Yasuda-Shedlovsky Result

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 11:54:49**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01011_CS000070_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	8.65	±0.06	-6.83	1342.1963	0.9712	0.203 M	26.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-01011 Points 106 to 156	19.84 %	Up	UV-metric pKa	76.8	45.1 M	0.208 M	27.0°C	☑	8.97
11I-01011 Points 54 to 105	26.33 %	Up	UV-metric pKa	76.7	41.7 M	0.204 M	26.5°C	☑	9.08
11I-01011 Points 3 to 53	35.20 %	Up	UV-metric pKa	75.9	37.0 M	0.197 M	26.8°C	☑	9.27

Graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 11:54:49**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01011_CS000070_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01011 Points 3 to 53

Graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 11:54:49**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01011_CS000070_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01011 Points 54 to 105

Graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 11:54:49**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01011_CS000070_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01011 Points 106 to 156

Graphs

Sample name:	**CS000070**	Experiment start time:	**01/09/2011 11:54:49**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01011_CS000070_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000070		
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	384.46		
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