Supporting Information

Influence of Surface-attachment Functionality on the Aggregation, Persistence, and Electron-transfer Reactivity of Chalcogenorhodamine Dyes on TiO₂

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Figure S1. Normalized absorbance spectra of thiophene-substituted dyes (a) and phenyl-substituted dyes (b) in CH₃OH.

Figure S2. Absorbance spectra of **1-Se** (a), **3-Se** (b), **2-O** (c), **4-O** (d), **2-S** (e), and **4-Se** (f) dissolved in CH₃OH and adsorbed to nanocrystalline TiO₂ films at various surface coverages.

Figure S3. Absorbance spectra of TiO₂ films functionalized with dyes **1-O** (a), **3-O** (b), **1-Se** (c), **3-Se** (d), **2-O** (e), **4-O** (f), **2-S** (g), and **4-Se** (h) as a function of time that the films were immersed in 0.1 M HCl in CH₃CN.

Figure S4. Absorptance and short-circuit photocurrent action spectra of FTO/TiO₂ electrodes functionalized with **1-Se** (a), **3-Se** (b), **2-O** (c), **4-O** (d), **2-S** (e), and **4-Se** (f). Absorptance spectra were acquired before assembly of DSSCs; IPCE data were acquired immediately after and either 20 min or 75 min after assembly of DSSCs.

Figure S5. Successive short-circuit photocurrent action spectra of FTO/TiO₂ electrodes functionalized with **1-O** (a), **3-O** (b), **1-Se** (c), **3-Se** (d), **2-O** (e), **4-O** (f), **2-S** (g), and **4-Se** (h). Data were acquired successively for 20-75 min after assembly of DSSCs.

Figure S6. Absorptance spectra of FTO/TiO₂ electrodes functionalized with **1-O** (a), **3-O** (b), **1-Se** (c), **3-Se** (d), **2-O** (e), **4-O** (f), **2-S** (g), and **4-Se** (h). Spectra were acquired before assembly of DSSCs and after 20 min (**1-E**, **3-E**) or 75 min (**2-E**, **4-E**) of successive photoelectrochemical measurements.

Figure S7. Best J-V data acquired for DSSCs with dyes **1-E** through **4-E** and N3.

Figure S8. Successive J-V data for DSSCs with dyes **1-Se** (a), **3-Se** (b), **2-O** (c), **4-O** (d), **2-S** (e), and **4-Se** (f).

Figure S9. Photoelectrochemical data for DSSCs with **1-O** and **3-O** (a), **1-Se** and **3-Se** (b), **2-O** and **4-O** (c), and **2-S** and **4-Se** (d) as a function of time during successive measurements.

Table S1. Photophysical data for dyes **1-E** and **2-E** in 0.1 M HCl in CH₃CN.

Table S2. Average photoelectrochemical data for DSSCs with dyes **1-E** through **4-E** and N3.

Table S3. Best photoelectrochemical data acquired for DSSCs with dyes **1-E** through **4-E** and N3.

Appendix S1. NMR spectra of dyes **3-Se**, **3-O**, **4-Se**, **4-O**, **7-Se**, **7-O**, **8-Se**, **8-O**, **9-Se**, and **9-O**.

Figure S1. Normalized absorbance spectra of thiophene-substituted dyes (a) and phenyl-substituted dyes (b) in CH₃OH.

Figure S2. Absorbance spectra of **1-Se** (a), **3-Se** (b), **2-O** (c), **4-O** (d), **2-S** (e), and **4-Se** (f) dissolved in CH_3OH and adsorbed to nanocrystalline TiO_2 films at various surface coverages. Spectra of solvated dyes are normalized to an absorbance of 1.0 at λ_{max} , and the baseline absorbance is offset such that the dashed line corresponds to 0. Arrows indicate the increase of absorbance with surface coverage.

Figure S3. Absorbance spectra of TiO_2 films functionalized with dyes **1-O** (a), **3-O** (b), **1-Se** (c), **3-Se** (d), **2-O** (e), **4-O** (f), **2-S** (g), and **4-Se** (h) as a function of time that the films were immersed in 0.1 M HCl in CH_3CN . Arrows indicate direction of spectral changes.

Figure S4. Absorbance and short-circuit photocurrent action spectra of FTO/TiO₂ electrodes functionalized with **1-Se** (a), **3-Se** (b), **2-O** (c), **4-O** (d), **2-S** (e), and **4-Se** (f). Absorbance spectra were acquired before assembly of DSSCs; IPCE data were acquired immediately after and either 20 min or 75 min after assembly of DSSCs. Error bars represent the standard deviations relative to the average IPCE values of 2 DSSCs.

Figure S5. Short-circuit photocurrent action spectra of FTO/TiO₂ electrodes functionalized with **1-O** (a), **3-O** (b), **1-Se** (c), **3-Se** (d), **2-O** (e), **4-O** (f), **2-S** (g), and **4-Se** (h). Data were acquired successively for 20-75 min after assembly of DSSCs.

Figure S6. Absorbance spectra of FTO/TiO₂ electrodes functionalized with **1-O** (a), **3-O** (b), **1-Se** (c), **3-Se** (d), **2-O** (e), **4-O** (f), **2-S** (g), and **4-Se** (h). Spectra were acquired before assembly of DSSCs (black lines) and after 20 min (**1-E**, **3-E**) or 75 min (**2-E**, **4-E**) of successive photoelectrochemical measurements (colored lines). Error bars represent the standard deviations relative to the average absorbances of 2 DSSCs.

Figure S7. Best J-V data acquired for DSSCs with dyes **1-E** through **4-E** and N3.

Figure S8. J-V data for DSSCs with dyes **1-Se** (a), **3-Se** (b), **2-O** (c), **4-O** (d), **2-S** (e), and **4-Se** (f); arrows indicate the changes of J_{sc} and V_{oc} with successive measurements.

Figure S9. Photoelectrochemical data for DSSCs with 1-O and 3-O (a), 1-Se and 3-Se (b), 2-O and 4-O (c), and 2-S and 4-Se (d) as a function of time during successive measurements. Error bars represent the standard deviations relative to the averages for 2 DSSCs.

Table S1. Photophysical data for dyes **1-E** and **2-E** in 0.1 M HCl in CH₃CN.

Dye	$\lambda_{\max}$ (nm) ^a	$\epsilon_{\max}$ (M ⁻¹ cm ⁻¹)
1-O	575 ^a	6.6×10^4 ^a
1-Se	607 ^a	6.5×10^4 ^a
2-O	554	5.0×10^4
2-S	574	2.9×10^4

^a From ref. 44.**Table S2.** Average photoelectrochemical data for DSSCs with dyes **1-E** through **4-E** and N3.^{a,b}

Dye	IPCE _{max} (%)		V _{oc} (mV)		J _{sc} (mA cm ⁻²)		ff		η (%)	
	initial ^c	final ^d	initial ^c	final ^d	initial ^c	final ^d	initial ^c	final ^d	initial ^c	final ^d
1-O	90 ± 15	38 ± 18	263 ± 5	307 ± 3	4.23 ± 0.15	1.64 ± 0.80	0.26 ± 0.01	0.42 ± 0.08	0.51 ± 0.05	0.43 ± 0.01
1-Se	91 ± 5	20.5 ± 0.1	230 ± 11	286 ± 5	3.46 ± 0.90	0.97 ± 0.28	0.26 ± 0.01	0.63 ± 0.03	0.34 ± 0.08	0.26 ± 0.04
2-O	95 ± 12	44 ± 5	284 ± 35	310 ± 9	4.0 ± 1.4	2.02 ± 0.08	0.27 ± 0.02	0.41 ± 0.18	0.51 ± 0.28	0.42 ± 0.16
2-S	53 ± 2	32 ± 2	304 ± 43	336 ± 6	2.88 ± 0.66	1.38 ± 0.07	0.33 ± 0.04	0.60 ± 0.10	0.54 ± 0.26	0.52 ± 0.12
3-O	81 ± 4	84 ± 6	240 ± 34	286 ± 48	3.25 ± 0.16	3.3 ± 1.1	0.28 ± 0.04	0.32 ± 0.12	0.36 ± 0.09	0.49 ± 0.10
3-Se	66 ± 5	67.8 ± 0.2	219 ± 12	261 ± 6	3.39 ± 0.11	3.28 ± 0.01	0.27 ± 0.01	0.31 ± 0.01	0.33 ± 0.04	0.44 ± 0.01
4-O	68 ± 1	56 ± 1	250 ± 7	306 ± 11	3.69 ± 0.02	3.86 ± 0.27	0.28 ± 0.06	0.34 ± 0.02	0.48 ± 0.03	0.76 ± 0.08
4-Se	53 ± 3	55 ± 7	218 ± 19	303 ± 4	3.07 ± 0.16	3.89 ± 0.38	0.27 ± 0.01	0.31 ± 0.07	0.34 ± 0.01	0.69 ± 0.08
N3	77 ± 8		814 ± 23		6.61 ± 0.94		0.52 ± 0.05		4.88 ± 0.59	

^a Electrolytes for chalcogenorhodamine DSSCs were 0.5 M LiI, 0.05 M I₂, 0.1 M 4tBP, 0.15 M HCl in CH₃CN; electrolyte for N3 was 0.1 M LiI, 0.05 M I₂, 0.1 M guanidinium thiocyanate, 0.5 M 4tBP, and 0.6 M PMII in CH₃CN; ^b data are averages of two DSSCs for each dye, and standard deviations are relative to average values; ^c initial values were measured immediately after assembling DSSCs; ^d final values were acquired after 25-35 min (dyes **1-E**, **2-E**) or 75-80 min (dyes **3-E**, **4-E**) of successive acquisitions of short-circuit photocurrent action spectra and J-V data.

Table S3. Best photoelectrochemical data acquired for DSSCs with dyes **1-E** through **4-E** and N3.^a

Dye	V _{oc} (mV)	J _{sc} (mA cm ⁻²)	ff	η (%)
1-O	293	3.03	0.365	0.606
1-Se	242	3.67	0.276	0.404
2-O	305	4.16	0.306	0.640
2-S	333	2.86	0.380	0.679
3-O	272	5.64	0.271	0.710
3-Se	326	4.10	0.369	0.799
4-O	311	4.03	0.338	0.793
4-Se	304	3.65	0.352	0.732
N3	793	7.72	0.505	5.91

^a Electrolytes for chalcogenorhodamine DSSCs were 0.5 M LiI, 0.05 M I₂, 0.1 M 4tBP, 0.15 M HCl in CH₃CN; electrolyte for N3 was 0.1 M LiI, 0.05 M I₂, 0.1 M guanidinium thiocyanate, 0.5 M 4tBP, and 0.6 M PMII in CH₃CN.

Appendix S1. NMR spectra of dyes **3-Se, 3-O, 4-Se, 4-O, 7-Se, 7-O, 8-Se, 8-O, 9-Se,** and **9-O.**

NMR spectrum number	Dye	Nucleus
1	3-Se	^1H
2	3-Se	^1H
3	3-Se	^{31}P
4	3-O	^1H
5	3-O	^1H
6	3-O	^{31}P
7	4-Se	^1H
8	4-Se	^1H
9	4-Se	^{31}P
10	4-O	^1H
11	4-O	^1H
12	4-O	^{31}P
13	7-Se	^1H
14	7-Se	^1H
15	7-Se	^{13}C
16	7-O	^1H
17	7-O	^1H
18	7-O	^{13}C
19	8-Se	^1H
20	8-Se	^1H
21	8-Se	^{13}C
22	8-O	^1H
23	8-O	^1H
24	8-O	^{13}C
25	8-O	^{13}C
26	9-Se	^1H
27	9-Se	^1H
28	9-Se	^{13}C
29	9-Se	^{13}C
30	9-O	^1H
31	9-O	^1H
32	9-O	^{13}C
33	9-O	^{13}C

NMR spectrum 1

STANDARD PROTON PARAMETERS

Sample Name: 2-A0-011-3

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3od
Data collected on: Jul 22 2011

Temp. 46.0 C / 319.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.9003771 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec

Saturated
CD₃OD solution

NMR spectrum 2

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Jul 22 2011

Temp. 46.0 C / 319.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.9003771 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec

Saturated
CD₃OD solution

NMR spectrum 3

STANDARD CARBON PARAMETERS

Sample Name: 2-AO-027-P31-2

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: alex1202012

Pulse Sequence: PHOSPHORUS (s2pul)

Solvent: dmsd

Data collected on: Jan 19 2012

Temp. 23.0 C / 296.1 K

Operator: Detty

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.078 sec

Width 30395.1 Hz

21120 repetitions

OBSERVE P31, 121.4727108 MHz

DECOUPLE H1, 300.0768683 MHz

Power 38 dB

on during acquisition

off during delay

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 603 hr, 33 min

NMR spectrum 4

STANDARD PROTON PARAMETERS

Sample Name: 2-A0-012-3

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3od
Data collected on: Jul 22 2011

Temp. 46.0 C / 319.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.9003771 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec

NMR spectrum 5

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3od
Data collected on: Jul 22 2011

Temp. 46.0 C / 319.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.9003771 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 38 sec

Saturated
CD₃OD solution

NMR spectrum 6

2-A0-012-P31-MeOH-DMSO

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: PHOSPHORUS

Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: dmsd / CD₃OD
Data collected on: Jan 23 2012

Temp. 22.5 C / 295.6 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.078 sec
Width 30395.1 Hz
16832 repetitions
OBSERVE P31, 121.4727108 MHz
DECOUPLE H1, 300.0768683 MHz
Power 38 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 603 hr, 33 min

Saturated
CD₃OD solution

NMR spectrum 7

1-A0-251-2

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Mar 10 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9404800 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec

Saturated
CD₃OD solution

NMR spectrum 8

1-A0-251-2

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3od
Data collected on: Mar 10 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9404800 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec

Saturated
CD₃OD solution

NMR spectrum 9

STANDARD CARBON PARAMETERS

Sample Name: 2-40-022-P31-2

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: PHOSPHORUS

Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: dmsd
Data collected on: Jan 20 2012

Temp. 23.0 C / 296.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.078 sec
Width 30395.1 Hz
20800 repetitions
OBSERVE P31, 121.4727108 MHz
DECOUPLE H1, 300.0768683 MHz
Power 38 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 603 hr, 33 min

NMR spectrum 10

2-A0-030-7

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Nov 28 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9003766 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

Saturated
CD₃OD solution

NMR spectrum 11

2-A0-030-7

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Nov 28 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9003766 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

Saturated
CD₃OD solution

NMR spectrum 12

STANDARD CARBON PARAMETERS

Sample Name: 2-40-030-P31-3

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: PHOSPHORUS

Pulse Sequence: PHOSPHORUS (s2pu1)
Solvent: dmsd
Data collected on: Jan 18 2012

Temp. 23.0 C / 296.1 K
Operator: Dettly

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.078 sec
Width 30395.1 Hz
22784 repetitions

OBSERVE P31, 121.4727108 MHz
DECOUPLE H1, 300.0768683 MHz
Power 38 dB
on during acquisition
off during delay
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 603 hr, 33 min

NMR spectrum 13

2-A0-005-3

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3od
Data collected on: Jul 13 2011

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.706 sec
Width 4803.1 Hz
8 repetitions
OBSERVE H1, 300.0750639 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 0 min 23 sec

NMR spectrum 14

2-A0-005-3

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cd3od

Data collected on: Jul 13 2011

Operator: Detty

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4803.1 Hz

8 repetitions

OBSERVE H1, 300.0750639 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 16384

Total time 0 min 23 sec

NMR spectrum 15

STANDARD CARBON PARAMETERS

Sample Name: [1-40-256-13C]

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Mar 20 2011

Temp. 25.1 C / 298.2 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
3456 repetitions
OBSERVE C13, 125.6997487 MHz
DECOUPLE H1, 499.9018501 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 58 min

NMR spectrum 16

1-A0-293-2

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 6 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993727 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

NMR spectrum 17

1-A0-293-2

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 6 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993727 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

NMR spectrum 18

STANDARD CARBON PARAMETERS

Sample Name: 1-A0-293-13C

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 7 2011

Temp. 22.0 C / 295.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2624 repetitions
OBSERVE C13, 75.4537562 MHz
DECOUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 53 hr, 41 min

NMR spectrum 19

2-A0-017-2

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Sep 13 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions

OBSERVE H1, 399.9410322 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec

NMR spectrum 20

2-A0-017-2

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3cn
Data collected on: Sep 13 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9410322 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec

NMR spectrum 21

2-A0-017-13C

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jan 6 2012

Temp. 21.9 C / 295.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2112 repetitions
OBSERVE C13, 75.4537539 MHz
DECOUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 5 hr, 22 min

NMR spectrum 22

2-A0-028-1

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Oct 31 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9410311 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec

NMR spectrum 23

2-A0-028-1

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3cn
Data collected on: Oct 31 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9410311 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec

NMR spectrum 24

2-A0-028-13C

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Jan 3 2012

Temp. 23.3 C / 296.4 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
21952 repetitions
OBSERVE C13, 125.7001162 MHz
DECOUPLE H1, 499.9035348 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 569 hr, 43 min

NMR spectrum 25

2-A0-028-13C

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Jan 3 2012

Temp. 23.3 C / 296.4 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
21952 repetitions
OBSERVE C13, 125.7001162 MHz
DECOUPLE H1, 499.9035348 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 569 43 min

NMR spectrum 26

2-A0-020-6

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jan 3 2012

Operator: Detty

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8000.0 Hz

8 repetitions

OBSERVE H1, 499.9010665 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 0 min 24 sec

NMR spectrum 27

2-A0-020-6

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Jan 3 2012

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9010665 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

NMR spectrum 28

2-A0-020-13C

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Jan 3 2012

Temp. 22.4 C / 295.6 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
3200 repetitions
OBSERVE C13, 125.7001172 MHz
DECOUPLE H1, 499.8035348 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 58 min

NMR spectrum 29

2-A0-020-13C

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Jan 3 2012

Temp. 22.8 C / 295.9 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
3840 repetitions
OBSERVE C13, 125.7001172 MHZ
DECOUPLE H1, 499.9035348 MHZ
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 58 min

NMR spectrum 30

2-A0-029-2

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Dec 12 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993712 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

NMR spectrum 31

2-A0-029-2

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Dec 12 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993712 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

NMR spectrum 32

STANDARD CARBON PARAMETERS

Sample Name: 2-A0-029-13C

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: 2-A0-029-13C

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2cl2
Data collected on: Dec 15 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
23040 repetitions
OBSERVE C13, 75.4537539 MHz
DECOUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 536 hr, 57 min

NMR spectrum 33

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: 2-A0-029-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Dec 15 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
23040 repetitions

OBSERVE C13, 75.4537539 MHz
DECOUPLE H1, 300.0760191 MHz

Power 38 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 536 hr, 57 min