Yasuda-Shedlovsky Result

Sample name:	**CS000110**	Experiment start time:	**25/08/2011 18:43:00**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25021_CS000110_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	8.14	±0.05	-8.47	1427.9068	0.9863	0.209 M	27.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25021 Points 104 to 154	20.87 %	Up	UV-metric pKa	76.7	44.6 M	0.211 M	27.3°C	☑	8.49
11H-25021 Points 53 to 103	27.01 %	Up	UV-metric pKa	76.6	41.4 M	0.211 M	26.7°C	☑	8.59
11H-25021 Points 3 to 52	37.07 %	Up	UV-metric pKa	75.7	36.0 M	0.204 M	26.9°C	☑	8.84

Graphs

Sample name:	**CS000110**	Experiment start time:	**25/08/2011 18:43:00**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25021_CS000110_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25021 Points 3 to 52

Graphs

Sample name:	**CS000110**	Experiment start time:	**25/08/2011 18:43:00**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25021_CS000110_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25021 Points 53 to 103

Graphs

Sample name:	**CS000110**	Experiment start time:	**25/08/2011 18:43:00**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25021_CS000110_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25021 Points 104 to 154

Graphs

Sample name:	**CS000110**	Experiment start time:	**25/08/2011 18:43:00**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25021_CS000110_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000110		
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	432.50		
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