Yasuda-Shedlovsky Result

Sample name:	**CS000110**	Experiment start time:	**26/08/2011 17:51:16**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26013_CS000110_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	8.13	±0.05	-6.09	1250.2195	0.9897	0.185 M	25.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-26013 Points 88 to 132	25.77 %	Up	UV-metric pKa	76.9	42.0 M	0.191 M	26.0°C	☑	8.53
11H-26013 Points 44 to 86	33.45 %	Up	UV-metric pKa	76.5	38.0 M	0.188 M	25.6°C	☑	8.69
11H-26013 Points 4 to 42	45.28 %	Up	UV-metric pKa	75.2	31.6 M	0.176 M	25.6°C	☑	9.02

Graphs

Sample name:	**CS000110**	Experiment start time:	**26/08/2011 17:51:16**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26013_CS000110_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-26013 Points 4 to 42

Graphs

Sample name:	**CS000110**	Experiment start time:	**26/08/2011 17:51:16**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26013_CS000110_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-26013 Points 44 to 86

Graphs

Sample name:	**CS000110**	Experiment start time:	**26/08/2011 17:51:16**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26013_CS000110_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-26013 Points 88 to 132

Graphs

Sample name: **CS000110**
Assay name: **UV-metric psKa**
Assay ID: **11H-26013**
Filename: **E:\T3 DATA\1108\11H-26013_CS000110_UV-metric psKa.t3r**

Experiment start time: **26/08/2011 17:51:16**
Analyst:
Instrument ID: **T311042**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000110	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
Sample by	Volume	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
Sample volume	0.0050 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
Molecular weight	432.50		
Individual pKa ionic environments	No		
Number of pKas	1	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
Sample is a	Base	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
pKa 1	4.00	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
logp (XH +)	-10.00	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r
logP (neutral X)	-10.00	26/08/2011 17:47:41	E:\T3 DATA\1108\11H-26010_CS000110_UV-metric psKa.t3r