Yasuda-Shedlovsky Result

Sample name:	**CS000034**	Experiment start time:	**29/08/2011 10:41:22**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29006_CS000034_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.73	±0.07	-13.92	1510.2700	0.9684	0.203 M	26.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-29006 Points 105 to 156	19.19 %	Up	UV-metric pKa	76.8	45.5 M	0.209 M	27.0°C	☑	4.06
11H-29006 Points 53 to 104	25.96 %	Up	UV-metric pKa	76.7	41.9 M	0.206 M	26.5°C	☑	4.18
11H-29006 Points 3 to 52	35.21 %	Up	UV-metric pKa	75.9	37.0 M	0.196 M	26.8°C	☑	4.41

Graphs

Sample name:	**CS000034**	Experiment start time:	**29/08/2011 10:41:22**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29006_CS000034_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-29006 Points 3 to 52

Graphs

Sample name:	**CS000034**	Experiment start time:	**29/08/2011 10:41:22**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29006_CS000034_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-29006 Points 53 to 104

Graphs

Sample name:	**CS000034**	Experiment start time:	**29/08/2011 10:41:22**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29006_CS000034_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-29006 Points 105 to 156

Graphs

Sample name:	**CS000034**	Experiment start time:	**29/08/2011 10:41:22**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29006_CS000034_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000034		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	436.92		
Individual pKa ionic environments	No		
Number of pKas	1	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r