Yasuda-Shedlovsky Result

Sample name:	**CS000064**	Experiment start time:	**26/07/2011 14:28:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26016_CS000064_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.31	±0.02	18.51	-965.2140	0.9938	0.196 M	27.9°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-26016 Points 101 to 150	21.35 %	Up	UV-metric pKa	76.6	44.3 M	0.205 M	27.5°C	☑	4.27
11G-26016 Points 51 to 100	27.94 %	Up	UV-metric pKa	76.3	40.9 M	0.199 M	27.2°C	☑	4.24
11G-26016 Points 3 to 50	36.42 %	Up	UV-metric pKa	75.1	36.3 M	0.185 M	29.0°C	☑	4.09

Graphs

Sample name:	**CS000064**	Experiment start time:	**26/07/2011 14:28:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26016_CS000064_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11G-26016 Points 3 to 50

Graphs

Sample name:	**CS000064**	Experiment start time:	**26/07/2011 14:28:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26016_CS000064_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11G-26016 Points 51 to 100

Graphs

Sample name:	**CS000064**	Experiment start time:	**26/07/2011 14:28:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26016_CS000064_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11G-26016 Points 101 to 150

Graphs

Sample name:	**CS000064**	Experiment start time:	**26/07/2011 14:28:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26016_CS000064_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000064		
Sample by	Volume		
Sample volume	0.0200 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
Molecular weight	329.40		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
pKa 1	4.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logp (XH +)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logP (neutral X)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r