Yasuda-Shedlovsky Result

Sample name:	**CS000109**	Experiment start time:	**26/08/2011 14:18:15**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26009_CS000109_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.36	±0.03	26.85	-1703.1930	0.9981	0.182 M	25.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-26009 Points 89 to 135	26.14 %	Up	UV-metric pKa	77.0	41.9 M	0.190 M	25.7°C	☑	3.11
11H-26009 Points 45 to 87	35.01 %	Up	UV-metric pKa	76.4	37.1 M	0.185 M	25.5°C	☑	2.97
11H-26009 Points 4 to 43	46.83 %	Up	UV-metric pKa	74.9	30.7 M	0.172 M	25.8°C	☑	2.63

Graphs

Sample name:	**CS000109**	Experiment start time:	**26/08/2011 14:18:15**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26009_CS000109_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-26009 Points 4 to 43

Graphs

Sample name:	**CS000109**	Experiment start time:	**26/08/2011 14:18:15**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26009_CS000109_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-26009 Points 45 to 87

Graphs

Sample name:	**CS000109**	Experiment start time:	**26/08/2011 14:18:15**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26009_CS000109_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-26009 Points 89 to 135

Graphs

Sample name:	**CS000109**	Experiment start time:	**26/08/2011 14:18:15**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26009_CS000109_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000109		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	481.96		
Individual pKa ionic environments	No		
Number of pKas	1	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r