Supplemental Information

Chemoselective Arylamidine Cyclizations: Mild Formation of 2-Arylimidazole-4-Carboxylic Acids

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General Procedure: All reactions were run under nitrogen. Solvents and reagents were from commercial sources and used without further purification.

Condition A: A 10 mL round bottom flask was charged with arylamidine hydrochloride (100 mol%), powdered KOH (120 mol%), and water (600 mM). Methyl-2-chloroacetoacetate (100 mol%) was added and the reaction was warmed to 60 °C for 2 hours. Concentration in vacuo followed by either silica gel chromatography (CH₂Cl₂/MeOH/AcOH, 90:10:1 v/v/v) or reverse phase HPLC (MeCN/aq 0.1% CF₃COOH) provided the 2-arylimidazole-4-carboxylic acid as the predominant product.

Condition B: A 10 mL round bottom flask was charged with arylamidine hydrochloride (100 mol%), MeCN (600 mM), and Et₃N (120 mol%). Methyl-2-chloroacetoacetate (100 mol%) was added and the reaction was warmed to 60 °C for 2 hours. Concentration in vacuo followed by either silica gel chromatography (CH₂Cl₂/MeOH, 95:5 → 90:10 v/v) or reverse phase HPLC (MeCN/aq 0.1% CF₃COOH) provided the 2-arylimidazole-4-carboxylic acid as the predominant product.

Condition C: All microwave experiments were conducted using a Discover-Explorer microwave reactor from CEM. Reactions were performed in sealed 10 mL tubes under an atmosphere of argon using reagent and solvent conditions identical to those reported in conditions A and B. Reaction temperature was monitored using a calibrated infrared temperature control system mounted below the reaction vessel. All samples were irradiated at 150W using a temperature gradient of 23 °C to 80 °C over the course of one minute followed by irradiation at 150W at 75 °C for an additional 10 minutes. Samples were cooled to room temperature and purified to homogeneity according to methods described in conditions A and B.

2-Phenyl:

(Imidazole) ¹H NMR (400 MHz, DMSO-*d*₆, 298 K) δ ppm 2.17 (s, 3 H) 7.43 (m, 3 H) 8.02 (m, 2 H). ¹³C NMR (100 MHz, DMSO-*d*₆, 298 K) δ ppm 158.7, 146.8, 139.9, 139.8, 131.8, 130.9, 128.7, 127.3, 16.9. Reverse phase HPLC (10 → 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, *t*_R = 0.4 min. HRMS-FAB *m/z* [M+H]⁺ calcd for C₁₁H₁₁N₂O₂⁺ 203.0815; found 203.0819.

(Pyrimidine) ¹H NMR (400 MHz, DMSO-*d*₆, 298 K) δ ppm 2.37 (s, 3 H) 7.44 (m, 3 H) 8.06 (m, 2 H) 13.13 (m, 1 H). ¹³C NMR (100 MHz, DMF-*d*₇, 298 K) δ ppm 161.1, 159.8, 155.3, 132.7, 129.6, 129.4, 128.8, 127.9, 22.5. Reverse phase HPLC (10 → 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, *t*_R = 1.4 min. HRMS-FAB *m/z* [M+H]⁺ calcd for C₁₁H₁₀N₂O₁Cl₁⁺ 221.0476; found 221.0481.

2-Pyridyl:

(Imidazole) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.19 (s, 3 H) 7.60 (m, 1 H) 8.44 (d, J = 9.30 Hz, 1 H) 8.70 (d, J = 4.40 Hz, 1 H) 9.19 (m, 1 H) 9.49 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 0.2 min. HRMS-FAB m/z [M+H]⁺ calcd for C₁₀H₁₀N₃O₂⁺ 204.0768; found 204.0775.

(Pyrimidine) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.39 (s, 3 H) 7.57 (m, 1 H) 8.41 (d, J = 7.80 Hz, 1 H) 8.72 (m, 1 H) 9.13 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 0.4 min. HRMS-FAB m/z [M+H]⁺ calcd for C₁₀H₉N₃O₁Cl₁⁺ 222.0429; found 222.0437.

2-Pyrazine:

(Imidazole) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.23 (s, 3 H) 8.70 (m, 2 H) 9.28 (m, 1 H) 9.66 (m, 1 H) 12.59 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 0.4 min. HRMS-FAB m/z [M+H]⁺ calcd for C₉H₉N₄O₂⁺ 205.0720; found 205.0726.

(Pyrimidine) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.45 (s, 3 H) 8.80 (m, 1 H) 8.87 (m, 1 H) 9.40 (m, 1 H) 12.96 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 1.0 min. HRMS-FAB m/z [M+H]⁺ calcd for C₉H₈N₄O₁Cl₁⁺ 223.0381; found 223.0391.

2-Furan:

(Imidazole) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.16 (s, 3 H) 7.02 (m, 1 H) 7.77 (m, 1 H) 8.40 (m, 1 H) 11.12 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 0.3 min. HRMS-FAB m/z [M+H]⁺ calcd for C₉H₉N₂O₃⁺ 193.0608; found 193.0612.

(Pyrimidine) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.36 (s, 3 H) 7.07 (m, 1 H) 7.82 (m, 1 H) 8.54 (m, 1 H) 13.01 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 1.2 min. HRMS-FAB m/z [M+H]⁺ calcd for C₉H₈N₂O₂Cl₁⁺ 211.0269; found 211.0270.

2-Thiophene:

(Imidazole) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.14 (s, 3 H) 7.61 (m, 2 H) 8.32 (m, 1 H) 9.25 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 0.4 min. HRMS-FAB m/z [M+H]⁺ calcd for C₉H₉N₂O₂S₁⁺ 209.0379; found 209.0382.

(Pyrimidine) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.35 (s, 3 H) 7.67 (d, J = 4.30 Hz, 1 H) 7.73 (d, J = 4.40 Hz, 1 H) 8.50 (m, 1 H) 13.03 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 1.4 min. HRMS-FAB m/z [M+H]⁺ calcd for C₉H₈N₂O₁S₁Cl₁⁺ 227.0040; found 227.0049.

2-Pyrazole:

(Imidazole) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.19 (s, 3 H) 6.56 (m, 1 H) 7.83 (m, 1 H) 8.37 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 0.4 min. HRMS-FAB m/z [M+H]⁺ calcd for C₈H₉N₄O₂⁺ 193.0720; found 193.0721.

(Pyrimidine) ^1H NMR (400 MHz, DMSO- d_6 , 298 K) δ ppm 2.39 (s, 3 H) 6.57 (m, 1 H) 7.87 (m, 1 H) 8.48 (m, 1 H). Reverse phase HPLC (10 $\rightarrow$ 90% MeCN / aq. 0.1% CF₃COOH over 3 minutes, 254 nm, t_R = 1.2 min. HRMS-FAB m/z [M+H]⁺ calcd for C₈H₈N₄O₁Cl₁⁺ 211.0381; found 211.0389.

Acquisition Time (sec)	0.6255	Comment	Imported from UXMNR.		Date	08 Jul 2005 13:11:28	
File Name							
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	17500	Original Points Count	16384
Points Count	16384	Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	26178.01
Temperature (degree C)	27.000

No.	(ppm)	(Hz)	Height
1	16.93	1704.0	0.2332
2	127.33	12812.5	0.5601
3	128.68	12948.3	0.5829
4	130.86	13167.2	0.2428
5	131.76	13258.3	0.1389
6	139.80	14066.8	0.1539
7	139.94	14081.2	0.0969
8	146.83	14774.6	0.1235
9	158.68	15966.7	0.1426

No.	Annotation	(ppm)
1	DMSO-d6	39.50

Acquisition Time (sec)		0.6259	Comment		Imported from UXNMR.	Date		09 Jul 2005 13:07:12
File Name			Nucleus			Original Points Count		
Frequency (MHz)			100.62			13C		
Points Count			16384			29pg30		
Sweep Width (Hz)			26178.01			Temperature (degree C) 27.000		
			Pulse Sequence			DIMETHYLFORMAMID-D7

No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	22.46	2260.2	0.2787	1	Dimethylformamide-d7	30.10
2	127.87	12866.9	0.0939	2	Dimethylformamide-d7	35.64
3	128.79	12959.5	1.0000	3	Dimethylformamide-d7	163.22
4	129.41	13021.9	0.1036			
5	129.57	13037.8	0.9597			
6	132.67	13349.4	0.4991			
7	155.25	15621.6	0.0370			
8	159.81	16080.2	0.0351			
9	161.09	16209.6	0.0413			

Acquisition Time (sec)		2.0447	Comment		Imported from UXNMR.		Date
File Name		Frequency (MHz)		400.13			
Nucleus	1H	Number of Transients		16		Original Points Count	
Pulse Sequence	zg30	Solvent		DMSO-D6		Sweep Width (Hz)	
						16384	
						8012.82	
						Points Count	
						16384	
						Temperature (degree C)	
						27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[1.94 .. 2.34]	3.000	8.40783e+8
2	[4.54 .. 6.84]	5.637	1.57976e+9
3	[7.28 .. 7.63]	3.192	8.94519e+8
4	[7.86 .. 8.18]	2.196	6.15447e+8

No.	Multiplet	Shift	(ppm)	J (Hz)	Type	H's
1	M3	2.17	[2.00 .. 2.34]	-	m	3
2	M2	7.43	[7.12 .. 7.73]	-	m	3
3	M1	8.02	[7.76 .. 8.28]	-	m	2

Acquisition Time (sec)	2.0447	Comment	Imported from UXNMR.		Date	08 Jul 2005 17:18:56
File Name						
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16	Original Points Count
Points Count	16384	Pulse Sequence	zg30	Solvent	DMSO-D6	16384
Temperature (degree C)	27.000				Sweep Width (Hz)	8012.82

No.	Annotation	(ppm)
1	DMSO-d6	2.49
2	D2O	3.37

No.	(ppm)	Value	Absolute Value
1	[2.28 .. 2.43]	3.000	1.70592e+9
2	[7.12 .. 7.65]	2.780	1.58084e+9
3	[7.84 .. 8.27]	1.837	1.04475e+9
4	[12.77 .. 13.36]	0.688	3.91206e+8

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M4	2.37	[2.31 .. 2.43]	-	m	3
2	M3	7.44	[7.24 .. 7.65]	-	m	3
3	M2	8.06	[7.88 .. 8.24]	-	m	2
4	M1	13.13	[12.87 .. 13.40]	-	m	1

Acquisition Time (sec)		Comment		Date	
File Name		Frequency (MHz)		400.13	
Nucleus		1H		Imported from Uxnmr.	
Pulse Sequence		zg30			
		Number of Transients		16	
		Solvent		DMSO-D6	
		Original Points Count		16384	
		Sweep Width (Hz)		8012.82	
		Points Count		16384	
		Temperature (degree C)		27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[2.07 .. 2.28]	3.000	1.35162e+9
2	[3.75 .. 6.08]	0.647	2.91519e+8
3	[7.42 .. 7.68]	0.985	4.43946e+8
4	[8.29 .. 8.53]	0.990	4.45867e+8
5	[8.65 .. 8.83]	0.929	4.18721e+8
6	[9.12 .. 9.27]	1.022	4.60389e+8
7	[9.28 .. 9.70]	0.262	1.17828e+8

No.	Multiplet	Shift1	(ppm)	J (Hz)	Type	H's
1	M6	2.19	[2.02 .. 2.36]	-	m	3
2	M5	7.60	[7.55 .. 7.66]	-	m	1
3	M4	8.44	[8.43 .. 8.45]	9.30	d	1
4	M3	8.70	[8.69 .. 8.71]	4.40	d	1
5	M2	9.19	[9.06 .. 9.32]	-	m	1
6	M1	9.49	[9.25 .. 9.74]	-	m	1

Acquisition Time (sec) 2.0447		Comment Imported from UXNMR.		Date
File Name		Frequency (MHz) 400.13		
Nucleus	¹ H	Number of Transients	16	Points Count
Pulse Sequence	zg30	Solvent	DMSO-D6	16384
		Original Points Count	16384	Temperature (degree C)
		Sweep Width (Hz)	8012.82	27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[2.28 .. 2.44]	3.000	1.64810e+9
2	[5.70 .. 7.35]	0.812	4.46116e+8
3	[7.45 .. 7.64]	0.938	5.15149e+8
4	[8.32 .. 8.49]	0.900	4.94581e+8
5	[8.66 .. 8.76]	0.895	4.91761e+8
6	[9.11 .. 9.23]	0.904	4.96895e+8

No.	Multiplet	Shift	(ppm)	J (Hz)	Type	H's
1	M5	2.39	[2.35 .. 2.42]	-	m	3
2	M4	7.57	[7.48 .. 7.67]	-	m	1
3	M3	8.41	[8.41 .. 8.42]	7.80	d	1
4	M2	8.72	[8.65 .. 8.79]	-	m	1
5	M1	9.13	[9.02 .. 9.24]	-	m	1

Acquisition Time (sec)		2.0447	Comment		Imported from UXNMR.	Date	20 Jun 2005 18:35:44
File Name		Frequency (MHz)	400.13			Points Count	16384
Nucleus		¹ H	Number of Transients	16	Original Points Count	16384	Temperature (degree C)
Pulse Sequence		zg30	Solvent	DMSO-D6	Sweep Width (Hz)	8012.82	27.000

Acquisition Time (sec)	2.0447	Comment	Imported from UXNMR.			Date	24 Jun 2005 20:09:36
File Name							
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16	Original Points Count	16384
Points Count	16384	Pulse Sequence	zg30	Solvent	DMSO-D6	Sweep Width (Hz)	8012.82
Temperature (degree C)	27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49
2	D2O	3.37

No.	(ppm)	Value	Absolute Value
1	[2.41 .. 2.47]	3.000	8.69407e+8
2	[8.75 .. 8.84]	0.851	2.46765e+8
3	[8.84 .. 8.91]	0.917	2.65600e+8
4	[9.34 .. 9.46]	0.797	2.31034e+8
5	[12.86 .. 13.37]	0.372	1.07879e+8

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M5	2.45	[2.42 .. 2.48]	-	m	3
2	M4	8.80	[8.77 .. 8.83]	-	m	1
3	M3	8.87	[8.84 .. 8.90]	-	m	1
4	M2	9.40	[9.36 .. 9.44]	-	m	1
5	M1	12.96	[12.45 .. 13.46]	-	m	1

Acquisition Time (sec)		Comment		Date	
File Name		Frequency (MHz)		400.13	
Nucleus		Number of Transients		16	
Pulse Sequence		Solvent		DMSO-D6	
		Original Points Count		16384	
		Sweep Width (Hz)		8012.82	
		Points Count		16384	
		Temperature (degree C)		27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value	No.	Multiplet	Shift	(ppm)	J (Hz)	Type	H's
1	[2.03 .. 2.29]	3.000	2.31193e+9	1	M5	2.16	[2.07 .. 2.24]	-	m	3
2	[6.59 .. 7.17]	0.786	6.05544e+8	2	M4	7.02	[6.95 .. 7.09]	-	m	1
3	[7.51 .. 7.98]	0.826	6.36316e+8	3	M3	7.77	[7.72 .. 7.83]	-	m	1
4	[8.21 .. 8.60]	0.829	6.39126e+8	4	M2	8.40	[8.31 .. 8.48]	-	m	1
5	[10.24 .. 12.09]	1.303	1.00411e+9	5	M1	11.12	[9.83 .. 12.41]	-	m	1

Acquisition Time (sec)		Comment		Date	
File Name		Frequency (MHz)		400.13	
Nucleus		Number of Transients		16	
Pulse Sequence		Solvent		DMSO-D6	
		Original Points Count		16384	
		Sweep Width (Hz)		8012.82	
		Points Count		16384	
		Temperature (degree C)		27.000

Acquisition Time (sec)		Comment		Date	
File Name		Frequency (MHz)		400.13	
Nucleus		1H		Imported from UXNMR.	
Pulse Sequence		zg30		20 Jun 2005 18:12:16	
		Number of Transients		16	
		Solvent		DMSO-D6	
		Original Points Count		16384	
		Sweep Width (Hz)		8012.82	
		Points Count		16384	
		Temperature (degree C)		27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[2.05 .. 2.29]	3.000	1.52422e+9
2	[7.41 .. 7.77]	2.385	1.21152e+9
3	[8.19 .. 8.49]	1.267	6.43878e+8
4	[8.49 .. 9.70]	1.315	6.67945e+8

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M4	2.14	[1.98 .. 2.30]	-	m	3
2	M3	7.61	[7.44 .. 7.79]	-	m	2
3	M2	8.32	[8.17 .. 8.47]	-	m	1
4	M1	9.25	[8.55 .. 9.95]	-	m	1

Acquisition Time (sec) 2.0447				Comment Imported from UXNMR.				Date
File Name		Frequency (MHz)		400.13				
Nucleus		1H		Number of Transients 16		Original Points Count 16384		Points Count 16384
Pulse Sequence		zg30		Solvent DMSO-D6		Sweep Width (Hz) 8012.82		Temperature (degree C) 27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[2.23 .. 2.45]	3.000	1.94995e+9
2	[7.39 .. 7.92]	1.939	1.26020e+9
3	[8.28 .. 8.77]	0.872	5.66578e+8
4	[12.63 .. 13.57]	0.514	3.33930e+8

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M5	2.35	[2.27 .. 2.43]	-	m	3
2	M4	7.67	[7.64 .. 7.71]	4.30	d	1
3	M3	7.73	[7.72 .. 7.74]	4.40	d	1
4	M2	8.50	[8.43 .. 8.57]	-	m	1
5	M1	13.03	[12.67 .. 13.40]	-	m	1

Acquisition Time (sec) 2.0447			Comment Imported from UXNMR.			Date 20 Jun 2005 18:25:04		
File Name			Frequency (MHz) 400.13			Points Count 16384		
Nucleus			1H			Temperature (degree C) 27.000		
Pulse Sequence			zg30			Sweep Width (Hz) 8012.82		
			Number of Transients 16			Original Points Count 16384		
			Solvent DMSO-D6

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[2.00 .. 2.39]	3.000	1.47565e+9
2	[6.35 .. 6.74]	1.108	5.44776e+8
3	[7.71 .. 7.97]	1.036	5.09752e+8
4	[8.29 .. 8.51]	1.050	5.16355e+8
5	[8.63 .. 9.55]	0.210	1.03538e+8

No.	Multiplet	Shift1	(ppm)	J (Hz)	Type	H's
1	M4	2.19	[2.15 .. 2.23]	-	m	3
2	M3	6.56	[6.52 .. 6.60]	-	m	1
3	M2	7.83	[7.78 .. 7.87]	-	m	1
4	M1	8.37	[8.15 .. 8.59]	-	m	1

Acquisition Time (sec)	2.0447	Comment	Imported from UXNMR.			Date	24 Jun 2005 20:16:00
File Name							
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	32	Original Points Count	16384
Points Count	16384	Pulse Sequence	zg30	Solvent	DMSO-D6	Sweep Width (Hz)	8012.82
Temperature (degree C)	27.000

No.	Annotation	(ppm)
1	DMSO-d6	2.49

No.	(ppm)	Value	Absolute Value
1	[2.34 .. 2.46]	3.000	1.63289e+9
2	[6.48 .. 6.75]	0.776	4.22566e+8
3	[7.82 .. 8.00]	0.868	4.72325e+8
4	[8.38 .. 8.59]	0.828	4.50723e+8

No.	Multiplet	Shift	(ppm)	J (Hz)	Type	H's
1	M4	2.39	[2.32 .. 2.46]	-	m	3
2	M3	6.57	[6.43 .. 6.72]	-	m	1
3	M2	7.87	[7.74 .. 8.00]	-	m	1
4	M1	8.48	[8.31 .. 8.65]	-	m	1

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Injection Date : 6/24/2005 10:09:52 AM Seq. Line : 12
Sample Name : Location : Vial 11
Acq. Operator : Inj : 1

Inj Volume : 1 µl

Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl

Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M

Last changed : 12/28/2004 10:00:33 AM

Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M

Last changed : 7/7/2005 3:19:48 PM

(modified after loading)

=====

PHENYL-IMIDAZOLE

=====

Injection Date : 6/24/2005 9:15:11 AM Seq. Line : 1
Sample Name : Location : Vial 1
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:10 PM
(modified after loading)

PHENYL-PYRIMIDINE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.117	BP	0.0414	32.86684	13.04334	0.1167
2	0.214	VB	0.1543	187.19838	16.76690	0.6647
3	1.228	PP	0.0651	22.77877	5.63791	0.0809
4	1.462	VV	0.1292	2.75891e4	3119.80615	97.9658
5	2.270	VP	0.0667	102.85040	21.92676	0.3652
6	2.861	VBA	0.3478	227.18912	9.27473	0.8067

Totals : 2.81619e4 3186.45578

=====

Injection Date : 6/24/2005 10:14:28 AM Seq. Line : 13
Sample Name : Location : Vial 12
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

PYRIDINE-IMIDAZOLE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.130	PV	0.0712	9994.20020	2112.57153	97.1466
2	1.002	VV	0.1575	88.84068	7.64859	0.8636
3	1.184	VV	0.0785	16.36482	2.95777	0.1591
4	1.387	VV	0.0682	30.65074	6.84891	0.2979
5	1.490	VV	0.0646	27.79655	6.67937	0.2702
6	1.812	VP	0.0488	24.46424	8.19441	0.2378
7	1.958	VP	0.0511	52.89843	16.63811	0.5142
8	2.867	VBA	0.1504	52.53753	7.81978	0.5107

Totals : 1.02878e4 2169.35847

=====

Injection Date : 6/24/2005 9:24:12 AM Seq. Line : 2
Sample Name : Location : Vial 2
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

PYRIDINE-PYRIMIDINE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.131	PV	0.0739	1.12571e4	2438.77100	29.7492
2	0.348	VV	0.1348	2.59543e4	3065.02832	68.5897
3	1.124	VV	0.1554	197.29648	18.06086	0.5214
4	1.263	VV	0.0894	105.35657	15.88632	0.2784
5	1.390	VP	0.0845	231.48581	38.30357	0.6118
6	1.814	VP	0.0389	33.49618	14.50573	0.0885
7	1.960	VP	0.0500	28.54417	9.24508	0.0754
8	2.868	VBA	0.1191	32.36241	8.01948	0.0855

Totals : 3.78399e4 5607.82035

=====

Injection Date : 6/24/2005 10:18:56 AM Seq. Line : 14
Sample Name : Location : Vial 13
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

PYRAZINE-IMIDAZOLE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.134	PV	0.0839	1.17419e4	2285.60693	69.9494
2	0.350	VB	0.1144	4899.39648	605.40411	29.1869
3	1.491	PV	0.0364	15.31842	7.99046	0.0913
4	1.814	VP	0.0511	35.59512	11.20823	0.2120
5	1.959	VP	0.0505	38.28029	12.22751	0.2280
6	2.868	VBA	0.1528	55.78897	7.86184	0.3323

Totals : 1.67863e4 2930.29908

=====

Injection Date : 6/23/2005 9:35:05 AM Seq. Line : 2
Sample Name : Location : Vial 2
Acq. Operator : Inj : 1
 Inj Volume : 1 µl

Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

PYRAZINE-PYRIMIDINE

=====

Area Percent Report

=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.132	PV	0.0314	29.16202	14.56886	0.5735
2	0.239	VV	0.1075	63.14036	8.23399	1.2418
3	0.386	VB	0.1329	56.15654	5.80316	1.1045
4	0.941	BV	0.0966	2111.53223	339.19785	41.5287
5	1.004	VP	0.0814	1757.69153	323.57257	34.5695
6	1.816	PV	0.0564	9.03442	2.48317	0.1777
7	1.958	VV	0.0579	12.50075	3.17590	0.2459
8	2.802	VBA	0.4042	1045.29883	38.56288	20.5585

Totals : 5084.51668 735.59838

=====

Injection Date : 6/24/2005 10:42:16 AM Seq. Line : 19
Sample Name : Location : Vial 14
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

FURAN-IMIDAZOLE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.134	PV	0.0544	7863.99463	2269.56836	20.7909
2	0.283	VB	0.1313	2.98428e4	3072.91699	78.8985
3	1.815	VP	0.0367	19.47955	10.01492	0.0515
4	1.960	VP	0.0504	33.50396	10.74154	0.0886
5	2.869	VBA	0.1705	64.51319	7.79907	0.1706

Totals : 3.78243e4 5371.04088

=====

Injection Date : 6/24/2005 9:33:20 AM Seq. Line : 4
Sample Name : Location : Vial 4
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

FURAN-PYRIMIDINE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.133	PB	0.0733	9800.98926	2143.98877	38.9721
2	0.633	BP	0.1349	55.74603	5.86547	0.2217
3	1.206	VV	0.0933	1.45479e4	2315.62427	57.8477
4	1.383	VV	0.0971	466.53314	65.47997	1.8551
5	1.544	VV	0.1081	119.52335	18.42142	0.4753
6	1.814	VV	0.0878	98.55101	15.58866	0.3919
7	1.958	VP	0.0590	43.29025	11.22353	0.1721
8	2.861	VBA	0.0946	16.13497	8.31907	0.0642

Totals : 2.51487e4 4584.51115

=====

Injection Date : 6/24/2005 10:46:55 AM Seq. Line : 20
Sample Name : Location : Vial 15
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

THIOPHENE-IMIDAZOLE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.132	BV	0.0700	9526.56738	2222.06982	28.3168
2	0.392	VB	0.1256	1.97012e4	2176.35522	58.5600
3	1.498	BV	0.2051	224.32610	13.69799	0.6668
4	1.814	VV	0.1556	372.00436	30.63942	1.1057
5	1.959	VV	0.0944	249.23839	36.18838	0.7408
6	2.862	VV	0.4190	3569.43359	104.88240	10.6098

Totals : 3.36428e4 4583.83323

=====

Injection Date : 6/24/2005 9:37:49 AM Seq. Line : 5
Sample Name : Location : Vial 5
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

THIOPHENE-PYRIMIDINE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.129	PB	0.0720	1.01122e4	2269.13208	37.7287
2	1.397	VV	0.0845	1.64588e4	3072.06104	61.4082
3	1.646	VV	0.0765	118.01122	25.72097	0.4403
4	1.812	VV	0.0569	51.55907	14.01488	0.1924
5	1.959	VP	0.0508	39.30931	12.45665	0.1467
6	2.858	VBA	0.0968	22.43738	8.48570	0.0837

Totals : 2.68023e4 5401.87132

=====

Injection Date : 6/24/2005 10:05:21 AM Seq. Line : 11
Sample Name : Location : Vial 6
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

PYRAZOLE-IMIDAZOLE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.133	PV	0.0680	8728.06934	2123.14258	44.4417
2	0.378	VB	0.1240	1.06699e4	1220.86047	54.3293
3	1.484	VV	0.0628	95.84547	23.90399	0.4880
4	1.814	VP	0.0477	52.77163	18.28872	0.2687
5	1.959	VP	0.0503	33.35411	10.70615	0.1698
6	2.870	VBA	0.1884	59.40174	7.66265	0.3025

Totals : 1.96394e4 3404.56457

=====

Injection Date : 6/24/2005 12:29:06 PM Seq. Line : 2
Sample Name : Location : Vial 92
Acq. Operator : Inj : 1
Inj Volume : 1 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 3 µl
Acq. Method : C:\HPCHEM\1\METHODS\230-305B.M
Last changed : 12/28/2004 10:00:33 AM
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed : 6/24/2005 2:27:50 PM
(modified after loading)

PYRAZOLE-PYRIMIDINE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.134	PV	0.0316	29.35318	13.89720	0.2921
2	0.200	VV	0.0742	123.70511	23.95509	1.2312
3	0.393	VB	0.1278	57.95327	6.39117	0.5768
4	1.179	BV	0.1043	5347.48584	758.07153	53.2214
5	1.510	VV	0.1035	97.69963	12.73400	0.9724
6	2.862	VBA	0.5509	4391.42334	106.54311	43.7061

Totals : 1.00476e4 921.59210