Yasuda-Shedlovsky Result

Sample name:	**CS000092**	Experiment start time:	**25/08/2011 15:56:35**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25014_CS000092_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.02	±0.07	24.35	-1533.1340	0.9736	0.199 M	25.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25014 Points 103 to 153	20.37 %	Up	UV-metric pKa	77.3	44.9 M	0.205 M	25.6°C	☑	2.89
11H-25014 Points 52 to 102	27.19 %	Up	UV-metric pKa	77.0	41.3 M	0.202 M	25.4°C	☑	2.79
11H-25014 Points 3 to 51	36.63 %	Up	UV-metric pKa	76.0	36.3 M	0.191 M	26.2°C	☑	2.63

Graphs

Sample name:	**CS000092**	Experiment start time:	**25/08/2011 15:56:35**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25014_CS000092_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25014 Points 3 to 51 Quality: Good

Graphs

Sample name:	**CS000092**	Experiment start time:	**25/08/2011 15:56:35**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25014_CS000092_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25014 Points 52 to 102 Quality: Good

Graphs

Sample name:	**CS000092**	Experiment start time:	**25/08/2011 15:56:35**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25014_CS000092_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25014 Points 103 to 153 Quality: Good

Graphs

Sample name:	**CS000092**	Experiment start time:	**25/08/2011 15:56:35**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25014_CS000092_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000092		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	345.40		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r