Yasuda-Shedlovsky Result

Sample name:	**CS000080**	Experiment start time:	**11/08/2011 15:57:46**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-11016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-11016_CS000080_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.33	±0.01	31.38	-1810.9331	0.9998	0.183 M	27.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-11016 Points 90 to 138	22.20 %	Up	UV-metric pKa	76.5	43.9 M	0.190 M	27.6°C	☑	6.06
11H-11016 Points 45 to 89	29.57 %	Up	UV-metric pKa	76.1	40.0 M	0.186 M	27.5°C	☑	5.98
11H-11016 Points 3 to 44	39.01 %	Up	UV-metric pKa	75.5	35.0 M	0.174 M	26.9°C	☑	5.86

Graphs

Sample name:	**CS000080**	Experiment start time:	**11/08/2011 15:57:46**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-11016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-11016_CS000080_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-11016 Points 3 to 44 Quality: Good

Graphs

Sample name:	**CS000080**	Experiment start time:	**11/08/2011 15:57:46**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-11016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-11016_CS000080_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-11016 Points 45 to 89 Quality: Good

Graphs

Sample name:	**CS000080**	Experiment start time:	**11/08/2011 15:57:46**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-11016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-11016_CS000080_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-11016 Points 90 to 138 Quality: Good

Graphs

Sample name:	**CS000080**	Experiment start time:	**11/08/2011 15:57:46**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-11016**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-11016_CS000080_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000080		
Sample by	Volume	11/08/2011 15:05:15	E:\T3 DATA\1107\11G-14011_CS000038_Fast UV pKa.t3r
Sample volume	0.0200 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	11/08/2011 15:05:15	E:\T3 DATA\1107\11G-14011_CS000038_Fast UV pKa.t3r
Molecular weight	340.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00	11/08/2011 15:05:15	E:\T3 DATA\1107\11G-14011_CS000038_Fast UV pKa.t3r
logp (XH +)	-10.00	11/08/2011 15:05:15	E:\T3 DATA\1107\11G-14011_CS000038_Fast UV pKa.t3r
logP (neutral X)	-10.00	11/08/2011 15:05:15	E:\T3 DATA\1107\11G-14011_CS000038_Fast UV pKa.t3r