Yasuda-Shedlovsky Result

Sample name:	**CS000076**	Experiment start time:	**26/07/2011 16:24:55**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26021_CS000076_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.70	±0.05	18.69	-792.6164	0.9727	0.210 M	28.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-26021 Points 117 to 175	24.19 %	Up	UV-metric pKa	76.2	42.8 M	0.215 M	28.3°C	☑	6.66
11G-26021 Points 59 to 116	31.96 %	Up	UV-metric pKa	75.8	38.7 M	0.212 M	27.9°C	☑	6.62
11G-26021 Points 3 to 58	42.83 %	Up	UV-metric pKa	74.5	32.9 M	0.201 M	28.7°C	☑	6.53

Graphs

Sample name:	**CS000076**	Experiment start time:	**26/07/2011 16:24:55**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26021_CS000076_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11G-26021 Points 3 to 58 Quality: Good

Graphs

Sample name:	**CS000076**	Experiment start time:	**26/07/2011 16:24:55**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26021_CS000076_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11G-26021 Points 59 to 116 Quality: Good

Graphs

Sample name:	**CS000076**	Experiment start time:	**26/07/2011 16:24:55**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26021_CS000076_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11G-26021 Points 117 to 175 Quality: Good

Graphs

Sample name:	**CS000076**	Experiment start time:	**26/07/2011 16:24:55**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26021**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26021_CS000076_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000076		
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	387.50		
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	6.00		
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		