Yasuda-Shedlovsky Result

Sample name:	**CS000032**	Experiment start time:	**09/08/2011 13:40:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.90	±0.10	32.09	-2054.3982	0.9688	0.203 M	27.4°C
Yasuda-Shedlovsky	9.31	±0.06	-0.73	915.2818	0.9435	0.203 M	27.4°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-09010 Points 105 to 157	19.99 %	Up	UV-metric pKa	76.6	45.1 M	0.206 M	27.7°C	☑	3.64
11H-09010 Points 53 to 104	27.39 %	Up	UV-metric pKa	76.4	41.2 M	0.205 M	27.2°C	☑	3.52
11H-09010 Points 3 to 52	38.69 %	Up	UV-metric pKa	75.4	35.1 M	0.196 M	27.4°C	☑	3.30

Graphs

Sample name:	**CS000032**	Experiment start time:	**09/08/2011 13:40:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-09010 Points 3 to 52 Quality: Good

Graphs

Sample name:	**CS000032**	Experiment start time:	**09/08/2011 13:40:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-09010 Points 53 to 104 Quality: Good

Graphs

Sample name:	**CS000032**	Experiment start time:	**09/08/2011 13:40:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-09010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-09010 Points 105 to 157 Quality: Good

Graphs

Sample name: **CS000032**
Assay name: **Fast UV psKa**
Assay ID: **11H-09010**
Filename: **E:\T3 DATA\1108\11H-09010_CS000032_Fast UV psKa.t3r**

Experiment start time: **09/08/2011 13:40:07**
Analyst:
Instrument ID: **T311042**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000032		
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	352.40		
Individual pKa ionic environments	No		
Number of pKas	2	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r
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
pKa 2	8.00	09/08/2011 12:20:47	E:\T3 DATA\1108\11H-04012_CS000100_pH-metric psKa.t3r
logP (XH2 2+)	-10.00	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