Yasuda-Shedlovsky Result

Sample name:	**cs000096**	Experiment start time:	**26/08/2011 10:15:26**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26005_cs000096_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.63	±0.05	38.79	-2606.1202	0.9968	0.181 M	26.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-26005 Points 90 to 134	23.54 %	Up	UV-metric pKa	76.6	43.2 M	0.188 M	27.1°C	☑	3.14
11H-26005 Points 45 to 88	31.34 %	Up	UV-metric pKa	76.2	39.1 M	0.184 M	26.8°C	☑	3.00
11H-26005 Points 4 to 43	41.38 %	Up	UV-metric pKa	75.6	33.7 M	0.172 M	25.8°C	☑	2.82

Graphs

Sample name:	**cs000096**	Experiment start time:	**26/08/2011 10:15:26**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26005_cs000096_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-26005 Points 4 to 43

Graphs

Sample name:	**cs000096**	Experiment start time:	**26/08/2011 10:15:26**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26005_cs000096_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-26005 Points 45 to 88

Graphs

Sample name:	**cs000096**	Experiment start time:	**26/08/2011 10:15:26**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26005_cs000096_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-26005 Points 90 to 134

Graphs

Sample name:	**cs000096**	Experiment start time:	**26/08/2011 10:15:26**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26005_cs000096_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000096		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/08/2011 10:12:49	E:\T3 DATA\1108\11H-02007_CS00067_pH-metric psKa.t3r
Molecular weight	419.89		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	26/08/2011 10:12:49	E:\T3 DATA\1108\11H-02007_CS00067_pH-metric psKa.t3r
pKa 1	3.50		
logp (XH +)	-10.00	26/08/2011 10:12:49	E:\T3 DATA\1108\11H-02007_CS00067_pH-metric psKa.t3r
logP (neutral X)	-10.00		