Yasuda-Shedlovsky Result

Sample name:	**CS000165**	Experiment start time:	**07/09/2011 16:56:23**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07019**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07019_CS000165_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	6.22	±0.00	6.88	85.2411	0.9632	0.202 M	25.2°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-07019 Points 105 to 156	19.76 %	Up	UV-metric pKa	77.5	45.2 M	0.208 M	25.1°C	☑	6.32
11I-07019 Points 53 to 104	26.82 %	Up	UV-metric pKa	77.2	41.5 M	0.203 M	25.0°C	☑	6.37
11I-07019 Points 3 to 52	35.77 %	Up	UV-metric pKa	76.3	36.7 M	0.196 M	25.5°C	☑	6.43

Graphs

Sample name:	**CS000165**	Experiment start time:	**07/09/2011 16:56:23**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07019**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07019_CS000165_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-07019 Points 3 to 52

Graphs

Sample name:	**CS000165**	Experiment start time:	**07/09/2011 16:56:23**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07019**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07019_CS000165_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-07019 Points 53 to 104

Graphs

Sample name:	**CS000165**	Experiment start time:	**07/09/2011 16:56:23**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07019**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07019_CS000165_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-07019 Points 105 to 156

Graphs

Sample name:	**CS000165**	Experiment start time:	**07/09/2011 16:56:23**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07019**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07019_CS000165_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000165		
Sample by	Volume	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	448.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	6.00		
logp (XH +)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00		