Yasuda-Shedlovsky Result

Sample name:	**cs000105**	Experiment start time:	**25/08/2011 14:46:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25011_cs000105_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.89	±0.09	26.90	-1666.7147	0.9700	0.195 M	25.5°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25011 Points 98 to 147	21.43 %	Up	UV-metric pKa	77.4	44.3 M	0.202 M	25.3°C	☑	3.75
11H-25011 Points 49 to 97	28.81 %	Up	UV-metric pKa	77.0	40.5 M	0.196 M	25.1°C	☑	3.61
11H-25011 Points 3 to 48	38.43 %	Up	UV-metric pKa	75.8	35.3 M	0.189 M	26.1°C	☑	3.39

Graphs

Sample name:	**cs000105**	Experiment start time:	**25/08/2011 14:46:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25011_cs000105_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25011 Points 3 to 48 Quality: Good

Graphs

Sample name:	**cs000105**	Experiment start time:	**25/08/2011 14:46:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25011_cs000105_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25011 Points 49 to 97 Quality: Good

Graphs

Sample name:	**cs000105**	Experiment start time:	**25/08/2011 14:46:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25011_cs000105_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25011 Points 98 to 147 Quality: Good

Graphs

Sample name:	**cs000105**	Experiment start time:	**25/08/2011 14:46:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25011_cs000105_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000105		
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	290.39		
Individual pKa ionic environments	No		
Number of pKas	1	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
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