Yasuda-Shedlovsky Result

Sample name:	**CS000093**	Experiment start time:	**29/08/2011 12:19:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29010_CS000093_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.65	±0.00	4.84	198.3433	0.9987	0.204 M	27.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-29010 Points 105 to 156	19.35 %	Up	UV-metric pKa	76.5	45.4 M	0.210 M	28.0°C	☑	5.77
11H-29010 Points 53 to 104	26.22 %	Up	UV-metric pKa	76.3	41.8 M	0.207 M	27.4°C	☑	5.81
11H-29010 Points 3 to 52	35.77 %	Up	UV-metric pKa	75.5	36.7 M	0.196 M	27.8°C	☑	5.90

Graphs

Sample name:	**CS000093**	Experiment start time:	**29/08/2011 12:19:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29010_CS000093_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-29010 Points 3 to 52

Graphs

Sample name:	**CS000093**	Experiment start time:	**29/08/2011 12:19:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29010_CS000093_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-29010 Points 53 to 104

Graphs

Sample name:	**CS000093**	Experiment start time:	**29/08/2011 12:19:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29010_CS000093_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-29010 Points 105 to 156

Graphs

Sample name:	**CS000093**	Experiment start time:	**29/08/2011 12:19:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29010_CS000093_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000093		
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	423.28		
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