only update adding the SOE and SOBD options to the Command Line Interface. The extra features (evaporation and binary distances) were requested by one user. If you are a CLI user, feel free to email for an updated version of the CLI document.

V5.0.07 Dec 2017

* The option to FindMols within your currently-loaded .hsd or .sof file has been added,
* A =>P button was added to the Polymer tab in DIY to transfer Polymer SMILES estimates directly to the last row in the Polymers form (similar to the =>SO button on the Y-MB tab)
* The evaporation calculations in the SO were added as an option to the CLI version, along with a special Pairwise method. The CLI documentation has been updated.
* Some minor bug fixes were made to the .mol2 file importer within Y-MB

V5.0.06 29 April 2017

* The following upgrades are the result of user requests from the HSP50 conference!
* You can now securely (no connection to the Internet) draw your own structures using (with kind permission) the powerful JSME (JavaScript Molecular Editor) package within your browser. When your structure is drawn, the SMILES string is available to copy and paste into Y-MB. You can even choose to draw an X for a Polymer SMILES.
* There is an XO (eXtra Optimization) button within SO that allows you to optimize for multiple attributes such as cost and safety as well as (or instead of) Distance. The Help file describes its functions. As this is the first version of this functionality, we will especially welcome feedback, good and bad, and suggestions for improvements.
* It is worth emphasising that although we provide a default properties table for the XO option, the user is responsible for populating it with whatever data they find to be relevant, especially cost and HSE data for which the HSPiP team can hold no responsibilities.
* A Reactions tab has been added to DIY. From a SMILES string, the functional groups are found and a list of the common reactions in which they can partake is provided. You may interpret this in a positive manner or (the point of the original user request) in a negative manner to see if the given solvent would participate in an unwanted chemical reaction if used in your process.
* Some extra .sof files have been added. Two sets of green solvents (from U York GCCE and two variants of lists from Prof Aubry’s group at Lille). A list of published Dowanol values has been included when it was pointed out that the Y-MB estimates (for complicated reasons) differ from Dow’s published values.

V5.0.05 29 October 2016

* A few obscure bugs were fixed in the Optimizer and the loading/conversion of .hsd files was improved.
* FindMols FG search had several bugs. These have been fixed.
* The Exclude option in FindMols now applies to FG search
* A bug in Open with Merge was fixed

V5.0.04 1 August 2016

* Historically there had been a need for separate Max values for δP and δH in the 3D view. 5.0.03 removed the option for non-spherical views so the separate Max values are redundant. Thus a single P/H Max option is now provided.
* If the Max and D-Min values or the Wire Frame option were changed the view was only refreshed via recalculation. Now the refresh is immediate.
* A new Miscibility graph has been added to the Miscibility tab in DIY. This implements an algorithm provided by Dr Robert Lacombe (co-developer of Sanchez-Lacombe solubility theory) and calculates the temperature at which miscibility occurs for any given volume fraction, rather than the Yes/No values of the simpler algorithm.
* When a Sphere is calculated the HSP and Radius are automatically added to the Target in the Optimizer. The How To has always said that this is what happened but it had not been implemented.
* Some minor bugs have been fixed including some issues with solvent names in the Solvent Optimizer.

V5.0.03 26 November 2015

* This is a major new release. Because it is compiled for 64x processors it will not work on old XP machines. It will install into c:\Program Files rather than c:\Program Files (x86) so your older version will not be affected and you can create your own shortcut link to the previous version if you wish. This means that you can continue to use the old calculations if you require them for consistency, patent purposes etc.
* It uses the newer DotNet Framework 4.6 rather than the old 4.0 so many of you will need to download and install the new Framework. Microsoft now make this especially easy and reliable.
* The change to 64x and Framework 4.6 is to re-align with Microsoft’s own longer term support for DotNet looking forward to the ongoing changes within the Windows 10 paradigm. In particular, the problems of Hi-Res displays is under better control with the new environment. A number of HSPiP users of previous versions have ended up with programs looking too small or not fitting onto the screen and have had to adjust screen settings to accommodate HSPiP. The new version is not guaranteed to be perfect because the “screen resolution” issue is an ongoing problem for all software providers. But it is certainly better when tested on a large variety of screens, including multi-monitor systems (though there can be a disconcerting shift as HSPiP moves from a small laptop screen onto a large external monitor). If you run HSPiP on a second monitor, then sub-forms now open in that second monitor.
* Win 7 does not have such “smart” automatic sizing so the program will not work at some resolutions. Older video projectors and older monitors may also have problems. It is simply not possible to have a good modern user experience and to work perfectly at all old-style resolutions.
* The shift to the new “screen resolution aware” layouts has required moving the positions of many of the standard buttons and check boxes. Whilst doing this we decided to bring in an improved “cleaner” look-and-feel to icons and buttons. Hopefully users will find the new layout to be rather neater and more logical.
* For technical reasons it is no longer possible to manually resize or expand the main HSPiP form.
* Many forms had a red X for closing the form rather than the consistent X at the top right of all Windows forms. Now all forms close using the consistent Windows X.
* The Y-MB engine has been significantly updated so predicted values of HSP and all other factors will change. In general these changes will be for the better but there are always some downsides so be alert and, if necessary, use the previous version if you require consistency.
* The outputs from Y-MB predictions imposed a new column structure onto the main data form. So at first it will look unfamiliar. To make it easier to know where you are, when you scroll horizontally through the columns, the Number and Name columns remain fixed, just like fixed columns in Excel.
* With many more columns of data available, the default option is to show just the selected few. The All option lets you see all the columns.
* Some previous parameter predictions such as thermal expansion coefficients, MIR and logKsoil are no longer provided. These were always unsatisfactory because they lacked a good experimental dataset. The expansion coefficients are replaced internally by a totally new algorithm for temperature-dependent effects. Those needing logKsoil estimates should build their own QSAR (a starting dataset is provided).
* The little-used “Squared” option in the Solvent Optimizer has been removed as there was no feedback to say that this (at one time) experimental option was of use. The Spherical option in the main form has also been removed because non-spherical plots have not been popular.
* There are fewer abbreviations on buttons. For example, the old O, P and δ buttons are now replaced with Optimizer, Polymer and DIY buttons and the old WF is now Wire Frame and the old X is now 3D Reset.
* When the Full Dataset option is selected in Y-MB you can now choose the No Header option so only the data and not Header + Data are put onto the Clipboard.
* Previous versions allowed a MyDB with your own values. This has become impossible to support given the large new set of functional parameters provided by Y-MB, so the functionality has been removed.
* The VLE (Vapour Liquid Equilibrium) calculations in the Azeotropes/VP portion of DIY have been totally re-written by Dr Yamamoto and are much more reliable and predictive. This is a major upgrade to HSPiP. One of the reasons for the new Y-MB with its parameter set was to make the VLE calculations more reliable. The VLE data can be exported for comparison to experimental values and/or experimental data can be imported for comparison.
* One key use of VLE is in the search for azeotrope solvent blends to meet demanding applications such as vapour degreasing, energy recovery systems and so forth. A function exists to load a set of solvents with their SMILES strings and calculate the azeotrope (existence then T and %) for all solvent pairs.
* A whole new QSAR (Quantitative Structure Activity Relationship) capability has been added within the HSPiP environment.
* The full power of the QSAR capability is discussed in a separate document. Many examples (including a logKsoil QSAR) are included, providing a crash course is QSARs – with examples of good and bad fits to show the harsh reality of QSAR work.
* The Diffusion form had a complicated way of estimating diffusion coefficients and surface concentrations. This has never been popular and the complexities of real polymers meant that the estimates were often unsatisfactory. These inputs cluttered up the interface. To reflect the new “cleaner” interface, these options have been removed and the form re-configured to be more user friendly.
* For those who like the sort of server-based workflow typical of Accelrys (Dassault Biovia) Pipeline Pilot there is now an option to buy a CLI (Command Line Interface) version of HSPiP. Pricing and compatibility information for the CLI is available on request. Because the CLI version always uses exactly the same routines as the stand-alone version, the results are always comparable.
* The full capability of the CLI version is discussed in a separate document.
* Some little-used functionalities that are no longer compatible with the new Y-MB engine have been removed: Analogs; automatic groups for SP; Functional Distance in the HSE part of DIY.
* The new Y-MB engine estimates enthalpy of fusion. The estimate is now included in the Solubility form – previously it was a user-defined entry only.
* When the Double Sphere is calculated via the GA option the values of both spheres are placed on the Clipboard for pasting into Word or Excel.
* When Names or Numbers options are selected for the Sphere the size of the text can now be varied from V.Small to V.Large via Medium which is equivalent to the previous versions.
* In FindMols the option exists to exclude elements (halogens, nitrogen, silicon etc.) from the suggested list of molecules.
* In the SO, copying solvents from the table no longer includes the greyed-out lines nor are they included in PW etc.
* Some minor changes to the 3D graphics in Y-MB have reduced some glitches in the main form.
* When the Solv.Check button is clicked within Polymers, there is now colour-coding of the solvents with respect to the various polymers: Red if outside all, Blue open if inside one polymer sphere, Blue solid if inside all spheres.
* Thanks to a fruitful partnership with Dr Eric Brendlé of Adscientis the IGC capability has been improved in two ways. First, it is now possible to load a simple text file of Vg values and their Chi values are automatically estimated. Second, those calculated Chi values no longer use the MVol of the stationary phase or, to put it another way, the MVol of the stationary phase is assumed to be large so the MVol\_Solvent/MVol\_Stationary\_Phase correction is essentially zero. This means that the absolute Chi values (for those who are interested) are not valid, but it also means that the HSP estimate no longer has to remove this Chi correction. Unfortunately previous versions did not account for this so HSP estimates of low MVol excipients were problematical. However, it is worth pointing out that far bigger errors have been caused by the effects of the supposedly neutral support phase. The Adscientis work showed that many typical supports have a large effect that often creates nonsensical HSP values, so the technique is only valid when truly near-neutral supports are used.
* We are grateful to the Toxics Use Reduction Institute (TURI) at the University of Massachusetts Lowell, for providing us with a large dataset of “Potentially safer chemicals” which we have jointly turned into .hsd and .sof files which you may wish to use in your own explorations for substituting toxic chemicals with safer one.
* The Help file now includes a list of the most used keyboard shortcuts.

v4.1.07

* This is a minor release with some small bug fixes, plus the addition of a LogS column in the Solvent Optimzer. The Default Solvent Optimizer.sof comes with reasonable values for all the solvents, S is in g/100ml.

v4.1.06

* This is a minor release with some small bug fixes

v4.1.05

* The PW and TW functions in the SO have extra output including the HSP of the mix and, for PW, the built-in miscibility check (without Donor/Acceptor) is applied.
* The calculation of Limits in SO has been tweaked to avoid the possibility of a slight excess for those with tight regulatory requirements.
* Although the eBook spoke about aroma chemicals no dataset was included in the install. The aroma dataset is now included in the install in both .hsd and .sof format. All the values are predicted from Y-MB and have not been confirmed against experimental data.
* A “Good-Bad only” plotting option was included to show all the Good solvents as solid blue spheres and all the Bad ones as solid red cubes, irrespective of whether they are in or out.
* The code for Polymer SMILES has been further tweaked – this remains experimental!
* A new Polymer Miscibility option is included in the Polymers section of DIY. This invokes the Donor/Acceptor concept inspired by Coleman-Painter theory which is described in the updated eBook. This work is very much experimental and user feedback will be much appreciated.
* The calculation of the interpenetration depth in the Adhesives form also includes the Donor/Acceptor option.
* Because the above work indicated that the Beerbower formula for Donor/Acceptor was the best option, Beerbower is now used in the D/A fit option for Sphere.
* To complement the book by Dr John Durkee, Cleaning with Solvents: Science and Technology, an extensive list of relevant solvents has been provided as a Solvent Optimizer file: CleaningWSolvents.sof

v4.1.04

* HSPiP showed layout problems on some high-resolution screens. These have been fixed.
* A user of SO wanted an option to not automatically sort the solvents during an Optimization or a 1, 2, 3 operation. The option has been added. It helps, for example if you wish to keep the same solvent order when pasting data into Excel.
* The X clear button in DIY was not consistent across all the tabs. This has been fixed.

v4.1.03

* An FAQ chapter has been added to the eBook. This addresses key questions about the meaning of the Radius (and why we can’t calculate it), the quality of the Sphere fit, the limitations of Y-MB for large molecules, issues about charged molecules and why we can’t predict them and finally a discussion about the HSP values of water and methanol.
* The HSPiP Help file (a .rtf) is now included in the HSPiP Data folder for those who want to read it in Word etc.
* A “Limit” option has been added to Solvent Optimizer so that a given solvent cannot be used at a value greater than that limit. For example, in cosmetics there might be a regulatory limit of 50% on the use of propylene glycol so an optimised formulation with 63% would not be useful. In that case L50 would be placed in the Weight column to signify a Limit of 50%. Another solvent might have L20 to show it cannot be used above 20%
* Copy All Solvents in SO had some column problems. This has been fixed, along with a bug in the FindMols import into SO.
* A new Line option has been added to SO. Select 2 good solvents and any solvent close to the line between them is also going to be a good solvent. To be able to select 2 solvents via the standard Ctrl-Click, the disabling of a solvent is now done via Ctrl-Shift Click, not Ctrl-Click
* It was sometimes a bit tedious to de-select a particular solvent blend so a Clear button has been provided (with a check to make sure you really want to un-check the solvents).
* Many users of the SO were frustrated to find that a suggested solvent pair was immiscible. A new Miscibility estimator has been added to Y-MB. Reliable miscibility prediction is surprisingly hard and defeats most approaches. The estimator is from a correlation of the data from 900+ solvent pairs and is ~ 90% accurate. The more feedback we get from users on failed predictions, the better we can upgrade the algorithms.
* As a shortcut for miscibility checking, the SO has a MChk button which does a miscibility check (using the same algorithm) on all selected solvent pairs.
* A new improved estimator of Antoine Coefficients has been added as part of the upgrade to higher quality calculations of vapour effects. In Y-MB the Antoines are now shown in their own boxes rather than as the “Other” text.
* The VLE calculations have been significantly improved. The previous Margules approach has been abandoned for a more sophisticated Wilson approach. To the user the interface has not changed (other than changing the names of the key parameters) but the results are generally much better, including the Azeotrope predictions.
* Within the improved Azeotrope/VLE it is possible to specify a Wt% Solvent1 within a blend and for the BPt of that solvent blend to be calculated for you.
* Using Wilson parameters, the Solubility calculations are somewhat improved over the previous Margules version.
* In DIY the FlashPt and MCI were not automatically added to the Clipboard after a calculation. That has been fixed.
* In SO there was a time-limit set on the 3 optimization. Now there is simply a warning that it might take a long time, and you can choose to Cancel if you wish.
* Column headers have been added to the TW output on the Clipboard
* In DIY Polymers it is possible to do a Batch Break (File Convert) of a set of Polymer SMILES in a text file (just like the File Convert in Y-MB). The output is placed on the Clipboard for pasting into Excel and also saved as a .pds file for loading into the Polymers table.
* The Surfactants calculations are now on their own tab instead of the Numbers tab.
* The EACN estimator in DIY has been updated with the latest extensive dataset from Prof Aubry’s group at U. Lille. It is now becoming a powerful tool for estimating these key parameters for HLD-NAC surfactant theory.
* Because so many users have found that methanol is anomalous we have decided to include an alternative set of values for “clustered” methanol. There is no doubt that methanol can form such clusters, and across a number of datasets the values we have provided do a good job of defining the opposite extreme of methanol (in the presence of long-chain carboxylic acids). It is up to you (as it is with our alternatives for water and 1,4-Dioxane) to decide which values to use.
* A few polymers were revised based on careful reassessment of datasets: PVP, PVC, PVdC, PLA, Cholesterol. A bug in the Save routine lost the extra data such as Rating. That has been fixed.
* In the Polymer Theory section a Flory-Rehner option has been added that describes the swelling of cross-linked polymers.
* In Y-MB a new button 🡪SO has been added. Clicking this puts all relevant data into a new line in the Solvent Optimizer, with the temporary name “From Y-MB”.
* In Y-MB the 3D importing for .xyz format has been refined and the simple Mopac Cartesian format (.mop) can also be read in. In both cases, bonds and bond orders (single, double, aromatic…) are implicit and have to be estimated via some complex routines that cannot be 100% reliable for complicated molecules.
* The Diffusion model now has a WLF (Williams-Landel-Ferry) option which is good for describing the huge changes in diffusion coefficient at temperatures above the Tg. If you know a D value at one temperature you can readily calculate it at another temperature, often finding surprisingly large differences. The WLF model is an alternative to the Arhenius-type temperature effects typically found in conventional polymers such as PE, PP or PET. Interestingly, both models are used in the food industry. WLF describes diffusion through, say, glassy sugars and Arhenius describes diffusion through typical packaging films.
* The Diffusion model had problems with very long time-scales under some circumstances. It is now more able to deal with complex, long-timescale issues.
* An expert user found that predictions of lactone structures from Y-MB were unsatisfactory. As we always welcome experimental data the lactone functionality was re-parameterised to better reflect reality.
* On the main form and in the SO when data are placed onto the Clipboard when the Temperature option is used, the calculated value is used, not the “differential” value shown in the form. So if a δD shows 18 -0.4, on the Clipboard it will be 17.6.
* A NADES dataset has been added in SO format. These are Natural Deep Eutectic Solvents which are of great interest in many areas. A discussion about NADES has been added (for convenience) to the Ionic Liquids chapter.
* The Y-Predict Power Tool has been completely updated. Using entirely new algorithms based on deep insights into thermal expansion, critical temperatures etc. it is now possible to predict many temperature-dependent properties. For example, the surface tension of chemicals from 298 to 408K can be calculated. This calculation has been made possible by a dataset of surface tensions of molecules such as tetralin at 400°K!
* For user convenience, the latest .msi installer is available from all 3 sites, Hansen-Solubility.com, Pirika.com, StevenAbbott.co.uk.

v4.0.08

* A new DPC menu option has been added on the main form. If you get data onto the Clipboard from anywhere in the program and your local standard is a Comma instead of a Point as the Decimal Separator, clicking DPC will convert the Decimal Points to Commas on the Clipboard so you can paste into, say, Excel and get numeric values.

v4.0.07

* In some circumstances the SMILES in the Clipboard data in FindMols lost their brackets. This has been fixed
* The diffusion coefficient settings were not correctly set on loading a .dif file into the modeller. This has been fixed
* MolFile import failed on V3000 (“extended”) files. That has been fixed

v4.0.05

* The Convert option in SO had been made more sophisticated for some users, but this introduced a bug for some files. This has been fixed
* Some minor revisions/clarifications to the Help file and to the eBook have been made.

v4.0.04

* A bug had crept into the new FindMols functionality affecting ranges starting at 0. – this was fixed

v4.0.03

* The new version 3.5 Y-MB engine gives higher-quality estimates of HSP values and key parameters
* The HSPiP Power Tools series is launched. These allow you to do extra things with your HSP data files, including sharing them with co-workers who can view them even if they do not have HSPiP installed. The Power Tools are app based so run on all standard platforms, PC, Mac, iPad, Android… *Please note that everything about each Power Tool is local to your machine – no internet access is used.*
* The main Sphere form can now be made full-screen, a popular request over the years. The aesthetics (the main reason for not doing it) are not perfect, but the extra viewing area of the 3D view and the tables might be useful for many users.
* The MVC (Molar Volume Correction) option now shows the solvents with their relative MVols (exaggerated for clarity) to make it easier to interpret wrong out or wrong in solvents in terms of MVol.
* The DIY Polymer tab now lets you estimate the HSP of an arbitrary co-polymer blend from the monomers in the table. The Polymer SMILES algorithm for n-mers has also been improved
* The Numbers tab now estimates from SMILES input the EACN (Equivalent Alkane Carbon Number) of oils, as used in surfactant HLD-NAC theory
* The FindMols and Solvent Optimizer now include a Donor/Acceptor option
* The Solvent Optimizer has a “Best +” option which finds solvent blends that are near the automatic optimums obtained by the 1 or 2 buttons. This lets you find alternative blends (within a specified extra distance) which may have failed to be optimal by only a small amount.
* A large user requested extra columns in the Solvent Optimizer to contain extra data: BPt, FlashPt, VP@25, MPt and MWt. These extra columns appear when the XC option is selected. The DefaultSolventOptimizer.sof file comes with these extra columns filled with data (to the best of our ability) but no attempt is made to fill these columns retrospectively – users who need them should create their own lists from the Default or make a new list – relevant data are automatically transferred from the Master Database using the Right-Click method.
* FindMols can create a .hsd file. If this was imported into the Solvent Optimizer the RER and Antoine values for molecules in the 10K dataset were missing. This has been fixed and the XC values are also imported. This is necessarily slower than before and only applies to FindMolsOutput.hsd. It is not realistic to expect RER and other data to be found from the 10K database if a hand-crafted .hsd file is used.
* If your test material has X% solvent in it when you do the Sphere test, you can now include the HSP of that solvent (which may itself be a blend) and its % in the test vial so that the actual HSP of the solvent blend in each test vial is used in the Sphere calculation. Read the Help file (search for DILUENT) to learn the trick for doing this.
* In Y-MB the “Check δTot” value was an historical remnant which should have been removed in earlier editions. It has now gone. The δTot value shown is the sum of the individual values, not an independently predicted value.
* There have been no changes to the HSP values in the master dataset. However, there has been one addition. An alternative value for 1,4-Dioxane has been added, representing the view that the low δP value of the original (matching the zero dipole moment) may not capture the essence of this solvent. It is up to you which version to use retrospectively or in the future. Of course the 10k dataset, based entirely on Y-MB values, has numerous changes because of the new Y-MB engine.

v3.1.26

* The % column in the SO has been renamed Vol% to make it unambiguous that HSPiP (and thermodynamics in general) use Vol% for mixtures.
* The ExpFit graph is now automatically hidden when appropriate
* When the Solvents button is clicked in Polymers, the optimal solvent intersection point is calculated and shown as an orange dot.
* A bug with the temperature option when swapping from IGC to the main form has been fixed

v3.1.25

* The Diffusion “Load” did not restore the surface concentrations – this has been fixed
* The Evaporation calculation of Antoine values did not place the correct values in the boxes – this has been fixed

v3.1.24

* The Distance calculator did not allow high δH values to be entered, this has been fixed
* In the Diffusion modeller h can now be input rather than just calculated from B. So if B is entered (as before) h is calculated but if h is entered, B is calculated
* The Diffusion modeller now allows saving and loading .dif diffusion setting files to make it easier to compare many different models

v3.1.23

* For the standard fit a new “Core” value is calculated which gives some idea of how sharp the fit is. If the width of the Core is small that means that even small deviations from the best fit give a large difference in the quality of the fit. If the width of the Core is large (sometimes just in one direction) then that shows that the fit is not very well defined.

V3.1.22

* A few minor interface bugs/inconsistencies were fixed

V3.1.21

* The default settings for Grid contained an immiscible pair. This has been changed.
* The Grid has been made somewhat easier to use – for example highlighting a row to delete is easier and Ctrl-D works within the Grid to allow values to be move around via Ctrl-P. The limit to 4 rows has been removed.
* An AutoGrid option has been added to create Grids automatically from the list of solvents in the Solvent Optimizer. This is currently experimental as it is proving difficult to identify a perfect algorithm.
* A Tw (Triplet-wise) option has been added to the Solvent Optimizer to find the best triplet matches to the current target. This works only on a selected list of solvents. The Pw mode now has the option to create a list from selected solvents only if more than 4 solvents are selected.
* The Master Database sometimes did not show a header. This has been fixed.
* A search in the Master Database made the Donor/Acceptor columns appear even when not selected. This has been fixed.
* The DIY Solubility form now has a Solubility Theory button which opens up a form showing the effects of MPt, Enthalpy of Fusion, Delta Heat Capacity and Enthalpy & Entropy of Mixing on the solubility curve of a crystalline molecule.
* A chapter on the Grid technique has been added to the eBook and the Solubility section has been expanded with an explanation of the extra terms.

V3.1.20

* A new Grid method has been added to generate solvent sets based on pairs of solvents. In principle this allows, say, 4 pairs of solvents to be used in combination as an alternative to 32 pure solvents for measuring HSP via the Sphere test. This is experimental, but the technique has been used successfully in some circumstances.
* A user pointed out that all the HPLC data files had become corrupted (just like the Gases.hsd) and these have been fixed.
* An FDA-approved method for estimating diffusion coefficients in some well-known polymers has been added to the Diffusion modeller.
* The “double-click trick” applied to very long lists such as EAFUS produced an error message. This has been fixed. Lists longer than EAFUS are not recommended as some molecules will not be plotted.
* Some minor changes to the Diffusion modeller have fixed the fact that some diffusions asymptoted to less than 100%, and the Excel outputs have had some extra default values added.

V3.1.19

* When the mouse is moved over the 3D plot, the solvent is shown. This is a much-asked-for improvement.
* A new chapter on Low Molecular-Mass Organic Gelators (LMOGs) has been added to the eBook
* At a user’s request a P button has been added to the Solvent Optimizer to open the Polymers form with polymers sorted according to the closeness to the Calculated values.
* The Diffusion modeller has been upgraded for Desorption mode – a “Loss” value (as opposed to a “Permeation” value for Absorption) is shown and the Loss data is available when the Data Capture button is clicked. Also an error in the “Year” timescale has been fixed.
* There has been a minor revision to the Donor/Acceptor algorithm that corrects for the cases where both materials are strong donors/acceptors, a rather rare case.
* When Activity Coeff. was selected in SO some numerical errors could appear at the end of the evaporation (values shown as NaN). This has been fixed.
* The Wet-Bulb calculation provided the “adiabatic” value uncorrected for the psychrometric ratio of the solvents. Because these ratios are known for only a few solvents, and because their calculation from first principles is complex, a ratio of 2 has been included in the calculation to give a more realistic value. From these calculations the “blush resistance at 80°F” values quoted in the literature are obtained.
* The Gases.hsd file had accidentally got corrupted during an earlier upgrade. The correct file is now included in the installation.

V3.1.18

* The Solvent Optimizer has a new button. 🡪V takes the current solvent mix and calculates the mix in the Vapour phase, replacing the % values with the vapour values and calculating the HSP of the vapour phase mix. This option was requested by a user.
* The search function in the Master Database is enhanced so that searching for, say, “hydroquinone” finds 1,4-Dihydroxybenzene (1,4-Benzenediol).
* On some PCs there were problems with the Camera picture of 3D images. This has been fixed
* A new “Exponential” fitting mode has been added for numerical data. This shows the quality of the fit via plots of experimental and calculated values.
* For ESC calculations where “Good” scores included 2 or more, the MVol corrected RED shown after the “/” (e.g. the 1.1 in 1.4/1.1) was incorrect. This error has been fixed.

V3.1.17

* When a Calculation is performed in the Solvent Optimizer, the calculated values are automatically added to the Clipboard and can therefore be Ctrl-P pasted into other parts of the program
* If the SSel (Show Selected) option was chosen and solvents shown from the Polymers form either the showing selected did not work or there was an error message. Both issues have been fixed
* It is now easier to select multiple solvents for the Right-Click transfer from the Master list to the Optimizer. Instead of having to select the whole line for each solvent, simply selecting one entry on each row will suffice
* The RER values in the Master database were supplied independently and values did not agree with those in the Solvent Optimizer. For many of the common solvents, the values in the Master database now match those in the Optimizer
* The Everything Added to Food in the United States (EAFUS) list has been added to the Examples folder in both .hsd and .sof format. This will be of great help to those who want to use ingredients that have such formal recognition – though you cannot necessarily conclude that being in EAFUS guarantees safety.

V3.1.16

* The RED values calculated when clicking the Solvents button in the Polymer form had a small “temperature” error. This should not have had a big effect on the final results. The error has been fixed.
* Some small changes to the 3D graphics have slightly improved the quality
* After Install there is an option to run the new version directly after finishing Install

V3.1.15

* In the Optimizer the Squared option was not correctly used in the Evaporation calculations. For technical reasons this isn’t feasible so the Squared option is automatically disabled for Evaporation calculations so that the user knows that it is not being used.
* Screen capture failed to work on some newer laptops for unexplained reasons. A new capture methodology has been introduced to fix the problem.
* In the Polymer form the Polymers button sometimes gave an error message. This has been fixed
* A user requested an RER calculator option for solvent mixes. This has been done – the nBuAc=100s option needs to be selected because it does the calculation by comparing to nBuAc. However, the “100s” in that option was always referenced to 100% evaporation. The ASTM standard is referenced to 90% evaporation so that the new RER value isn’t skewed by some small amount of very slow solvent. If you have used this option before then the new numbers will be changed by ~10%.
* When solvents with predicted RER values were added from the Master data to Solvent Optimizer, the parentheses were brought in. These have been removed
* The ShowRED option in the Solvent Optimizer now shows the RED in the full table. When deselected the Distance is shown as before.

V3.1.14

* For GA calculations the Total solubility parameter was erroneously reported. This has been fixed.
* Some people had issues with v3.1.13 install. The causes were unclear, so this version is hopefully problem free.

V3.1.13

* If an empty .hsd or .ssd file is opened a message appears to explain the issue, rather than a general error message that appeared in previous versions.
* Some users want to optimize solvent blends to the Radius rather than the Target. A “RED fit” option has been added to make this possible.
* A revision to the chapter on diffusion on glove materials resolves a complex issue on surface resistance.
* For some complex MolFiles, creating the SMILES from which the Y-MB is calculated can take too long. A No SMILES option bypasses the SMILES generation and can significantly speed up the Y-MB process.

V3.1.12

* A bug was found that in some circumstances produced a Classic GA Sphere fit rather than the standard version. In most circumstances the results are very similar. However, both Force Fit and Minimum Sphere could be affected by this issue. This version ensures that GA calculations can never happen unless specifically requested.

V3.1.11

* From the first edition, the Target value in the Solvent Optimizer was automatically set according to the current selected value in the main form. This was a good idea at the time. But several users have asked that the Target values in SO be preserved so the Target is no longer automatically set. We apologise to anyone who preferred the previous version.
* When a Sphere has been calculated and an .hsd file is saved, the calculated values (in the Results box at the top right) are saved in the file and are shown when the file is re-loaded. This was a convenience requested by users in a large corporation who regularly send .hsd files to each other and wanted the others to see the precise results they had obtained.
* If you calculate the HSP of a solvent blend in the Solvent Optimizer its values can be transferred to the bottom of the Sphere solvent table by clicking the new S button. This allows you very easily to add solvent blends to your solubility table.
* If you have done a GA fit using Classic GA or Double Sphere then close the GA window, the program automatically does a fit using the standard methodology. This is to avoid confusion – you don’t see a double sphere or a GA fit when the GA window is not open.

V3.1.10

* When the Solvent Optimizer is called from the Polymers form, the polymer radius is automatically carried across
* A bug in the multi-Polymer “Solvents” command introduced with the SSel option has been fixed
* In Find Molecules it was never possible to find HSP values =0. This has been fixed.

V3.1.09

* The δTot Force Fit function was made a little more aggressive – to suit cases where moving the original fit exacts a large penalty.
* A new option SSel has been added to the main form so that the 2D and 3D plots show selected solvents in a distinctive colour and, if the Name option is chosen, show the name(s) only of the selected solvent(s). This is useful for identifying interesting features in your data.
* The “2nd surface resistance” algorithm in the diffusion modeller has been updated

V3.1.08

* In Find Molecules, extra ≤ options have been added for a wider choice of functional groups
* In the Solvent Optimizer the “Convert” importer checks the internal database. If there is an exact match of name or number then the RER and Antoine values are imported.
* In the Numbers section of DIY the “surfactant” section allows much greater versatility. You can now mix and match custom and pre-packaged heads and tails. This allows you, for example, to calculate HSP of your own hydrophobic tail with a long EO chain which is inefficient to calculate with Y-MB.

V3.1.07

* The SRC option was not working properly. This has been fixed
* The old algorithm for calculating the Ra of multiple polymers via the Polymer “Solvents” button was unsatisfactory. It now finds the maximum Ra of any polymer with respect to the solvent and reports that – this lets you see the worst-case possibility.

V3.1.06

* Sphere and Cylinder options were added to the Diffusion modeller
* A bug in the Optimizer “Convert” importer was fixed

V3.1.05

* A new option was added to the Solvent Optimizer that tries to optimize a (small) range of solvents to match either the overall evaporation curve or the shape of the Ra/RED curve.
* In obscure circumstances, the GA option would not recognise “in” and “out” solvents correctly. This has been fixed.
* Some errors in InChIKeys crept into the large Master database. These have been fixed. However, InChIs created in Y-MB for aromatic molecules that use lower case (e.g. c1ccccc1 for Benzene) are incorrect – they come out as the saturated version (cyclohexane in this example). Aromatics shown in upper case (C1=CC=CC=C1) work correctly. This issue only affects InChIs, all other properties work irrespective of the aromatic nomenclature. Fixing this issue will be a challenge.
* The δD for 1-decene has been revised down slightly as has the δH for 1-octanol.

V3.1.04

Minor bug fixes and tweaks to eBook text.

V3.1.03

This is a major update with many features.

First, we have moved to the DotNet Framework 4. There are many reasons for this, not least the fact that the download of FW4 is *much* smaller than previous Frameworks.

* The database has been tidied up and in the master database for the non-10,000 chemicals predicted values are shown in brackets to distinguish them from real values – something frequently requested but impossible till the new methodology of this release. The MIR data are based on the more recently published data and predictive algorithms have been updated for many of the parameters.
* A new, more flexible file system is used to replace the .ssd file. Of course .ssd files are still respected, but the new .hsd (Hansen Solubility Data) file is now the default.
* We have modified a very few HSP values in the database. The important solvent DBE has been slightly modified based on new experimental data on Dimethyl Succinate from an HSPiP user. Other changes are to: N-Acetylmorpholine; N-Ethyl Formamide; Propionamide; 1,2,3-Trichloro Propene; Ethylene Carbonate. All such changes were made after considerable cross-checking. The “green” solvents methyl and ethyl succinates/glutarates/adipates have been added along with glycerol carbonates and Dimethyl Isosorbide.
* On some XP machines Ctrl-Shift click does not work to transfer solvents from the Master Dataset to the Solvent Optimizer. Right Click has been added as an alternative method. In addition, the RER from the Master list is now transferred instead of the calculated RER from the Antoine Constants.
* For those who wish to copy a Full line of data from the Master database, a Ctrl-F option has been added.
* In Solvent Optimizer the **Pw** button does a PairWise calculation of all solvent combinations and places the (sorted) results onto the Clipboard for pasting into Excel. This is useful for an exhaustive list of all solvent blends that are, for example, inside the polymer sphere.
* For users of video projectors (or NetBooks) with a size too small for the program, a Microsoft AutoScroll kicks in and lets you scroll to find missing bits of the various forms.
* A Clear option has been added to the Polymers form – this resets everything to the original view.
* You can now load/save your own polymer data sets, with the file format .pds. This replaces the olds system with a single Polymers.dat.
* A **WF** option has been added to allow a WireFrame view of the Sphere. This is particularly useful for viewing multiple polymers from the Polymers form using the Solvents button.
* In FindMols the BPt column was filled with the MVol values during the functional group search. This has been fixed. Also an option to *not* limit searches to 200 molecules has been added at a user’s request.
* Some fits with insufficient data can produce high δD values, beyond the range of and δD values used in the tests. A warning is placed at the top of the fitted values: “Possible δD bad fit”.
* Some excellent polymers were given wrong overlap values in the double-click method on the Polymers form. This has been fixed.
* For VLE calculations, if the molecule is found in the database then the database values are used instead of predicted ones.
* InChIKeys are added to the database and can be searched in the same manner as CAS, Formula etc.
* There are new Advanced Sphere fitting techniques: Double and Data. These allow the advanced user to explore alternatives to the standard single Sphere. The old “GA” option now opens up the Advanced fitting form where you can use the classic GA as well as the two new options. There is a setting for accuracy v speed and you can input initial guesses which can sometimes help send the GA fit into the right part of a complex fitting space.
* If the user wants their own dataset to override the master dataset then by placing a valid MyMasterDataSet.hsd file in the HSPiPData folder their own data gets loaded instead. Such a dataset can be created in many way, though the DIY File Convert method may be the one most frequently used.
* After a Y-MB calculation the user can choose to have the full data or just the HSP data put onto the Clipboard. In either case the HSP can be Ctrl-P’d into any of the standard inputs as per normal.
* Most forms now have an option to print the relevant table. There are no print options with this functionality. Users who want fancier formatting can use the Copy Table options to place the data into a program (such as Excel) with many more print options.
* Data from an HSPiP user has caused us to significantly revise the HSP values for sodium lauryl sulphate (and similar surfactants) and for the sodium sulphate head group.
* The Solubility estimator now allows manual override of HSP and MVol data – this allows, for example, solubility calculations for solvent mixtures if you know the HSP of the mixture. The Yalkowsky approximation has been improved and entropic effects can no-longer over-ride the Ideal solubility.
* When the Solubility Graph is shown in the Optimizer, the Relative Solubilities shown in the graph appear in the Distance column, which is renamed to Rel.Sol. The Excel capture also captures the Relative Solubilities rather than the Distance.
* Optimizer parameters are included in the Clipboard transfer to Excel to give a permanent record of the parameters used. A further option allows the user to Load/Save their parameter settings within a .sof file. It’s an option because sometimes you don’t want to override your current settings if you load a different .sof file.
* In the Optimizer you can now graph how the Ra changes during evaporation. You can also show the RED instead of Ra within the table and the graph, using the Radius in the Optimizer form. You can also show (where appropriate) the previous Total and Ra or RED graph so you can see how things change when you alter parameters.
* In the Optimizer there is an option to plot the Web-bulb temperature during the evaporation for those who have a serious interest in the issues of blushing during drying.
* The GCRI form allows you to use manual BPt inputs instead of the values estimated from the SMILES input.

V3.0.38 Resolution of Evaporation issues. Stable evaporation code. Sphere Radius Check for identifying “holes” in Sphere fit. Autocheck for update of old data sets to latest database values. Merge of two .ssd files with autoalert of different values

V3.0.30-37 Debates in user community about correct Evaporation model. Different version gave different comments for and against. Gradual evolution of revised algorithm. Addition of InChI input/output.

V3.0.20-29 Small additions to user interface, minor changes to database

V3.0.03-19 Response to release version issues, requests, bugs. Addition of “bad solvent only” option for the Solvent Optimizer.

V3.0.02 Release of HSPiP 3rd Edition. Many improvements, described to user community, from 2nd Edition

V2 First release of Y-MB automated method. Major update of database after extensive checking/revision. Many improvements from feedback of user community.

V1 1st Edition. Implementation of all the basic HSP functionality from Hansen book. Manual methods for HSP estimation.