Yasuda-Shedlovsky Result

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 16:13:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09016_CS000080_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.19	±0.08	25.09	-1331.4139	0.9640	0.202 M	27.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-09016 Points 105 to 156	20.24 %	Up	UV-metric pKa	76.5	44.9 M	0.206 M	27.8°C	☑	6.06
11H-09016 Points 53 to 104	27.88 %	Up	UV-metric pKa	76.3	40.9 M	0.204 M	27.4°C	☑	5.98
11H-09016 Points 3 to 52	39.69 %	Up	UV-metric pKa	75.2	34.6 M	0.195 M	27.7°C	☑	5.84

Graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 16:13:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09016_CS000080_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-09016 Points 3 to 52 Quality: Good

Graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 16:13:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09016_CS000080_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-09016 Points 53 to 104 Quality: Good

Graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 16:13:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09016_CS000080_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-09016 Points 105 to 156 Quality: Good

Graphs

Sample name:	**CS000080**	Experiment start time:	**09/08/2011 16:13:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09016_CS000080_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000080		
Sample by	Volume		
Sample volume	0.0200 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r
Molecular weight	340.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r
pKa 1	4.00	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r
logp (XH +)	-10.00	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r
logP (neutral X)	-10.00	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r