Supporting Information for:

Radiosynthesis and Evaluation of [^{11}C-*Carbonyl*]-Labeled Carbamates as Fatty Acid Amide Hydrolase Radiotracers for Positron Emission Tomography.

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Contents:

1. Time-dependent inhibition of rat brain FAAH by **1** and **8**
2. Regional brain biodistribution of [^{11}C-*carbonyl*]carbamates in rats.
3. Kinetics of irreversible binding of [^{11}C-*carbonyl*]carbamates to FAAH ex vivo in rat brain.
4. Select RadioHPLC chromatograms from radiosynthesis of [^{11}C- *carbonyl*]carbamates
5. ^{1}H and ^{13}C NMR spectra of reported compounds.

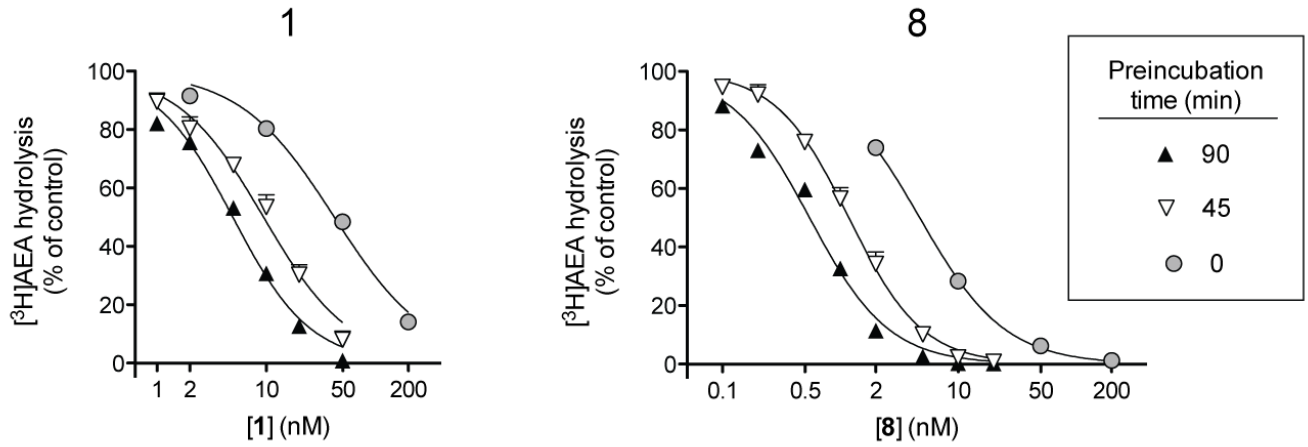
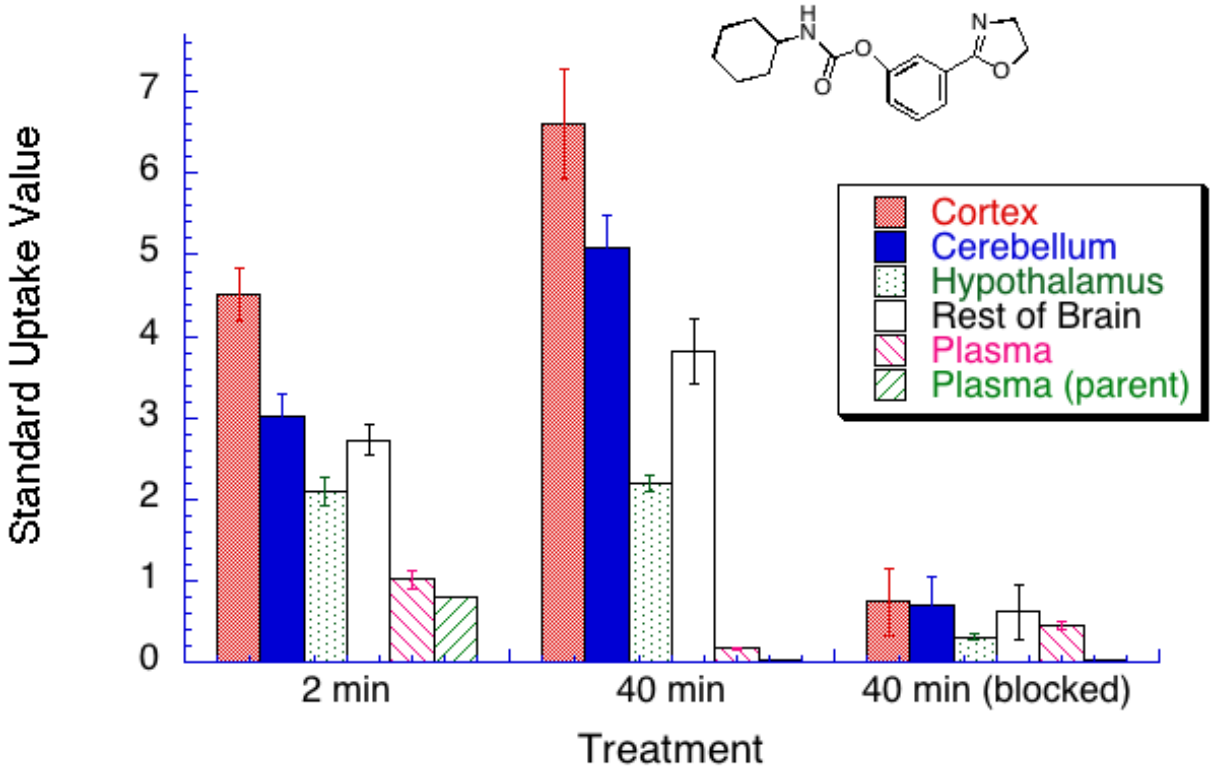
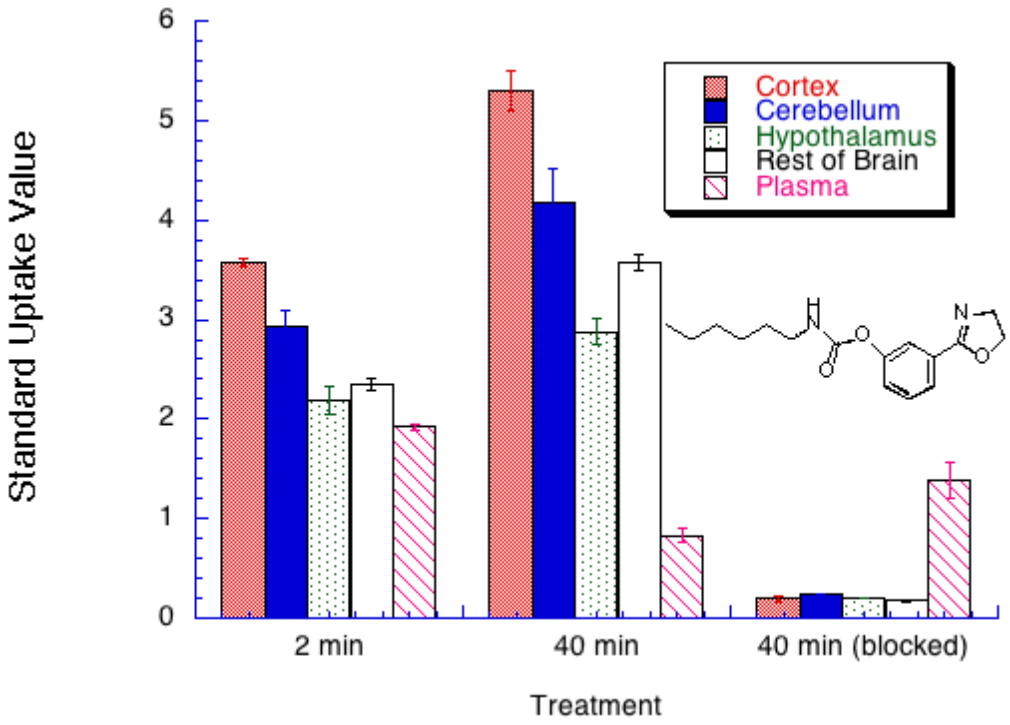


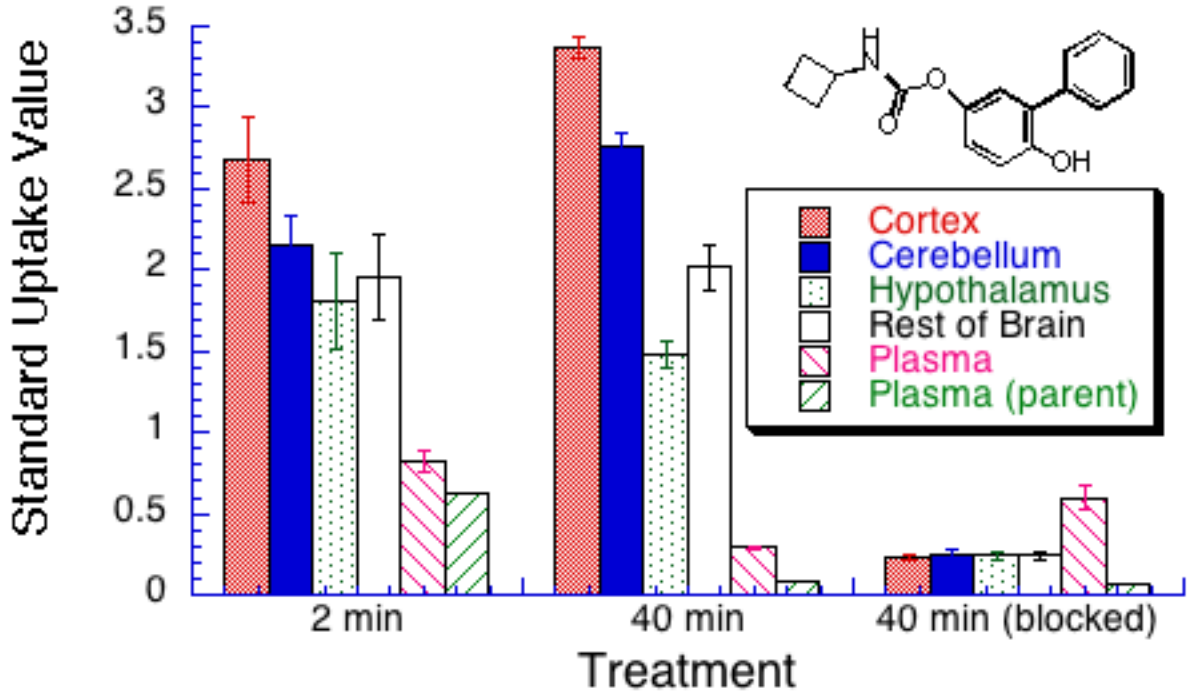
Figure S1. Time-dependent incubation by **8** (top panel) and **1** (bottom panel) of 0.5 μM [^{3}H]anandamide hydrolysis by rat brain homogenates. Shown are means ± s.e.m. (when not enclosed by the symbols), n=3, of the activity as % of the vehicle controls.



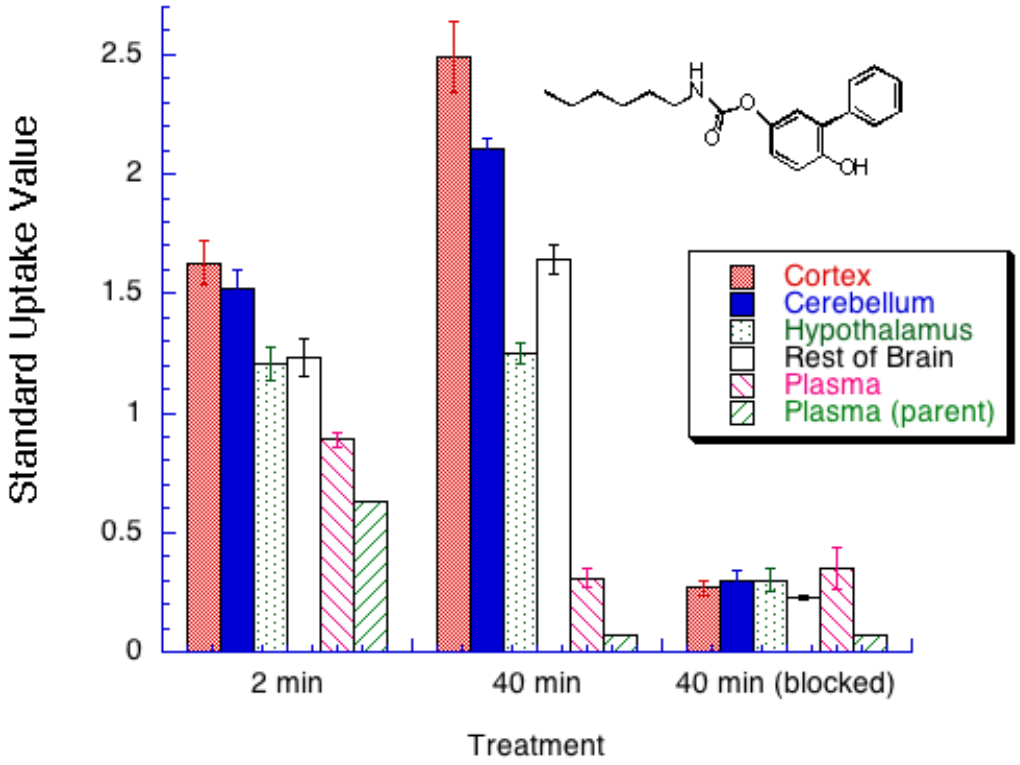
Figures S2. Regional uptake of radioactivity in rat brain [^{11}C]**6** at 2 and 40 min post iv injection. The blocked group was pre-treated with URB597 (2mg/kg, ip). Each value represents the mean (n=5) ± SD.



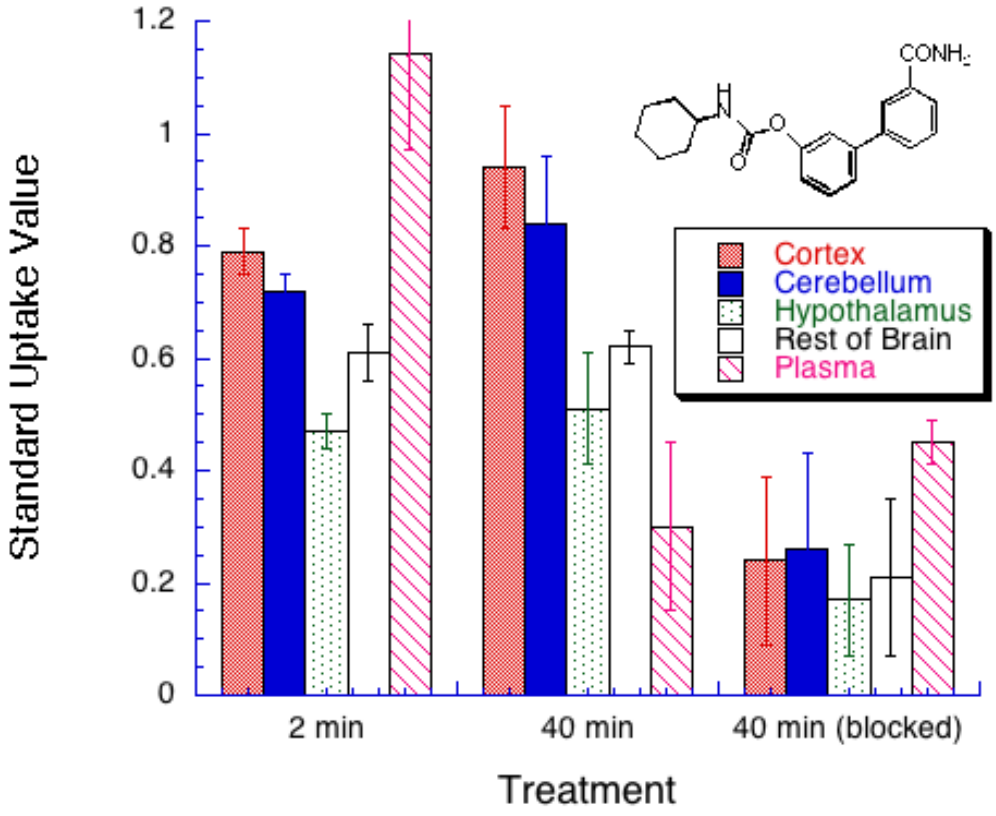
Figures S3. Regional uptake of radioactivity in rat brain [^{11}C]**8** at 2 and 40 min post iv injection. The blocked group was pre-treated with URB597 (2mg/kg, ip). Each value represents the mean (n=5) ± SD.



Figures S4. Regional uptake of radioactivity in rat brain [^{11}C]**4** at 2 and 40 min post iv injection. The blocked group was pre-treated with URB597 (2mg/kg, ip). Each value represents the mean (n=5) ± SD.



Figures S5. Regional uptake of radioactivity in rat brain [^{11}C]**5** at 2 and 40 min post iv injection. The blocked group was pre-treated with URB597 (2mg/kg, ip). Each value represents the mean (n=5) ± SD.



Figures S6. Regional uptake of radioactivity in rat brain [^{11}C]**2** at 2 and 40 min post iv injection. The blocked group was pre-treated with URB597 (2mg/kg, ip). Each value represents the mean (n=5) ± SD.

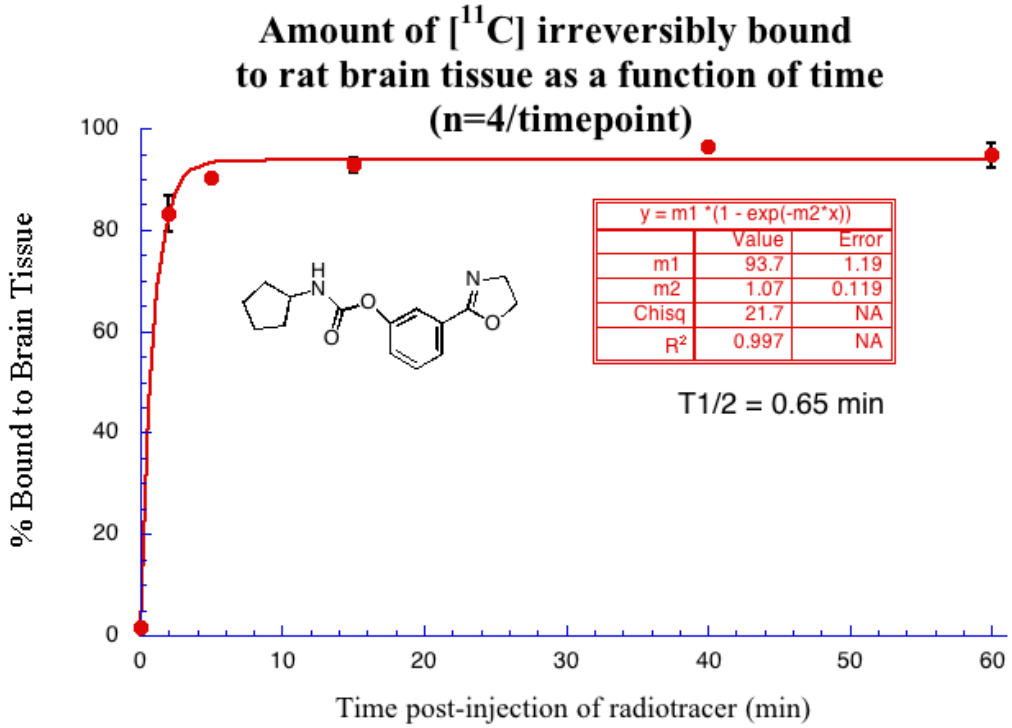


Figure S7. % of radioactivity irreversibly bound to rat brain parenchyma post-intravenous injection of [^{11}C]**7** (n=4/group) at various time points.

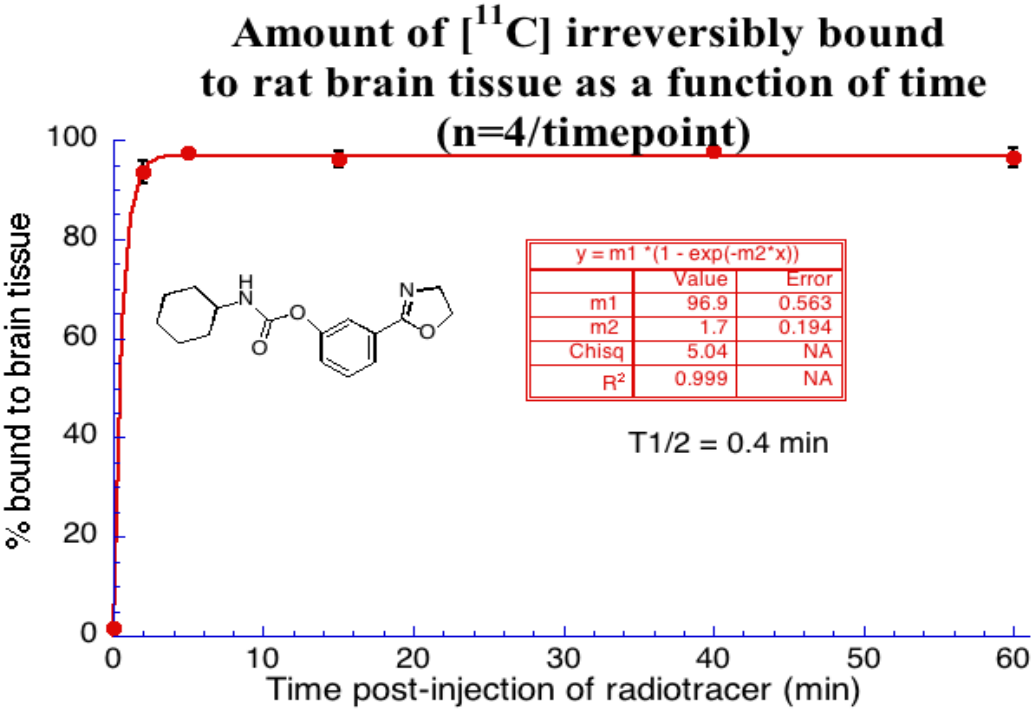


Figure S8. % of radioactivity irreversibly bound to rat brain parenchyma post-intravenous injection of [^{11}C]**6** (n=4/group) at various time points.

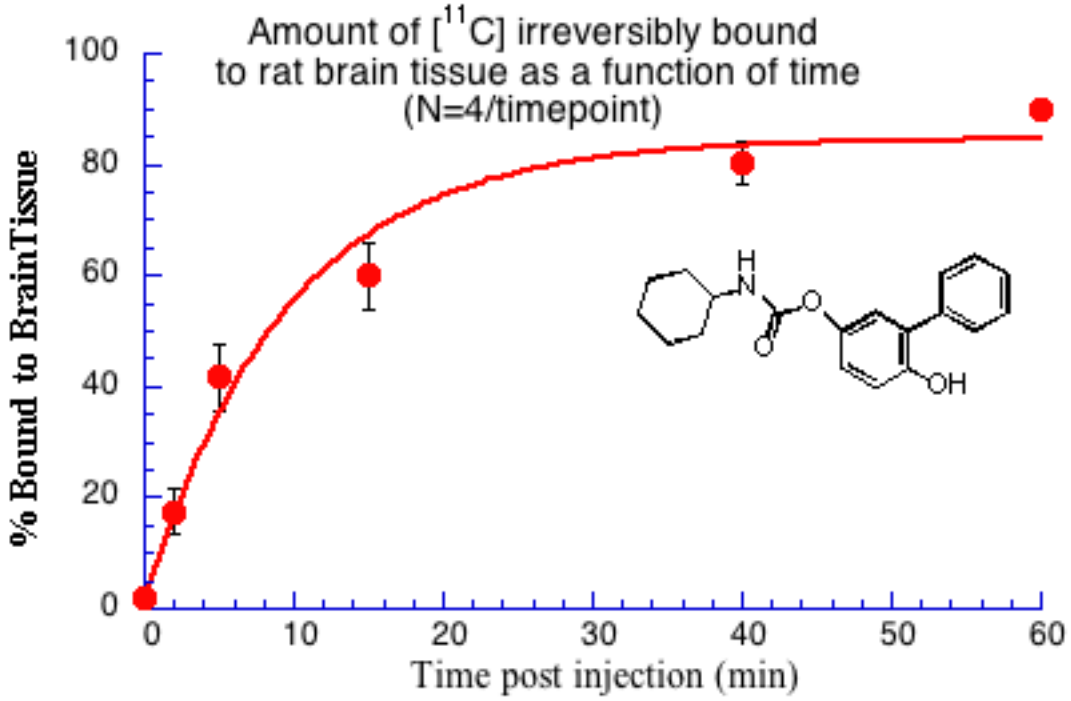


Figure S9. % of radioactivity irreversibly bound to rat brain parenchyma post-intravenous injection of [^{11}C]**1** (n= 4/group) at various time points.

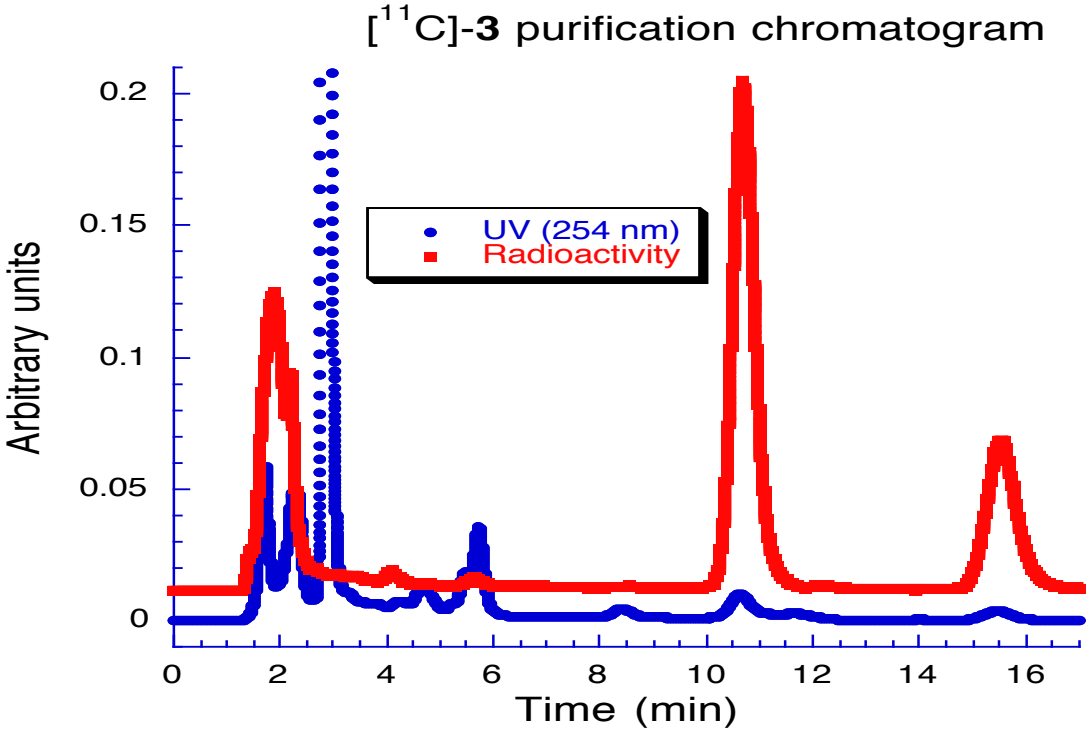


Figure S10. Radio-HPLC chromatogram: purification of [^{11}C]**3** which elutes at 15.5 min. The large radioactivity peak at 11 min corresponds to the unwanted regioisomer. Conditions: Phenomenex Luna C18(2), 250x10mm, 10 µ, 60/40 MeOH/H_2O +0.1N ammonium formate, 254nm, 9 mL/min.

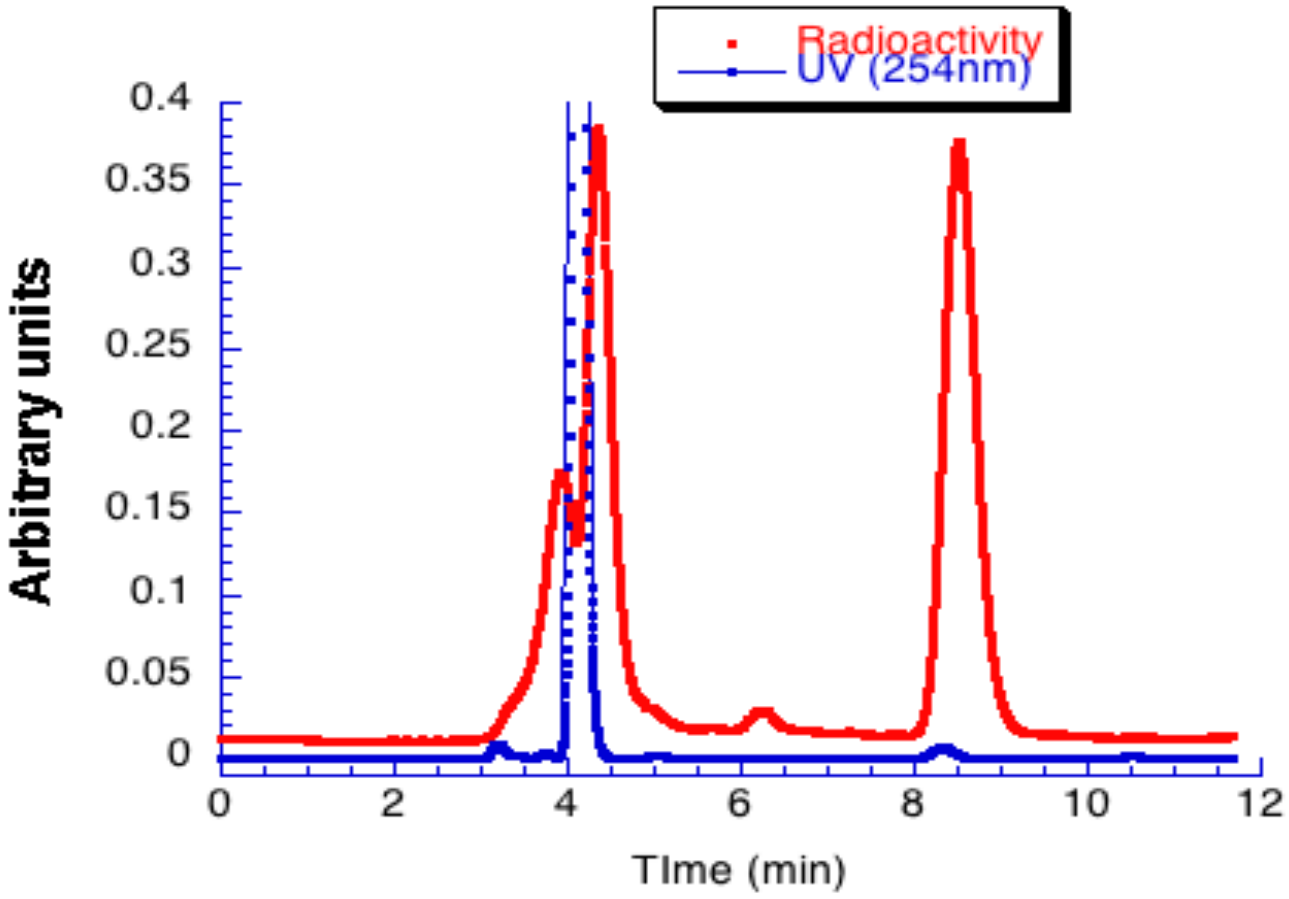


Figure S11. Radio-HPLC chromatogram: purification of [^{11}C]**6** which elutes at 8.4 min. Conditions: Phenomenex Luna C18(2), 250x10mm, 10 μ, 40/60 CH_3CN/H_2O +0.1N ammonium formate, 254nm, 7 mL/min.

^{1}H and ^{13}C NMR of **2**

6/8/2012 11:08:13 AM

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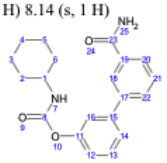
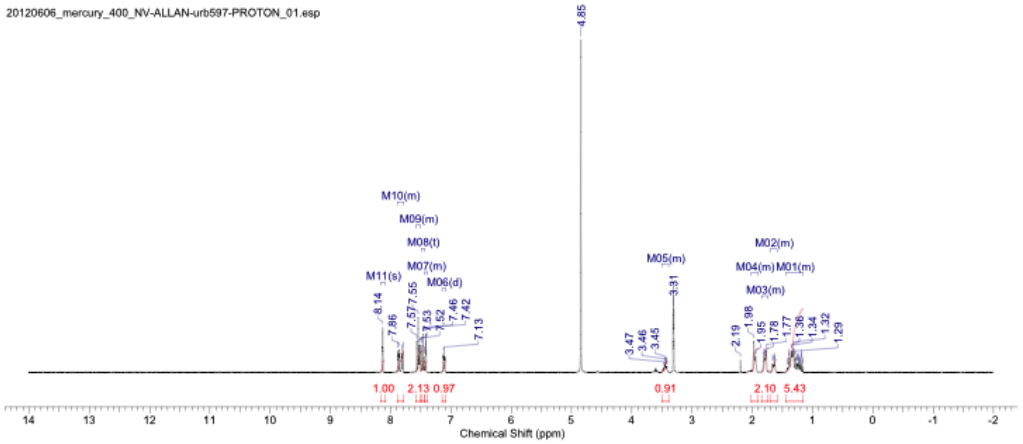
Spectrum Offset (Hz)	2398.0574	Sweep Width (Hz)	6389.78	Temperature (degree C)	25.000		

1H NMR (399 MHz, METHANOL-d_4) δ ppm 1.16 - 1.45 (m, 5 H) 1.59 - 1.71 (m, 1 H) 1.75 - 1.85 (m, 2 H) 1.90 - 2.02 (m, 2 H) 3.39 - 3.50 (m, 1 H) 7.12 (d, =7.02 Hz, 1 H) 7.39 - 7.43 (m, 1 H) 7.46 (t, =7.80 Hz, 1 H) 7.51 - 7.58 (m, 2 H) 7.78 - 7.89 (m, 2 H) 8.14 (s, 1 H)





6/8/2012 11:14:26 AM

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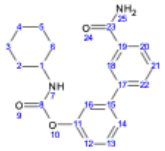
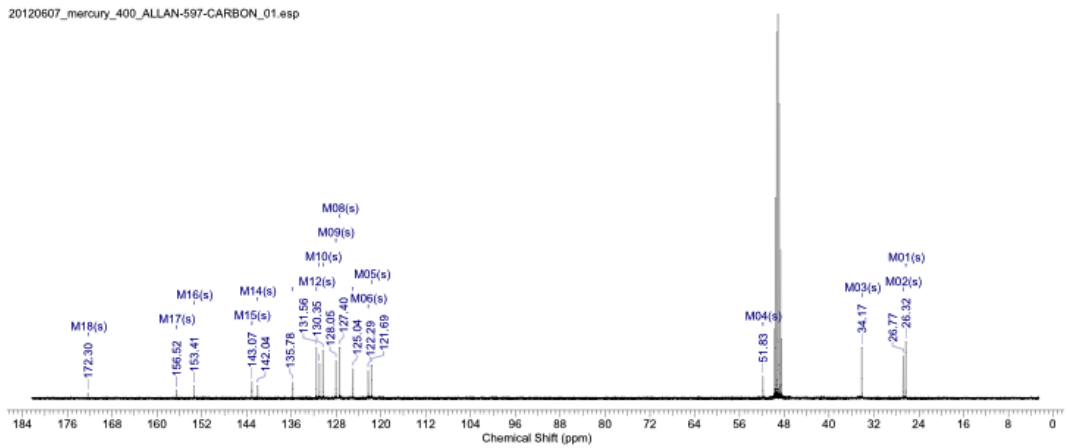
Pulse Sequence	s2pul	Receiver Gain	39.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	9281.7891
Sweep Width (Hz)	18050.54	Temperature (degree C)	25.000				

13C NMR (100 MHz, DMSO-d_6) δ ppm 26.32 (s, 1 C) 26.77 (s, 1 C) 34.17 (s, 1 C) 51.83 (s, 1 C) 121.69 (s, 1 C) 122.29 (s, 1 C) 125.04 (s, 1 C) 127.40 (s, 1 C) 128.05 (s, 1 C) 130.35 (s, 1 C) 131.01 (s, 1 C) 131.56 (s, 1 C) 135.78 (s, 1 C) 142.04 (s, 1 C) 143.07 (s, 1 C) 153.41 (s, 1 C) 156.52 (s, 1 C) 172.30 (s, 1 C)





^{1}H and ^{13}C NMR of **3**

4/15/2011 4:39:53 PM

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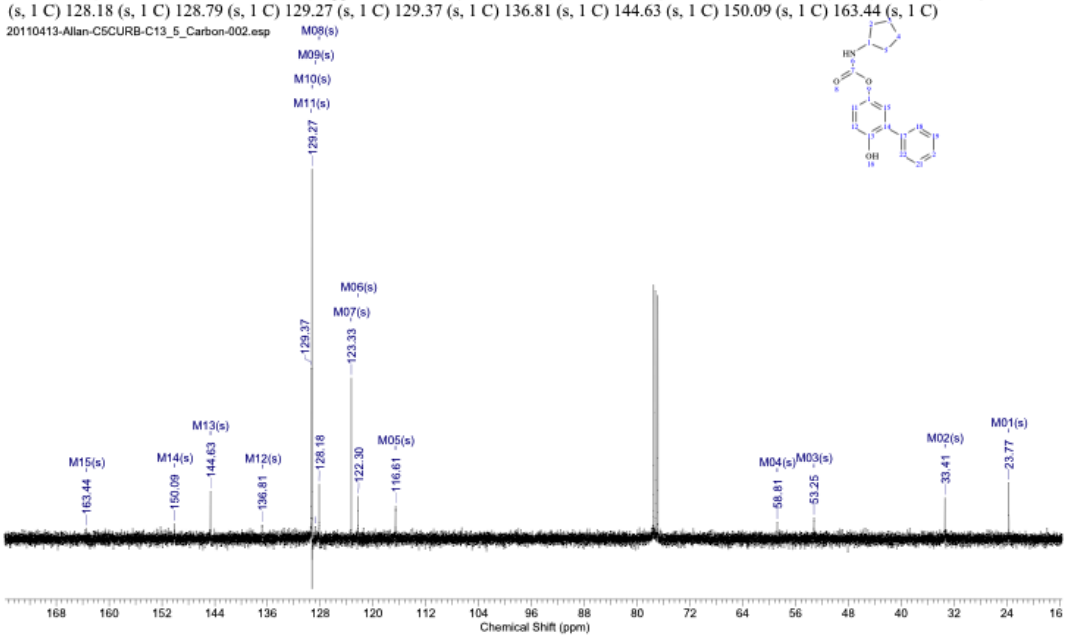
Pulse Sequence	s2pul	Receiver Gain	39.00	Solvent	CHLOROFORM-d	
Spectrum Offset (Hz)	10544.9658	Sweep Width (Hz)	24096.38	Temperature (degree C)	25.000	

13C NMR (100 MHz, CHLOROFORM-*d*) δ ppm 23.77 (s, 1 C) 33.41 (s, 1 C) 53.25 (s, 1 C) 58.81 (s, 1 C) 116.61 (s, 1 C) 122.30 (s, 1 C) 123.33 (s, 1 C) 128.18 (s, 1 C) 128.79 (s, 1 C) 129.27 (s, 1 C) 129.37 (s, 1 C) 136.81 (s, 1 C) 144.63 (s, 1 C) 150.09 (s, 1 C) 163.44 (s, 1 C)



4/15/20114:19:36 PM

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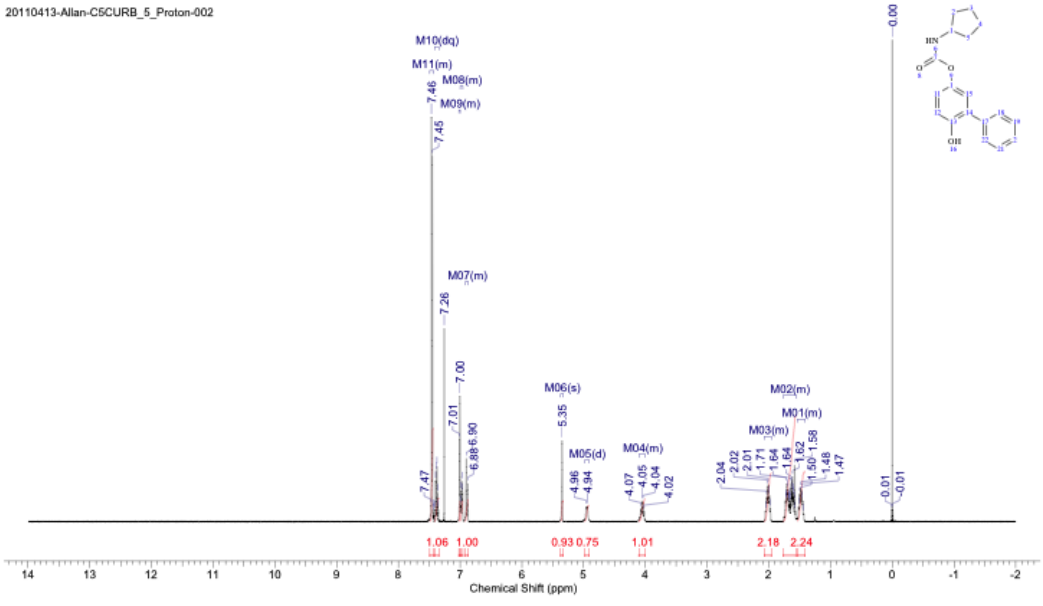
Numberof Transients	16	OriginalPoints Count	19109	PointsCount	32768	PulseSequence	s2pul
ReceiverGain	30.00	Solvent	CHLOROFORM-d			SpectrumOffset (Hz)	2395.6104
SweepWidth (Hz)	6385.70	Temperature(degree C)	25.000				

1H NMR (399 MHz, CHLOROFORM- *d*) δppm 1.42 - 1.54 (m, 2 H) 1.56 - 1.77 (m, 4 H) 1.96 - 2.07 (m, 2 H) 4.00 - 4.11 (m, 1 H) 4.95 (d, =6.63 Hz,1 H) 5.35 (s, 1 H) 6.87 - 6.92 (m, 1 H) 6.96 - 7.00 (m, 1 H) 7.00 - 7.02 (m, 1 H) 7.38 (dq, =8.50,4.31 Hz, 1 H) 7.43 - 7.49 (m, 4 H)



^{1}H and ^{13}C NMR of **4**

6/8/2012 10:58:54 AM

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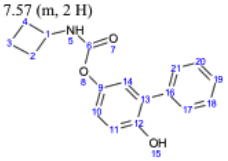
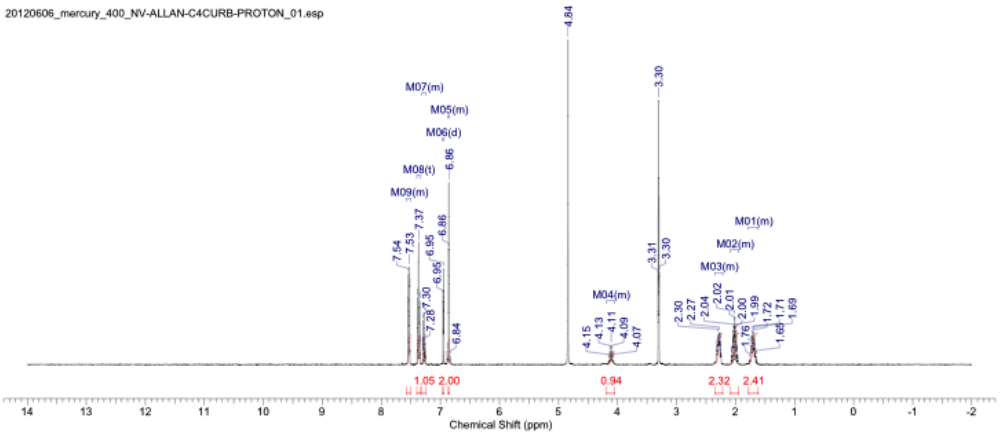
Nucleus	1H	**Number of Transients**	16	**Original Points Count**	16384	**Points Count**	16384
Pulse Sequence	s2pul	**Receiver Gain**	39.00	**Solvent**	METHANOL-d4		
Spectrum Offset (Hz)	2395.9661	**Sweep Width (Hz)**	6389.78	**Temperature (degree C)**	25.000		

1H NMR (399 MHz, METHANOL-d_4) δ ppm 1.62 - 1.78 (m, 2 H) 1.94 - 2.09 (m, 2 H) 2.22 - 2.35 (m, 2 H) 4.04 - 4.18 (m, =8.58, 8.29, 8.14, 8.14 Hz, 1 H) 6.85 - 6.87 (m, 2 H) 6.95 (d, =3.12 Hz, 1 H) 7.25 - 7.31 (m, 1 H) 7.37 (t, =7.41 Hz, 2 H) 7.50 - 7.57 (m, 2 H)





6/8/2012 11:06:34 AM

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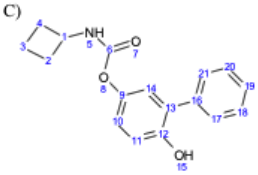
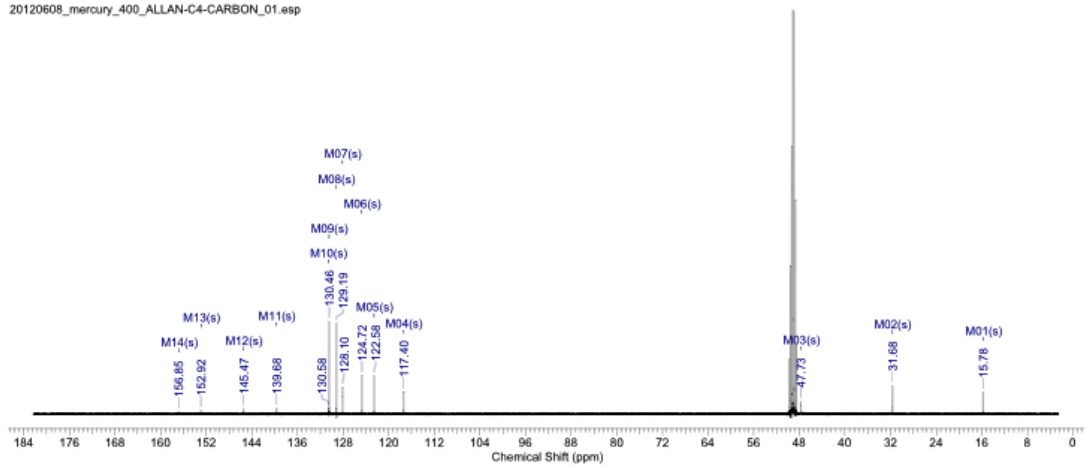
Nucleus	13C	**Number of Transients**	5000	**Original Points Count**	23541	**Points Count**	32768
Pulse Sequence	s2pul	**Receiver Gain**	39.00	**Solvent**	DMSO-d6	**Spectrum Offset (Hz)**	9281.7891
Sweep Width (Hz)	18050.54	**Temperature (degree C)**	25.000				

13C NMR (100 MHz, DMSO-d_6) δ ppm 15.78 (s, 1 C) 31.68 (s, 1 C) 47.73 (s, 1 C) 117.40 (s, 1 C) 122.58 (s, 1 C) 124.72 (s, 1 C) 128.10 (s, 1 C) 129.19 (s, 1 C) 130.46 (s, 1 C) 130.58 (s, 1 C) 139.68 (s, 1 C) 145.47 (s, 1 C) 152.92 (s, 1 C) 156.85 (s, 1 C)





^{1}H and ^{13}C NMR of **5**

xx

^{1}H NMR of **6**

4/14/2011 8:08:19 AM

Formula $C_{16}H_{20}N_2O_3$	*FW*	288.3416					
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File Name	G:\NV-NMR-2\20110413-Allan-FAAH-12_1_Proton-002			*Frequency (MHz)*	399.40	*Nucleus*	1H
Number of Transients	16	*Original Points Count*	19109	*Points Count*	32768	*Pulse Sequence*	s2pul
Receiver Gain	39.00	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	2400.7354
Sweep Width (Hz)	6385.70	*Temperature (degree C)*	25.000				

1H NMR (399 MHz, CHLOROFORM-*d*) δ ppm 1.14 - 1.30 (m, 3 H) 1.32 - 1.45 (m, 2 H) 1.50 - 1.68 (m, 3 H) 1.76 (dt, =9.16, 4.58 Hz, 2 H) 2.03 (d, =9.55 Hz, 2 H) 3.51 - 3.66 (m, 1 H) 4.06 (t, =9.45 Hz, 1 H) 4.43 (t, =9.65 Hz, 2 H) 7.22 - 7.31 (m, 2 H) 7.36 - 7.45 (m, 1 H) 7.53 - 7.63 (m, 1 H) 7.71 (s, 1 H) 7.79 (d, =7.99 Hz, 1 H)

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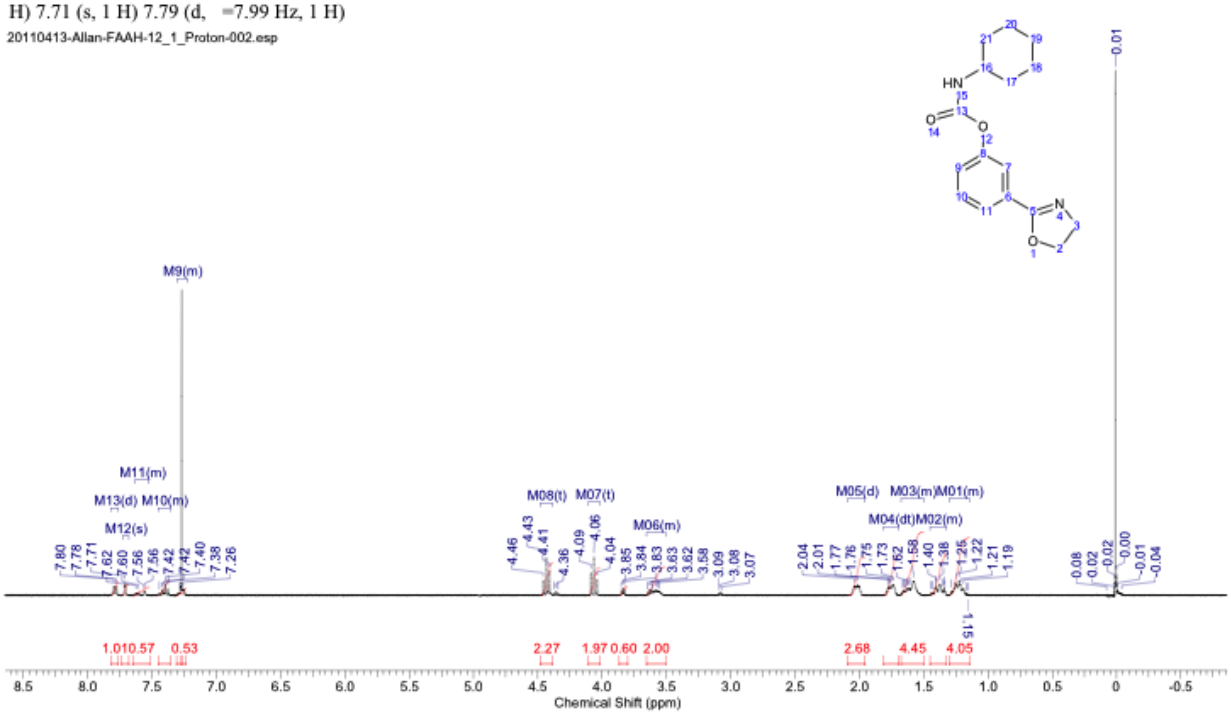

^{1}H NMR of **7**

4/14/2011 8:22:33 AM

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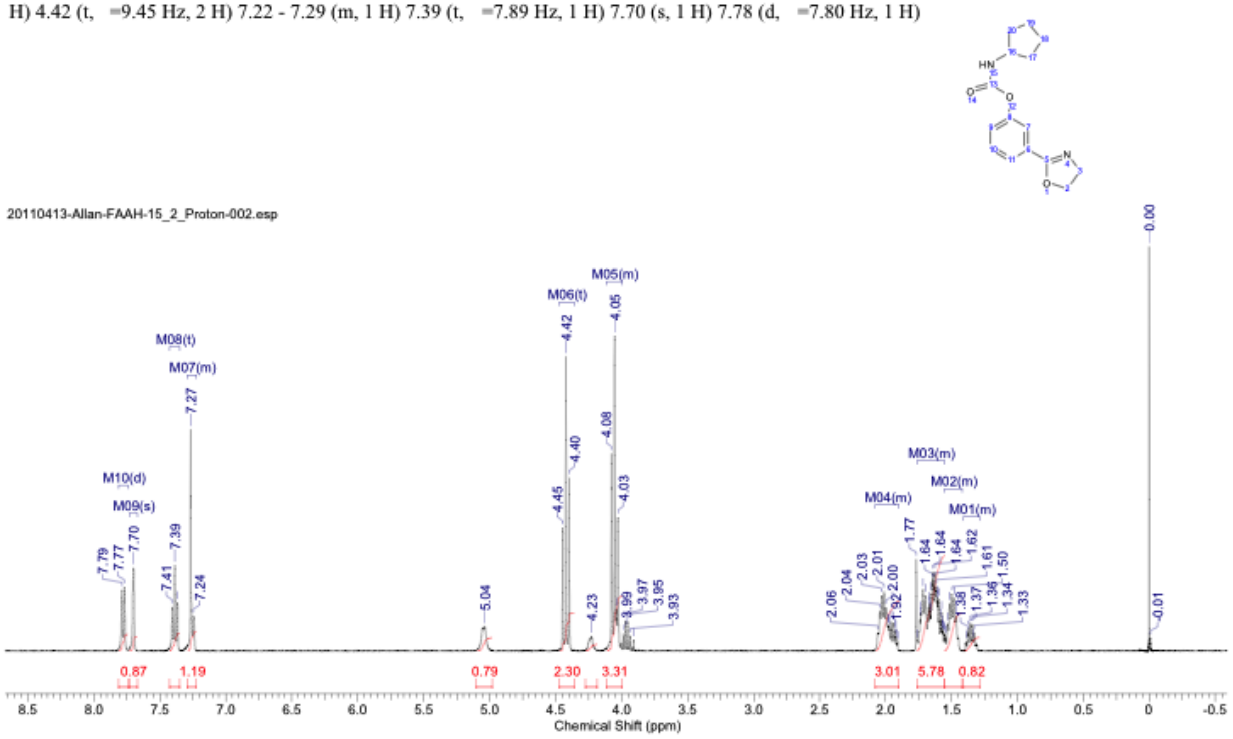
Number of Transients	16	Original Points Count	19109	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	30.00	Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2398.5334
Sweep Width (Hz)	6385.70	Temperature (degree C)	25.000				

1H NMR (399 MHz, CHLOROFORM-*d*) δ ppm 1.28 - 1.41 (m, 1 H) 1.42 - 1.55 (m, 2 H) 1.55 - 1.76 (m, 4 H) 1.90 - 2.07 (m, 2 H) 4.00 - 4.11 (m, 2 H) 4.42 (t, =9.45 Hz, 2 H) 7.22 - 7.29 (m, 1 H) 7.39 (t, =7.89 Hz, 1 H) 7.70 (s, 1 H) 7.78 (d, =7.80 Hz, 1 H)



^{1}H and ^{13}C NMR of **8**

xx

^{1}H and ^{13}C NMR of **9**

11/2/2011 1:16:55 PM

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Date Stamp	02 Nov 2011 15:21:36						
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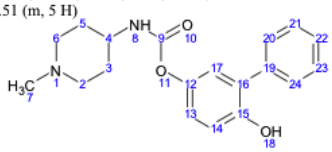
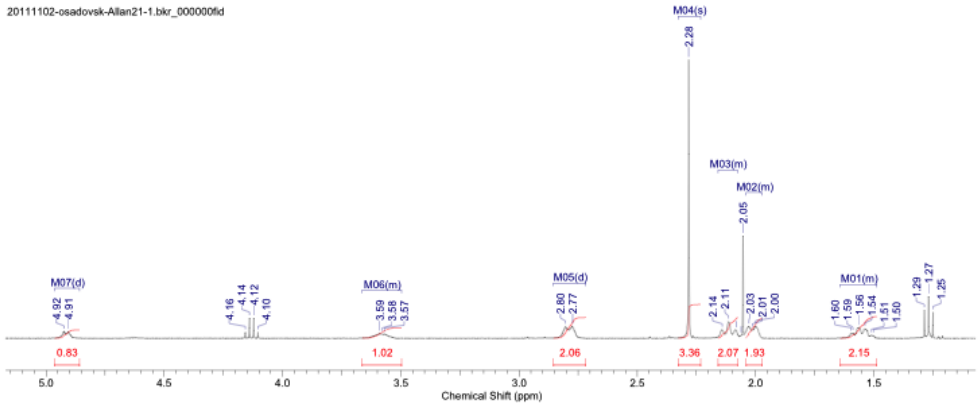
Frequency (MHz)	400.22	Nucleus	1H	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	walkup	Points Count	16384	Pulse Sequence	zg45
Receiver Gain	161.00	SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2392.5789
Sweep Width (Hz)	6409.87	Temperature (degree C)	25.160				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 1.49 - 1.64 (m, 2 H) 1.97 - 2.04 (m, 2 H) 2.08 - 2.16 (m, 2 H) 2.28 (s, 3 H) 2.79 (d, =11.74 Hz, 2 H) 3.50 - 3.66 (m, 1 H) 4.92 (d, =7.82 Hz, 1 H) 6.89 - 6.95 (m, 1 H) 6.97 - 7.04 (m, 2 H) 7.36 - 7.51 (m, 5 H)





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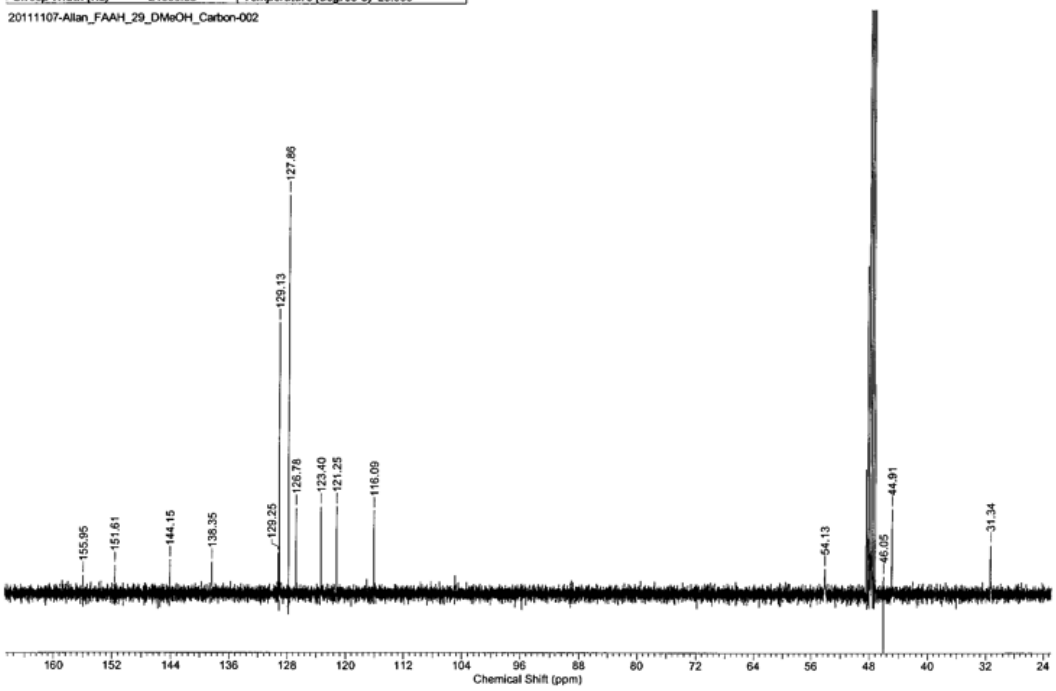
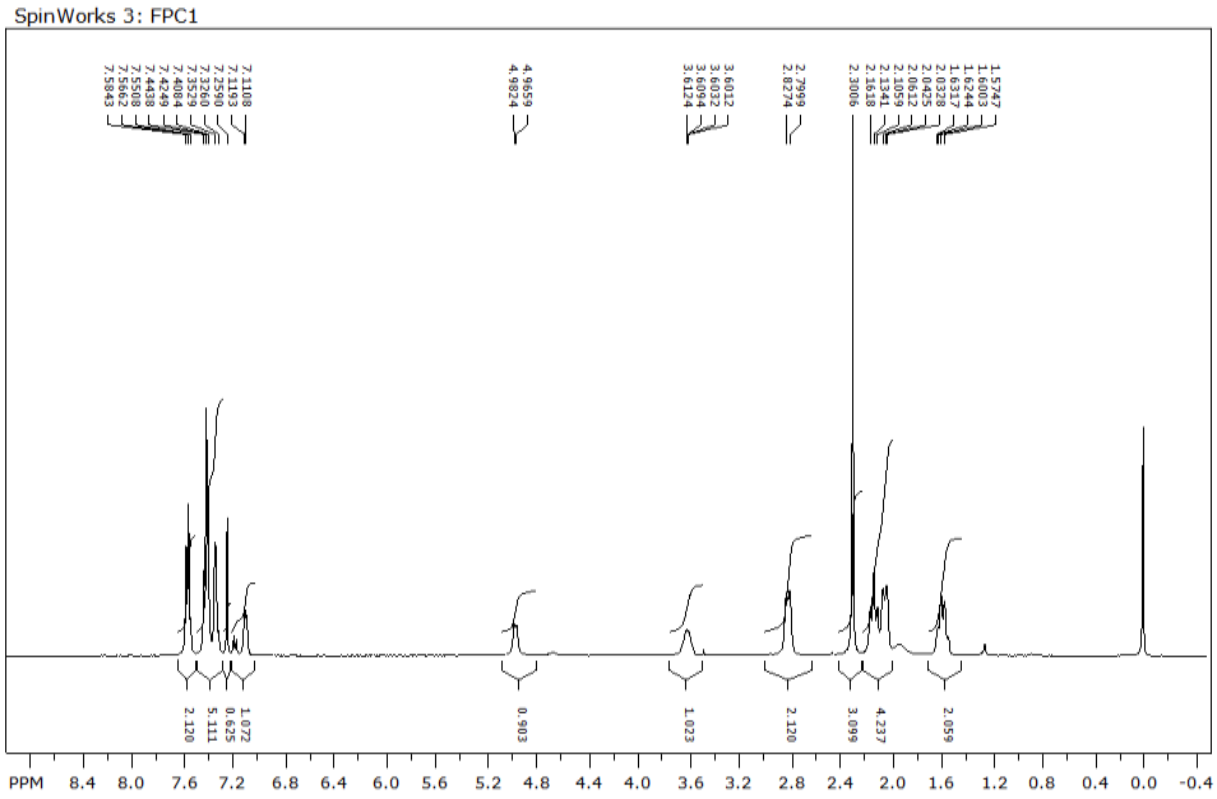
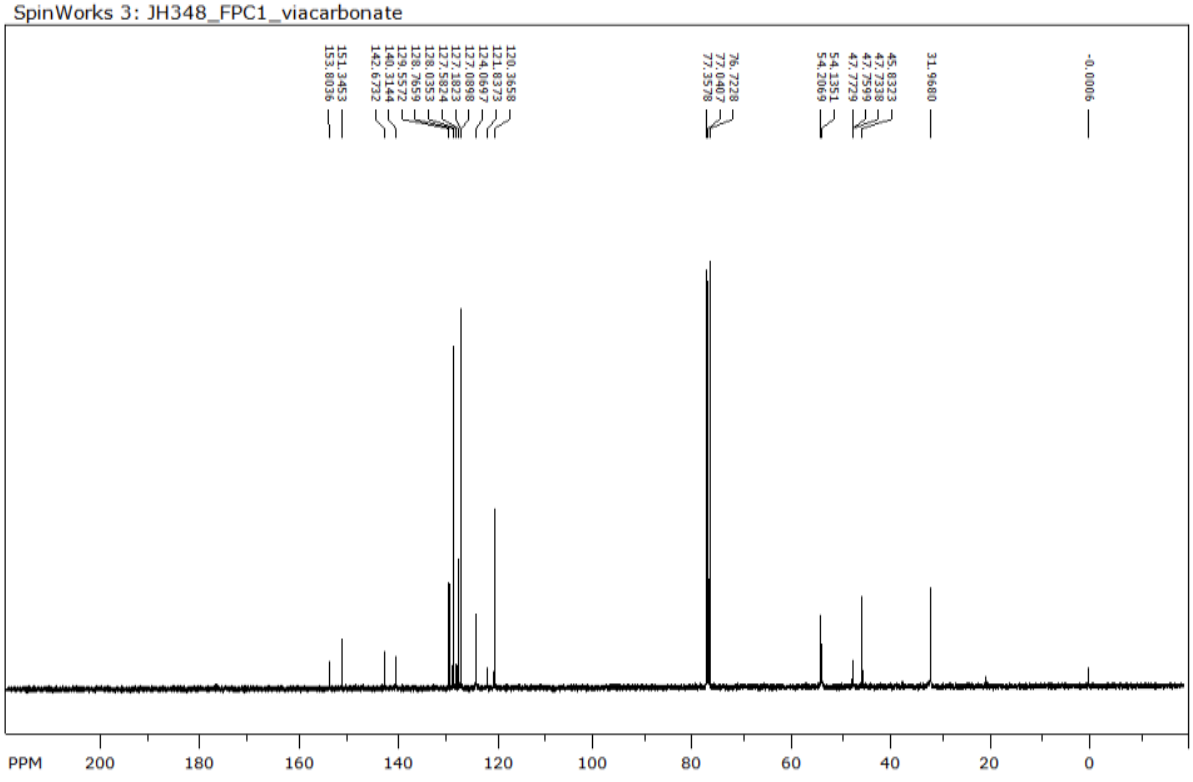
Pulse Sequence	s2pul	Receiver Gain	39.00	Solvent	METHANOL-d4	Spectrum Offset (Hz)	10544.0352
Sweep Width (Hz)	24096.38	Temperature (degree C)	25.000				

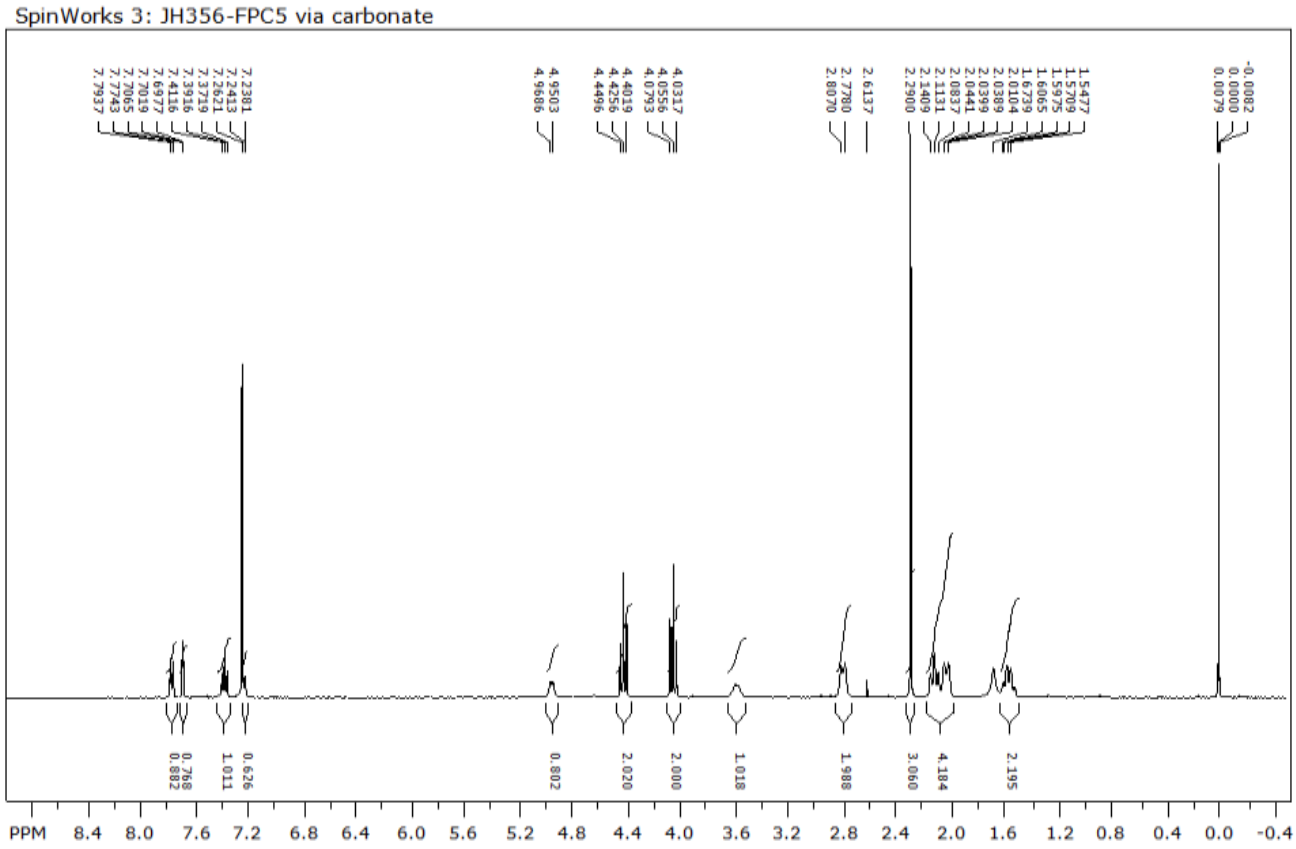


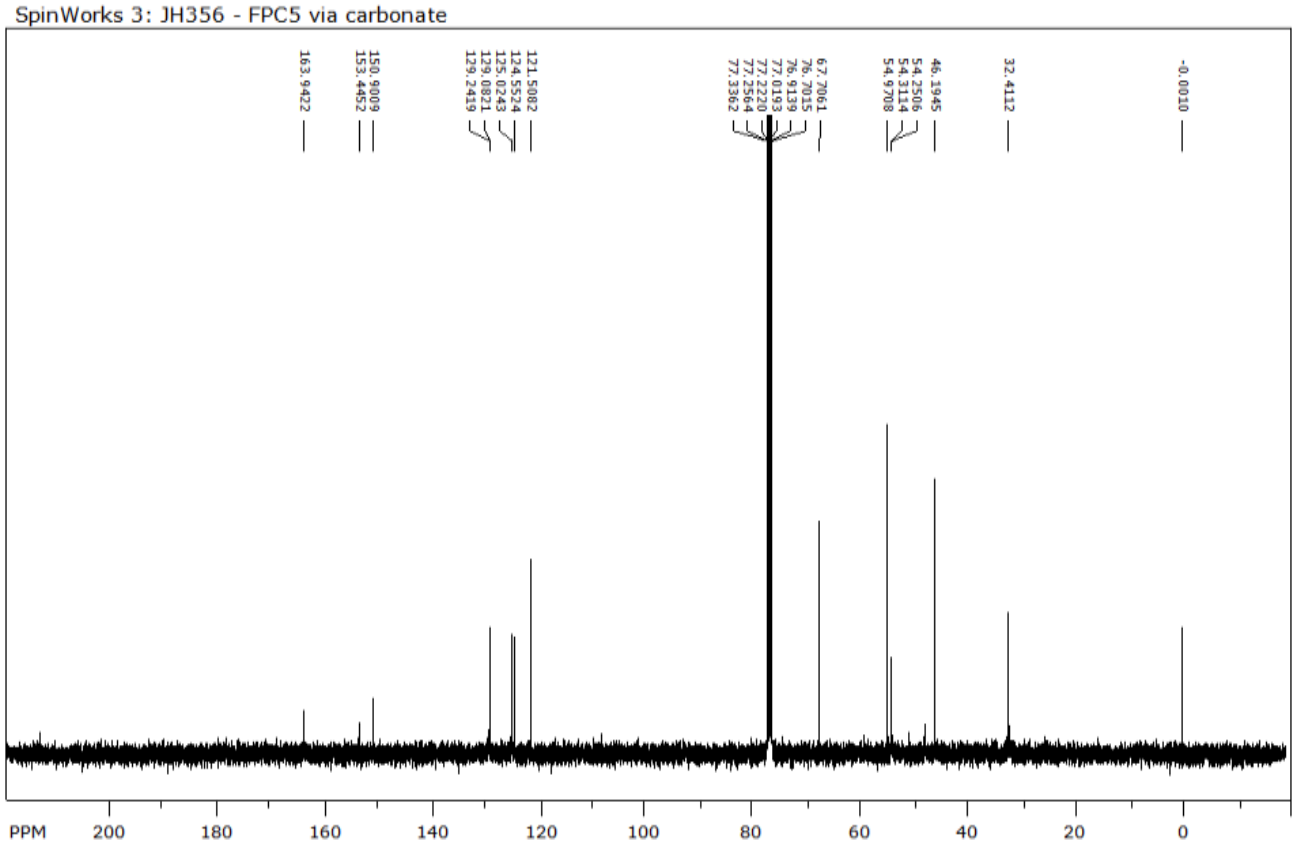
^{1}H and ^{13}C NMR of **10**





^{1}H and ^{13}C NMR of **11**


SpinWorks 3: JH356-FPC5 via carbonate
PPM

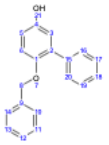

SpinWorks 3: JH356 - FPC5 via carbonate
PPM

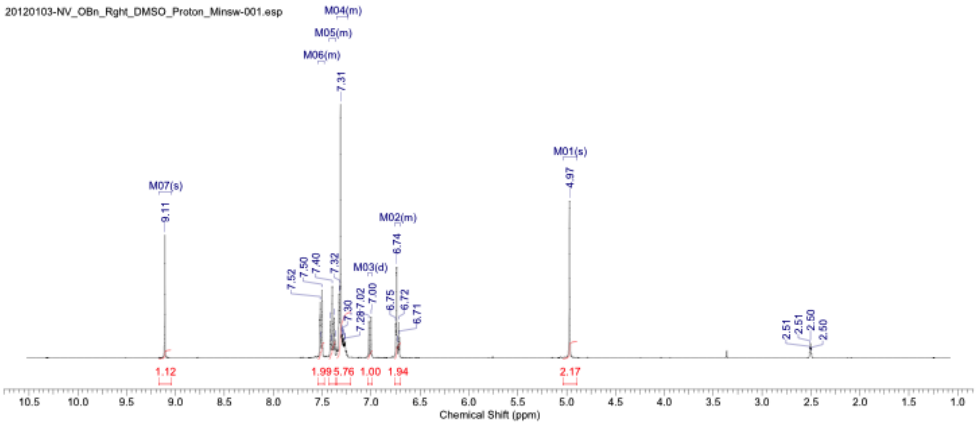
^{1}H and ^{13}C NMR of **14**

9/24/2012 11:17:25 AM

Formula $C_{19}H_{16}O_2$	FW	276.3291					
Acquisition Time (sec)	2.9924	Date	Jan 3 2012	Date Stamp	Jan 3 2012		
File Name	F:\Flesh-BASI-RABOTA\NV\NV-NMR-2\20120103-NV_OBn_Rght_DMSO_Proton_Minsw-001					Frequency (MHz)	399.36
Nucleus	1H	Number of Transients	16	Original Points Count	11292	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	22.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2316.0420
Sweep Width (Hz)	3773.58	Temperature (degree C)	25.000				

1H NMR (399 MHz, DMSO-d_6) δ ppm 4.97 (s, 2 H) 6.70 - 6.76 (m, 2 H) 7.01 (d, =8.52 Hz, 1 H) 7.24 - 7.35 (m, 6 H) 7.36 - 7.43 (m, 2 H) 7.48 - 7.54 (m, 2 H) 9.11 (s, 1 H)

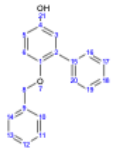


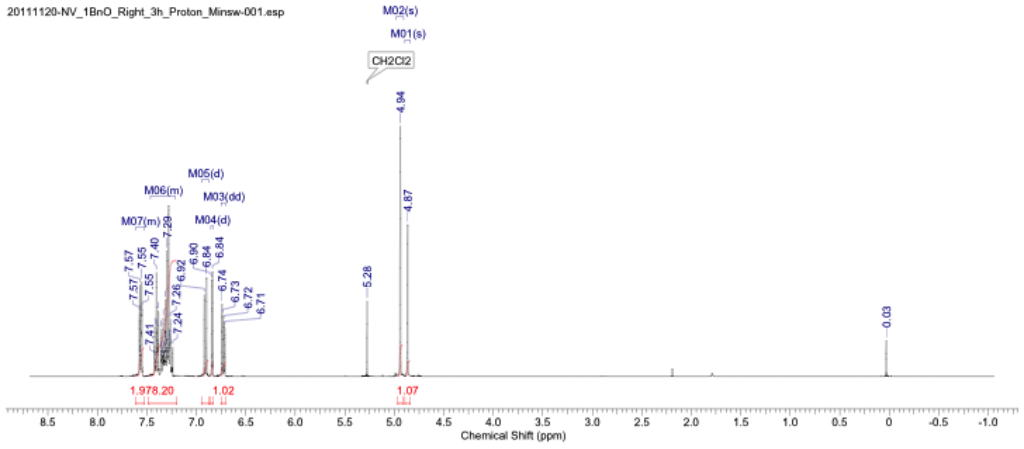


9/24/2012 11:22:56 AM

Formula $C_{19}H_{16}O_2$	FW	276.3291					
Acquisition Time (sec)	2.9925	Date	Nov 20 2011	Date Stamp	Nov 20 2011		
File Name	F:\Flesh-BASI-RABOTA\NV\NV-NMR-2\20111120-NV_1BnO_Right_3h_Proton_Minsw-001					Frequency (MHz)	399.36
Nucleus	1H	Number of Transients	16	Original Points Count	11644	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	18.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	1522.0955	Sweep Width (Hz)	3891.05	Temperature (degree C)	25.000		

1H NMR (399 MHz, CHLOROFORM-*d*) δ ppm 4.87 (s, 1 H) 4.94 (s, 2 H) 6.73 (dd, =8.79, 3.09 Hz, 1 H) 6.84 (d, =3.09 Hz, 1 H) 6.91 (d, =8.79 Hz, 1 H) 7.21 - 7.46 (m, 8 H) 7.53 - 7.61 (m, 2 H)

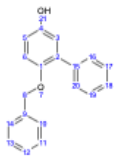


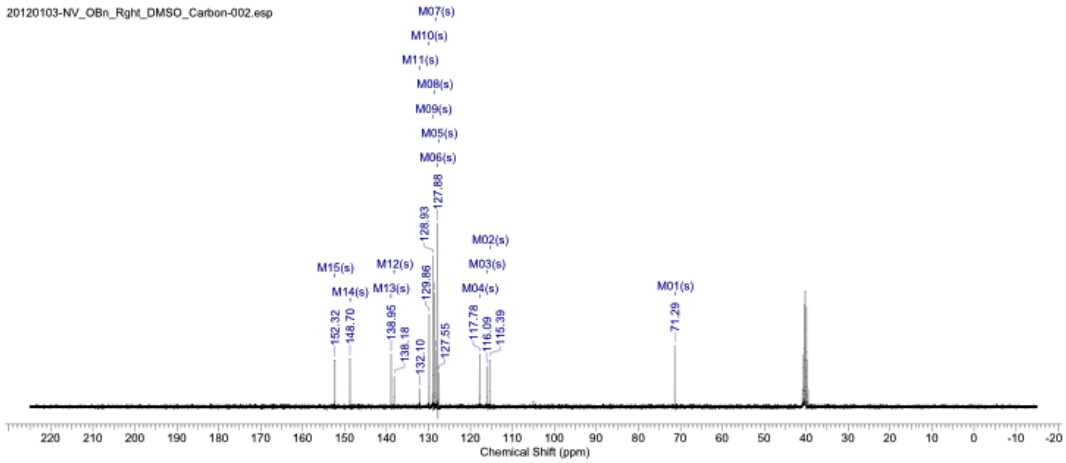


9/21/2012 11:55:08 AM

Formula $C_{19}H_{16}O_2$	FW	276.3291					
Acquisition Time (sec)	1.3005	Date	Jan 3 2012	Date Stamp	Jan 3 2012		
File Name	F:\Flesh-BASI-RABOTA\NV\NV-NMR-Z\20120103-NV_OBn_Rght_DMSO_Carbon-002					Frequency (MHz)	100.43
Nucleus	13C	Number of Transients	512	Original Points Count	31337	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	39.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	10544.0293
Sweep Width (Hz)	24096.38	Temperature (degree C)	25.000				

13C NMR (100 MHz, DMSO-d_6) δ ppm 71.29, 115.39, 116.09, 117.78, 127.55, 127.88, 128.18, 128.61, 128.93, 129.86, 132.10, 138.18, 138.95, 148.70, 152.32



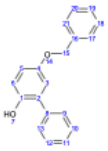


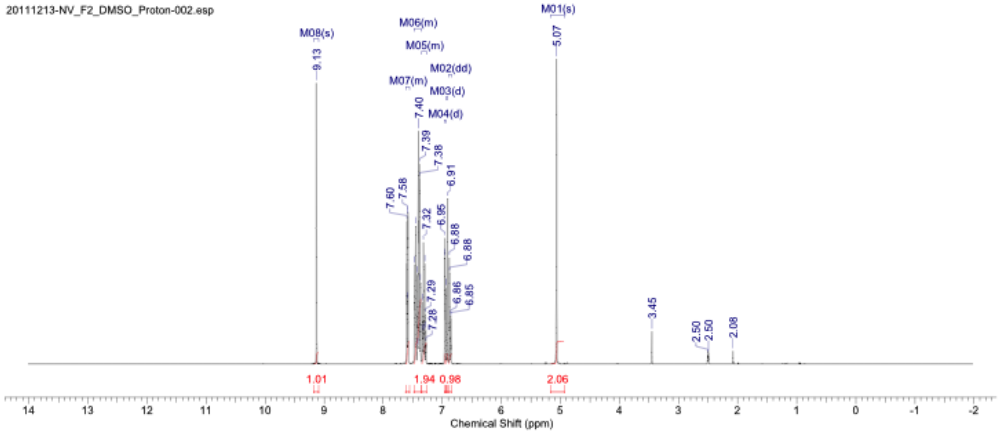
^{1}H and ^{13}C NMR of **15**

9/21/2012 11:14:10 AM

Formula $C_{19}H_{16}O_2$	FW	276.3291					
Acquisition Time (sec)	2.9925	Date	Dec 13 2011	Date Stamp	Dec 13 2011		
File Name	F:\Flesh-BASI-RABOTA\NV\NV-NMR-Z\20111213-NV_F2_DMSO_Proton-002					Frequency (MHz)	399.36
Nucleus	1H	Number of Transients	16	Original Points Count	19109	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	12.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2402.2405
Sweep Width (Hz)	6385.70	Temperature (degree C)	25.000				

1H NMR (399 MHz, DMSO-*d*$_6$) δ ppm 5.07 (s, 2 H) 6.87 (dd J=8.77 Hz, J=2.92 Hz,, 1 H) 6.92 (d, J=8.77 Hz, 1 H), 6.96 (d, =2.92 Hz, 1 H) 7.27 - 7.35 (m, 2 H) 7.36 - 7.48 (m, 6 H) 7.55 - 7.62 (m, 2 H) 9.13 (s, 1 H)

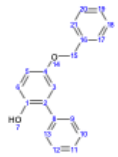


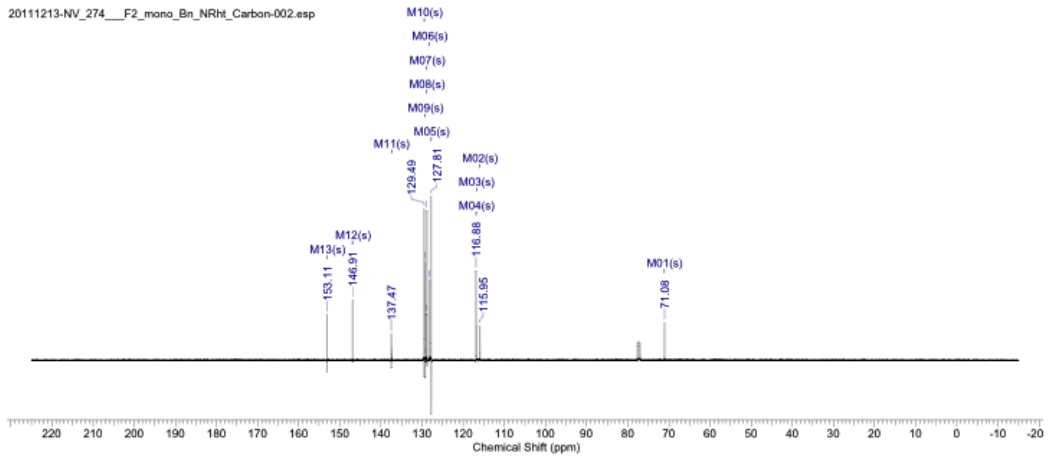


9/21/2012 11:17:13 AM

Formula $C_{19}H_{16}O_2$	FW	276.3291					
Acquisition Time (sec)	1.3005	Date	Dec 13 2011	Date Stamp	Dec 13 2011		
File Name	F:\Flesh-BASI-RABOTA\NV\NV-NMR-Z\20111213-NV_274___F2_mono_Bn_NRht_Carbon-002					Frequency (MHz)	100.43
Nucleus	13C	Number of Transients	512	Original Points Count	31337	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	39.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10543.9844	Sweep Width (Hz)	24096.38	Temperature (degree C)	25.000		

13C NMR (100 MHz, CHLOROFORM-*d*) δ ppm 71.08, 115.95, 116.84, 116.88, 127.81, 128.18, 128.83, 128.98, 129.29, 129.49, 137.47, 146.91, 153.11



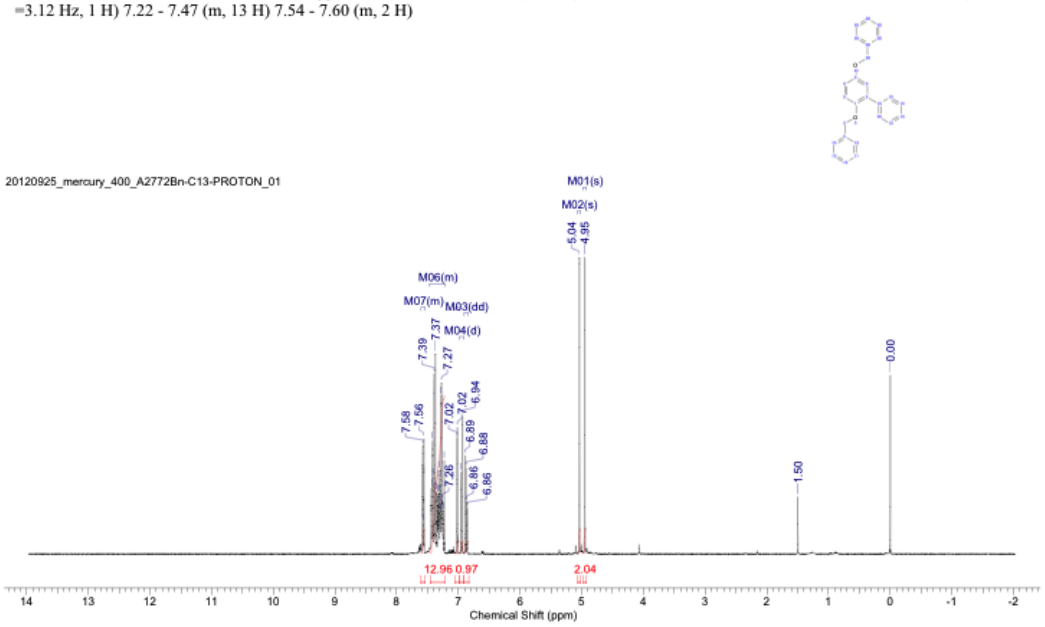


^{1}H and ^{13}C NMR of **16**

9/25/2012 1:16:23 PM

Formula $C_{26}H_{22}O_2$	FW	366.4517					
Acquisition Time (sec)	2.5641	Date	Sep 25 2012	Date Stamp	Sep 25 2012		
File Name	F:\NV-NMR-2\20120925_mercury_400_A2772Bn-C13-PROTON_01					Frequency (MHz)	399.31
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2383.6860	Sweep Width (Hz)	6389.78	Temperature (degree C)	25.000		

1H NMR (399 MHz, CHLOROFORM-*d*) δ ppm 4.95 (s, 2 H) 5.04 (s, 2 H) 6.87 (dd, =8.97 Hz, =3.12 Hz, 1 H) 6.95 (d, =8.97 Hz, 1 H) 7.02 (d, =3.12 Hz, 1 H) 7.22 - 7.47 (m, 13 H) 7.54 - 7.60 (m, 2 H)



9/25/2012 1:37:11 PM

Formula $C_{26}H_{22}O_2$	FW	366.4517					
Acquisition Time (sec)	1.3042	Date	Sep 25 2012	Date Stamp	Sep 25 2012		
File Name	F:\NV-NMR-2\20120925_mercury_400_A2772Bn-C13-CARBON_01					Frequency (MHz)	100.42
Nucleus	13C	Number of Transients	256	Original Points Count	32768	Points Count	32768
Pulse Sequence	s2pul	Receiver Gain	39.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	11044.5479	Sweep Width (Hz)	25125.63	Temperature (degree C)	25.000		

13C NMR (100 MHz, CHLOROFORM-*d*) δ ppm 70.67, 71.65, 114.29, 115.52, 117.73, 127.02, 127.08, 127.52, 127.55, 127.93, 127.97, 128.36, 128.57, 129.56, 132.72, 137.20, 137.42, 138.33, 150.04, 153.44