Yasuda-Shedlovsky Result

Sample name:	**CS000034**	Experiment start time:	**01/09/2011 11:30:36**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01010_CS000034_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.80	±0.09	-9.55	1176.7895	0.9189	0.201 M	26.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-01010 Points 108 to 154	19.90 %	Up	UV-metric pKa	76.9	45.1 M	0.206 M	26.8°C	☑	4.07
11I-01010 Points 55 to 107	26.36 %	Up	UV-metric pKa	76.8	41.7 M	0.203 M	26.1°C	☑	4.18
11I-01010 Points 3 to 54	35.40 %	Up	UV-metric pKa	75.9	36.9 M	0.193 M	26.9°C	☑	4.39

Graphs

Sample name:	**CS000034**	Experiment start time:	**01/09/2011 11:30:36**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01010_CS000034_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01010 Points 3 to 54

Graphs

Sample name:	**CS000034**	Experiment start time:	**01/09/2011 11:30:36**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01010_CS000034_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01010 Points 55 to 107

Graphs

Sample name:	**CS000034**	Experiment start time:	**01/09/2011 11:30:36**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01010_CS000034_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01010 Points 108 to 154

Graphs

Sample name:	**CS000034**	Experiment start time:	**01/09/2011 11:30:36**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01010_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	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	436.92		
Individual pKa ionic environments	No		
Number of pKas	1	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r