Yasuda-Shedlovsky Result

Sample name:	**CS000093**	Experiment start time:	**01/09/2011 12:18:05**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01012_CS000093_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.66	±0.00	5.60	139.9273	0.9970	0.202 M	26.9°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-01012 Points 107 to 155	19.81 %	Up	UV-metric pKa	76.8	45.2 M	0.207 M	27.2°C	☑	5.77
11I-01012 Points 55 to 106	26.21 %	Up	UV-metric pKa	76.7	41.8 M	0.205 M	26.4°C	☑	5.81
11I-01012 Points 3 to 54	35.10 %	Up	UV-metric pKa	75.8	37.1 M	0.196 M	27.1°C	☑	5.88

Graphs

Sample name:	**CS000093**	Experiment start time:	**01/09/2011 12:18:05**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01012_CS000093_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01012 Points 3 to 54

Graphs

Sample name:	**CS000093**	Experiment start time:	**01/09/2011 12:18:05**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01012_CS000093_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01012 Points 55 to 106

Graphs

Sample name:	**CS000093**	Experiment start time:	**01/09/2011 12:18:05**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01012_CS000093_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01012 Points 107 to 155

Graphs

Sample name:	**CS000093**	Experiment start time:	**01/09/2011 12:18:05**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01012_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	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	423.28		
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