Yasuda-Shedlovsky Result

Sample name:	**CS000066**	Experiment start time:	**26/07/2011 14:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26017_CS000066_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.12	±0.05	22.00	-1326.2300	0.9850	0.197 M	28.2°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-26017 Points 101 to 150	21.51 %	Up	UV-metric pKa	76.5	44.3 M	0.205 M	27.7°C	☑	3.03
11G-26017 Points 51 to 100	28.16 %	Up	UV-metric pKa	76.1	40.8 M	0.198 M	27.7°C	☑	2.94
11G-26017 Points 3 to 50	36.60 %	Up	UV-metric pKa	75.0	36.2 M	0.188 M	29.1°C	☑	2.76

Graphs

Sample name:	**CS000066**	Experiment start time:	**26/07/2011 14:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26017_CS000066_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11G-26017 Points 3 to 50

Graphs

Sample name:	**CS000066**	Experiment start time:	**26/07/2011 14:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26017_CS000066_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11G-26017 Points 51 to 100

Graphs

Sample name:	**CS000066**	Experiment start time:	**26/07/2011 14:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26017_CS000066_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11G-26017 Points 101 to 150

Graphs

Sample name:	**CS000066**	Experiment start time:	**26/07/2011 14:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26017_CS000066_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000066		
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	381.50		
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