Yasuda-Shedlovsky Result

Sample name:	**CS000070**	Experiment start time:	**29/08/2011 11:55:37**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29009_CS000070_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	8.54	±0.09	-12.27	1751.1428	0.9519	0.208 M	27.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-29009 Points 105 to 156	19.01 %	Up	UV-metric pKa	76.5	45.6 M	0.213 M	28.1°C	☑	8.93
11H-29009 Points 53 to 104	25.54 %	Up	UV-metric pKa	76.4	42.1 M	0.211 M	27.3°C	☑	9.04
11H-29009 Points 3 to 52	34.57 %	Up	UV-metric pKa	75.8	37.3 M	0.201 M	27.3°C	☑	9.25

Graphs

Sample name:	**CS000070**	Experiment start time:	**29/08/2011 11:55:37**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29009_CS000070_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-29009 Points 3 to 52

Graphs

Sample name:	**CS000070**	Experiment start time:	**29/08/2011 11:55:37**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29009_CS000070_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-29009 Points 53 to 104

Graphs

Sample name:	**CS000070**	Experiment start time:	**29/08/2011 11:55:37**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29009_CS000070_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-29009 Points 105 to 156

Graphs

Sample name:	**CS000070**	Experiment start time:	**29/08/2011 11:55:37**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29009_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	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	384.46		
Individual pKa ionic environments	No		
Number of pKas	1	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r