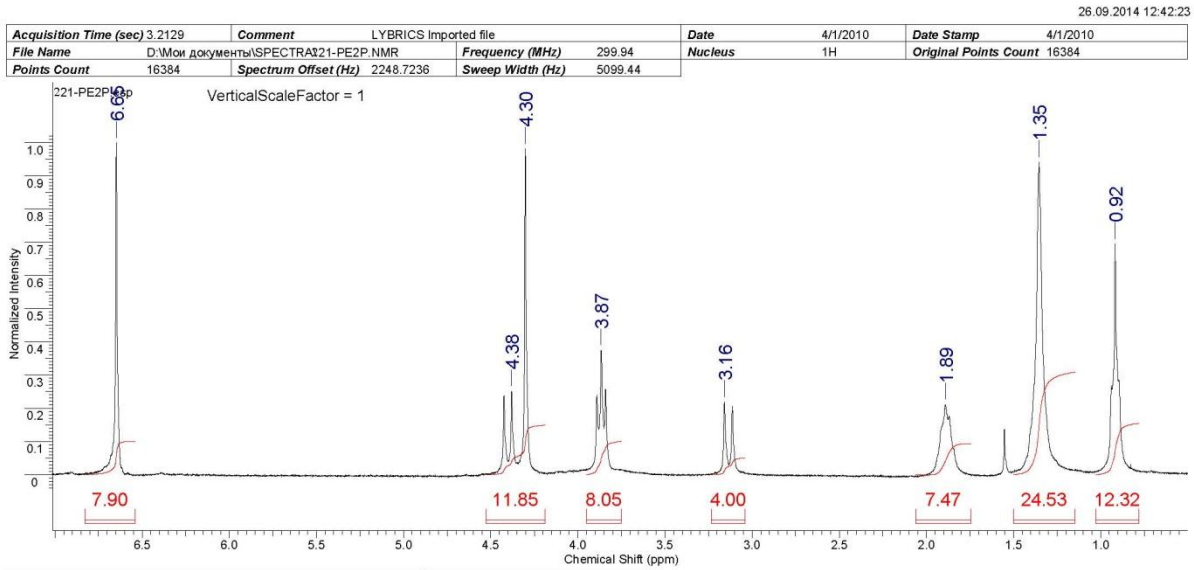
New Journal of Chemistry

Electronic supplementary information

Cationic amphiphilic calixarenes for DNA compaction into small nanoparticles and gene delivery

Roman V. Rodik, Ann-Sophie Anthony, Vitaly I. Kalchenko, Yves Mély Andrey S. Klymchenko

^{1}H NMR, ^{13}C NMR and FT-IR spectra for the synthesized compounds.



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.7812 .. 1.02	12.3187818	1.49431690e+7	12.31878185
2	[1.1484 .. 1.50	24.5281581	2.97536260e+7	24.52815819
3	[1.7453 .. 2.06	7.46528912	9.05569100e+6	7.46528912
4	[3.0410 .. 3.23	4.00000000	4.85215800e+6	4.00000000
5	[3.7501 .. 3.94	8.05417347	9.77003100e+6	8.05417347
6	[4.1888 .. 4.52	11.8505468	1.43751810e+7	11.85054684
7	[6.5405 .. 6.82	7.89795542	9.58053200e+6	7.89795542

No.	(ppm)	(Hz)	Height
1	0.92	275.2	0.6961
2	1.35	406.2	0.9419
3	1.89	567.1	0.2113
4	3.16	947.2	0.2190
5	3.87	1159.5	0.3747
6	4.30	1290.2	0.9817
7	4.38	1313.5	0.2511
8	6.65	1994.0	1.0000

Fig. S1. ^{1}H NMR of compound **5**.

26.09.2014 12:34:49

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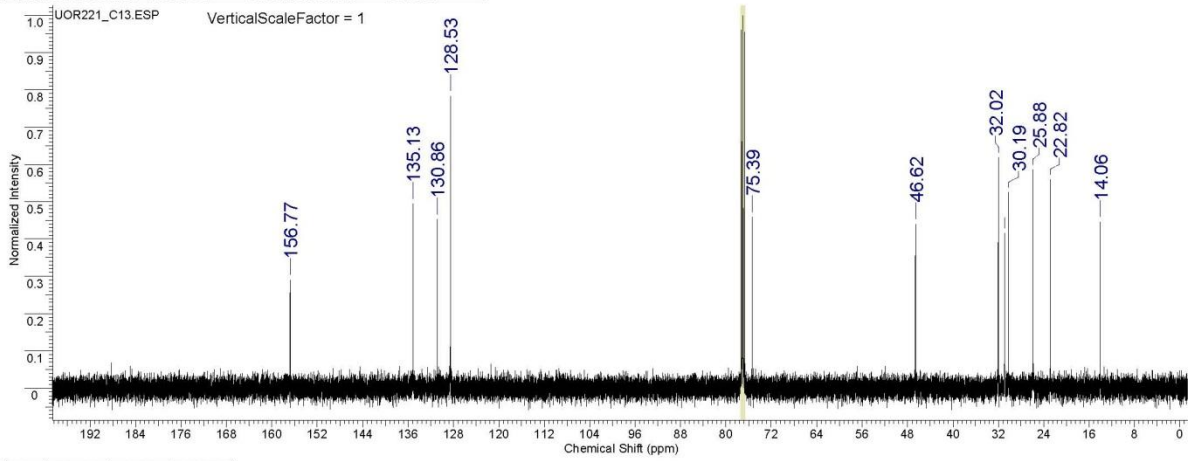
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	253	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	14996.9111	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	14.06	1767.4	0.4458
2	22.82	2868.9	0.5589
3	25.88	3254.4	0.5856
4	30.19	3795.4	0.5246
5	30.89	3883.2	0.4148
6	32.02	4025.8	0.6184
7	46.62	5860.8	0.4395
8	75.39	9479.1	0.4587
9	128.53	16160.0	0.7834
10	130.86	16452.7	0.4527
11	135.13	16989.3	0.4938

No.	(ppm)	(Hz)	Height
12	156.77	19710.9	0.2910

Fig. S2. ^{13}C NMR of compound **5**.

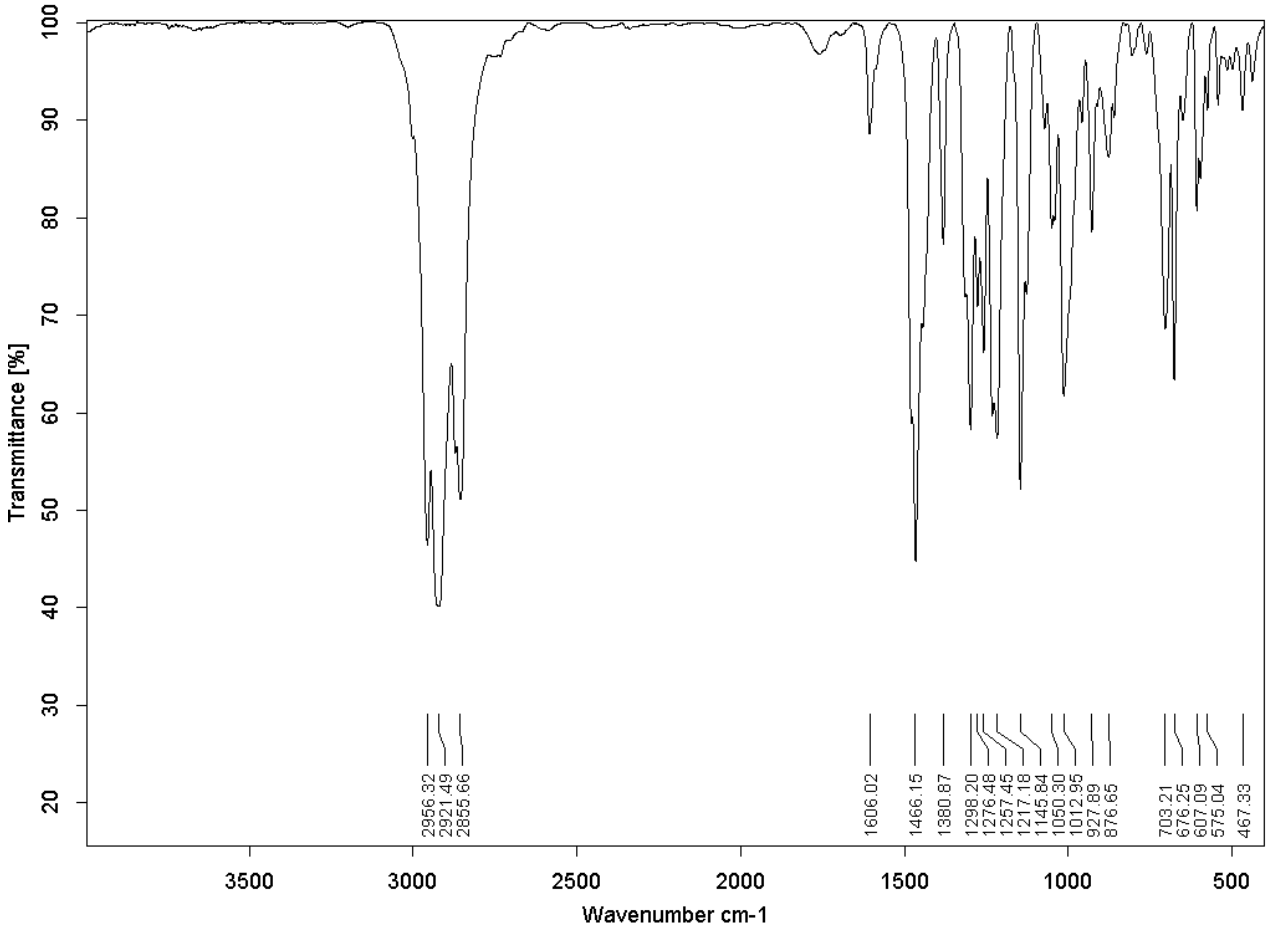


Fig. S3. FT-IR of compound **5**.

25.09.2014 13:22:42

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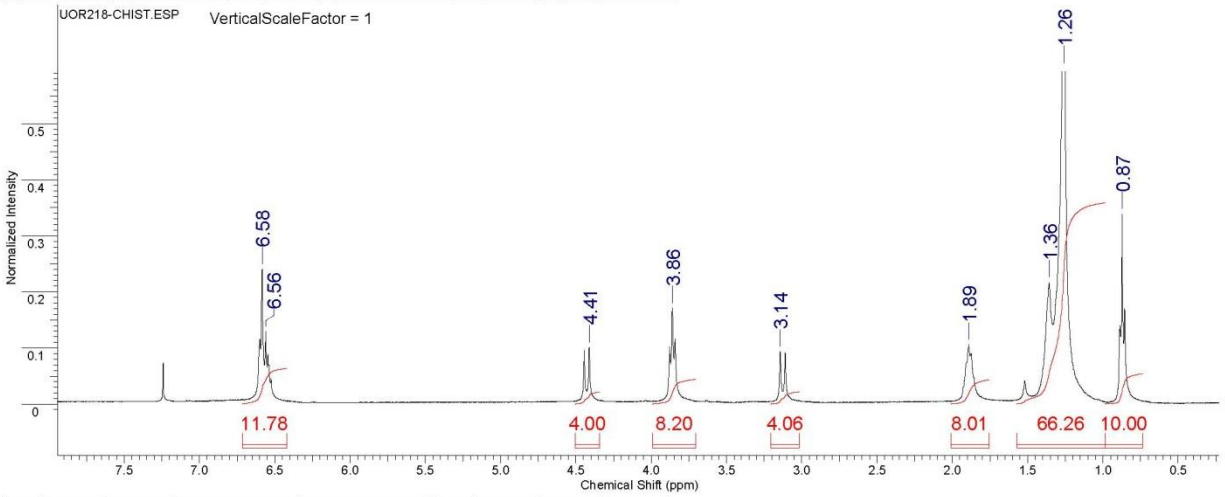
Spectrum Offset (Hz)	3348.2568	***Sweep Width (Hz)***	7260.85	***Temperature (degree C)***	20.000				



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.7349 .. 0.98	0.0002336	1.77867320e+7	10.00023365
2	[0.9874 .. 1.57	66.2566146	1.17846112e+8	66.25661469
3	[1.7582 .. 2.00	8.01140976	1.42493460e+7	8.01140976
4	[3.0172 .. 3.20	4.05783129	7.21738700e+6	4.05783129
5	[3.7045 .. 3.98	8.20361710	1.45912120e+7	8.20361710
6	[4.3424 .. 4.50	4.00000000	7.11452650e+6	4.00000000
7	[6.4191 .. 6.71	11.7772417	2.09473740e+7	11.77724171

No.	(ppm)	(Hz)	Height
1	0.87	348.9	0.3388
2	1.26	503.6	1.0000
3	1.36	542.6	0.2171
4	1.89	756.7	0.1058
5	3.14	1257.5	0.0938
6	3.86	1543.8	0.1706
7	4.41	1764.5	0.1011
8	6.56	2623.9	0.1299
9	6.58	2633.6	0.2406

Fig. S4. ^{1}H NMR of compound **8**.

26.09.2014 12:34:49

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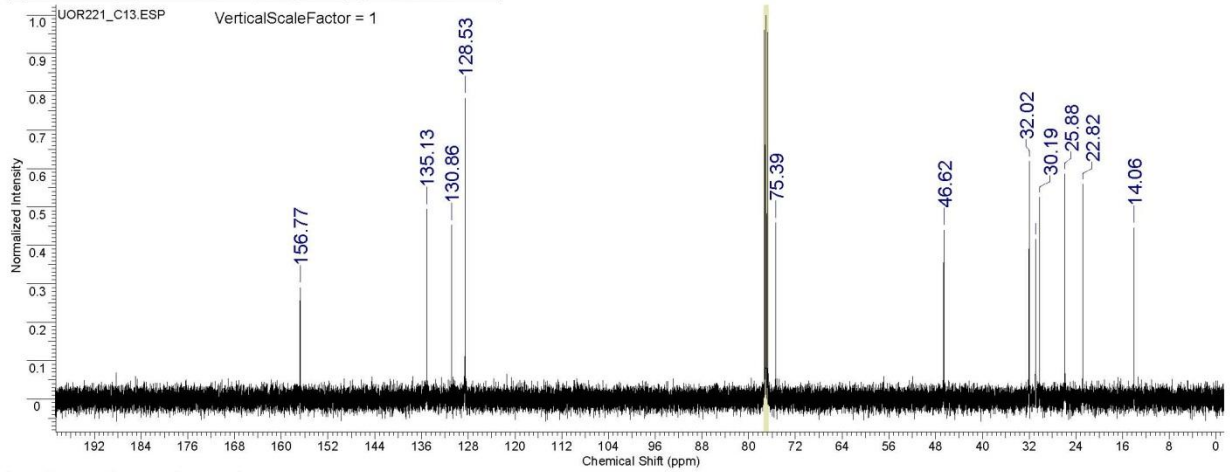
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	253	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	14996.9111	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	14.06	1767.4	0.4458
2	22.82	2868.9	0.5589
3	25.88	3254.4	0.5856
4	30.19	3795.4	0.5246
5	30.89	3883.2	0.4148
6	32.02	4025.8	0.6184
7	46.62	5860.8	0.4395
8	75.39	9479.1	0.4587
9	128.53	16160.0	0.7834
10	130.86	16452.7	0.4527
11	135.13	16989.3	0.4938

No.	(ppm)	(Hz)	Height
12	31.72	3987.9	0.6958
13	74.89	9415.2	0.4771
14	121.58	15285.4	0.3874
15	127.81	16069.8	0.7996
16	134.90	16960.4	0.3946
17	156.34	19656.6	0.2676

Fig. S5. ^{13}C NMR of compound **8**.

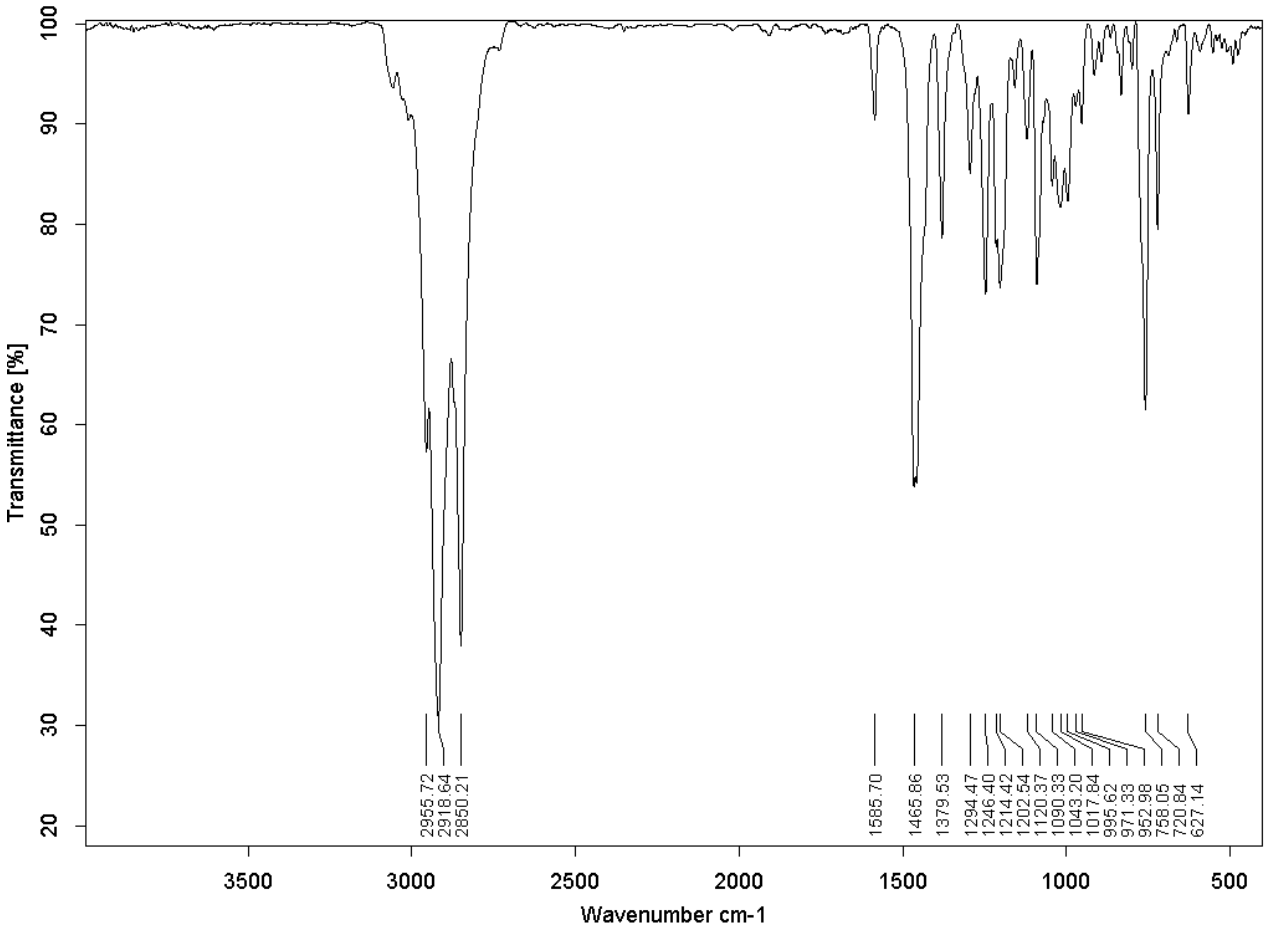
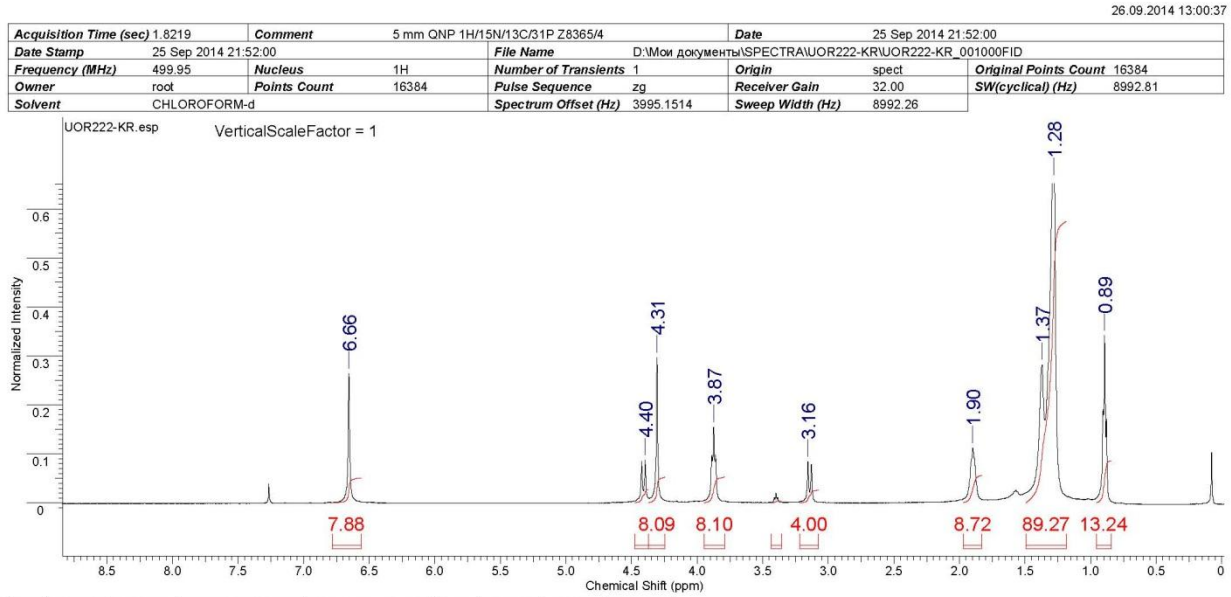


Fig. S6. FT-IR of compound **8**.



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8434 .. 0.95	3.2373542	2.76916380e+7	13.23735428
2	[1.1837 .. 1.49	89.2694625	1.86745584e+8	89.26946259
3	[1.8292 .. 1.97	8.71701050	1.82353880e+7	8.71701050
4	[3.0755 .. 3.21	4.00000000	8.36772550e+6	4.00000000
5	[3.3597 .. 3.43	0.67913145	1.42069637e+6	0.67913145
6	[3.7910 .. 3.94	8.10274887	1.69503960e+7	8.10274887
7	[4.2453 .. 4.36	8.08849239	1.69205700e+7	8.08849239
8	[4.3717 .. 4.47	4.29660130	8.98819500e+6	4.29660130
9	[6.5623 .. 6.78	7.88235283	1.64893410e+7	7.88235283

No.	(ppm)	(Hz)	Height
1	0.89	446.9	0.3410
2	1.28	640.7	1.0000
3	1.37	685.1	0.2817
4	1.90	949.2	0.1122
5	3.16	1577.6	0.0839
6	3.87	1936.6	0.1541
7	4.31	2152.8	0.2960
8	4.40	2197.9	0.0872
9	6.66	3327.4	0.2637

Fig. S7. ^{1}H NMR of compound **9**.

26.09.2014 12:48:32

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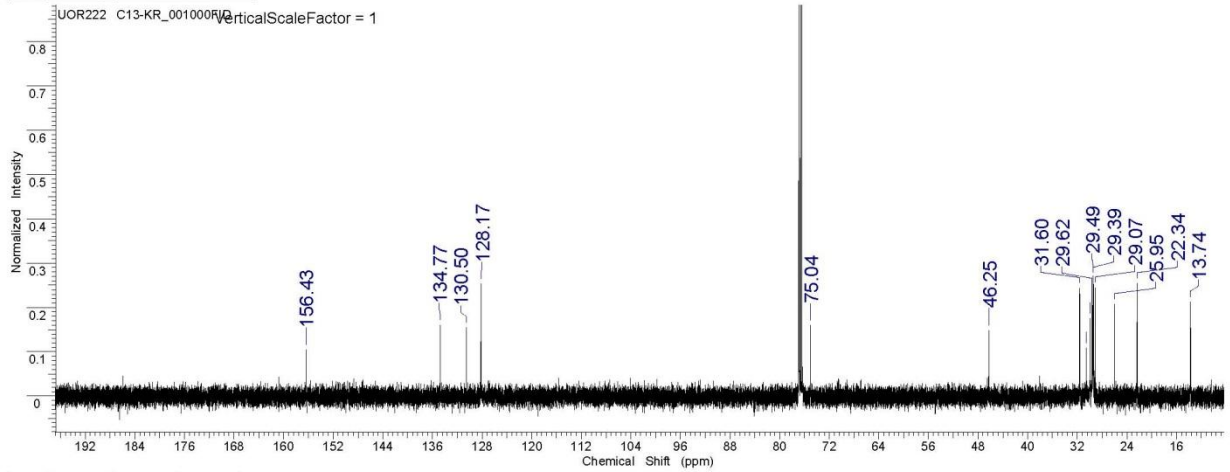
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	293	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	14952.5186
Sweep Width (Hz)	32679.24						



No.	(ppm)	(Hz)	Height
1	13.74	1728.0	0.2129
2	22.34	2809.1	0.2547
3	25.95	3262.3	0.2076
4	29.07	3654.8	0.2448
5	29.39	3695.7	0.2661
6	29.45	3703.2	0.2691
7	29.49	3707.1	0.2712
8	29.58	3719.6	0.2180
9	29.62	3724.6	0.2417
10	29.92	3761.5	0.1752
11	30.53	3838.8	0.1080

No.	(ppm)	(Hz)	Height
12	31.60	3972.9	0.2433
13	46.25	5815.4	0.1481
14	75.04	9434.2	0.1596
15	128.17	16114.6	0.2524
16	130.50	16407.3	0.1542
17	134.77	16944.4	0.1599
18	156.43	19667.5	0.1046

Fig. S8. ^{13}C NMR of compound **9**.

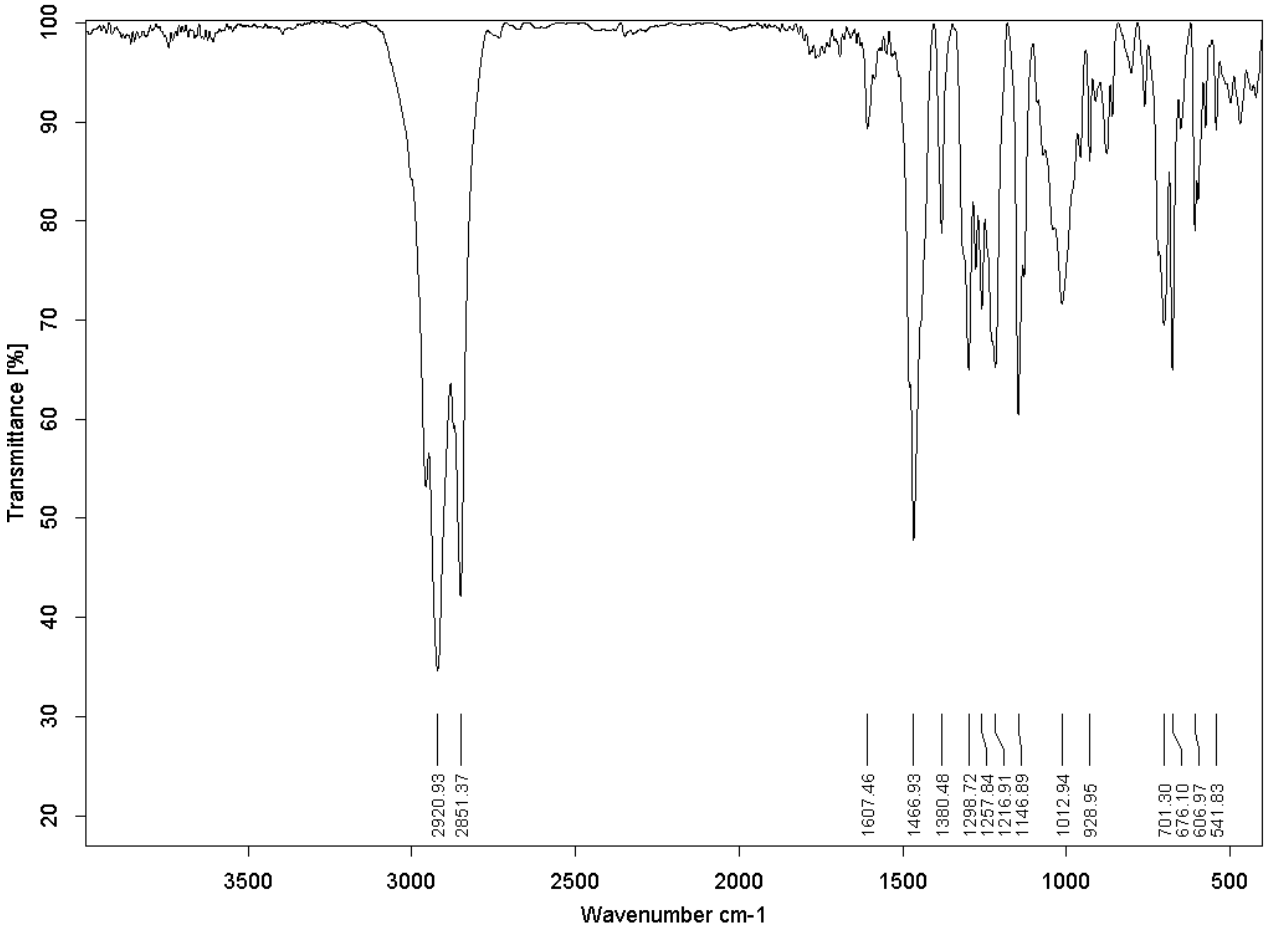
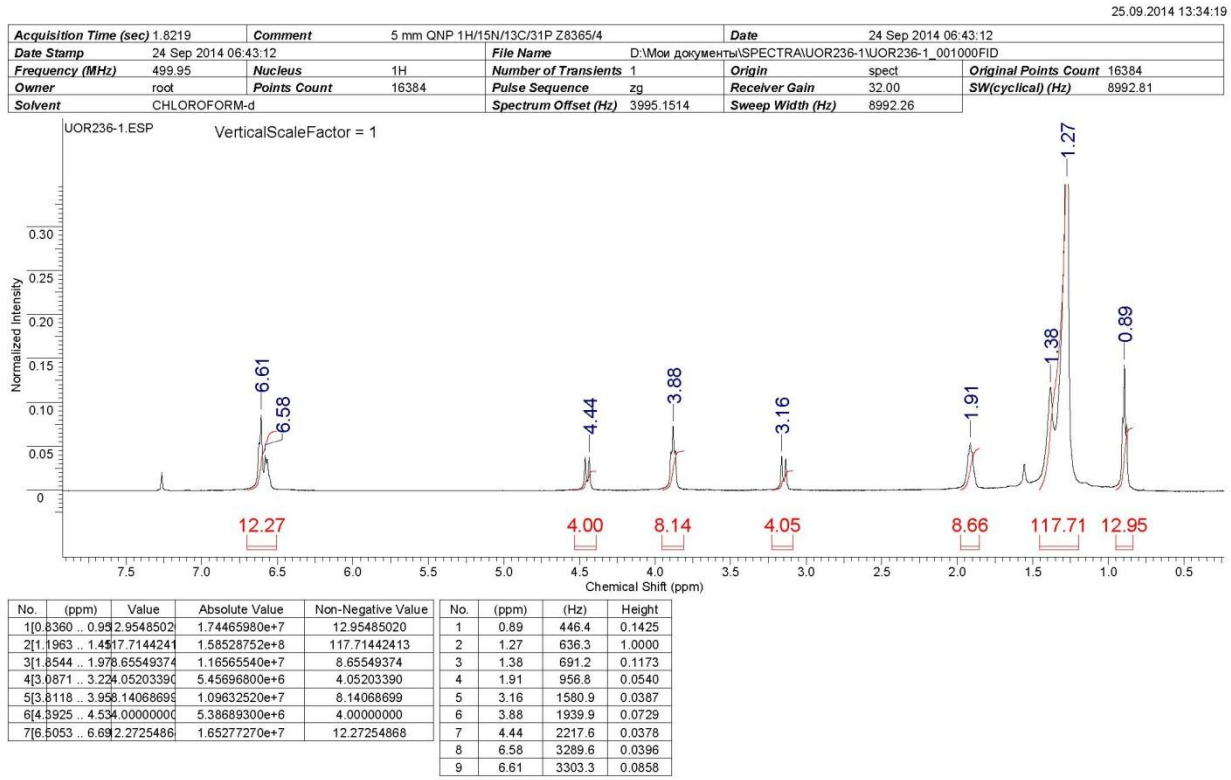


Fig. S9. FT-IR of compound **9**.



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8360 .. 0.95	12.9548502	1.74465980e+7	12.95485020
2	[1.1963 .. 1.45	117.7144241	1.58528752e+8	117.71442413
3	[1.8544 .. 1.97	8.65549374	1.16565540e+7	8.65549374
4	[3.0871 .. 3.22	4.05203390	5.45696800e+6	4.05203390
5	[3.8118 .. 3.95	8.14068699	1.09632520e+7	8.14068699
6	[4.3925 .. 4.53	4.00000000	5.38689300e+6	4.00000000
7	[6.5053 .. 6.69	12.2725486	1.65277270e+7	12.27254868

No.	(ppm)	(Hz)	Height
1	0.89	446.4	0.1425
2	1.27	636.3	1.0000
3	1.38	691.2	0.1173
4	1.91	956.8	0.0540
5	3.16	1580.9	0.0387
6	3.88	1939.9	0.0729
7	4.44	2217.6	0.0378
8	6.58	3289.6	0.0396
9	6.61	3303.3	0.0858

Fig. S10. ^{1}H NMR of compound **10**.

25.09.2014 13:39:12

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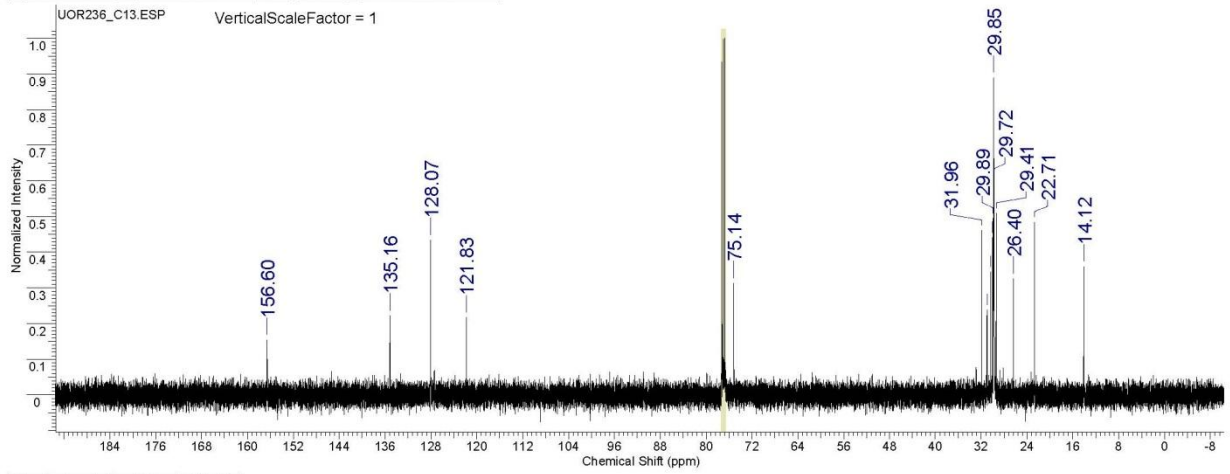
Spectrum Offset (Hz)	14998.4082	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	14.12	1774.9	0.3594
2	22.71	2855.5	0.4842
3	26.40	3318.7	0.3257
4	29.41	3697.7	0.5092
5	29.72	3737.1	0.6050
6	29.79	3745.1	0.6625
7	29.81	3747.5	0.6617
8	29.83	3750.0	0.6176
9	29.85	3753.0	0.8896
10	29.89	3757.5	0.4955
11	30.00	3771.5	0.4235

No.	(ppm)	(Hz)	Height
12	30.03	3775.5	0.4411
13	30.37	3817.9	0.3452
14	31.00	3898.1	0.2389
15	31.96	4018.3	0.4610
16	75.14	9447.2	0.3129
17	121.83	15317.3	0.2173
18	128.07	16101.7	0.4339
19	135.16	16992.8	0.2224
20	156.60	19689.0	0.1546

Fig. S11. ^{13}C NMR of compound **10**.

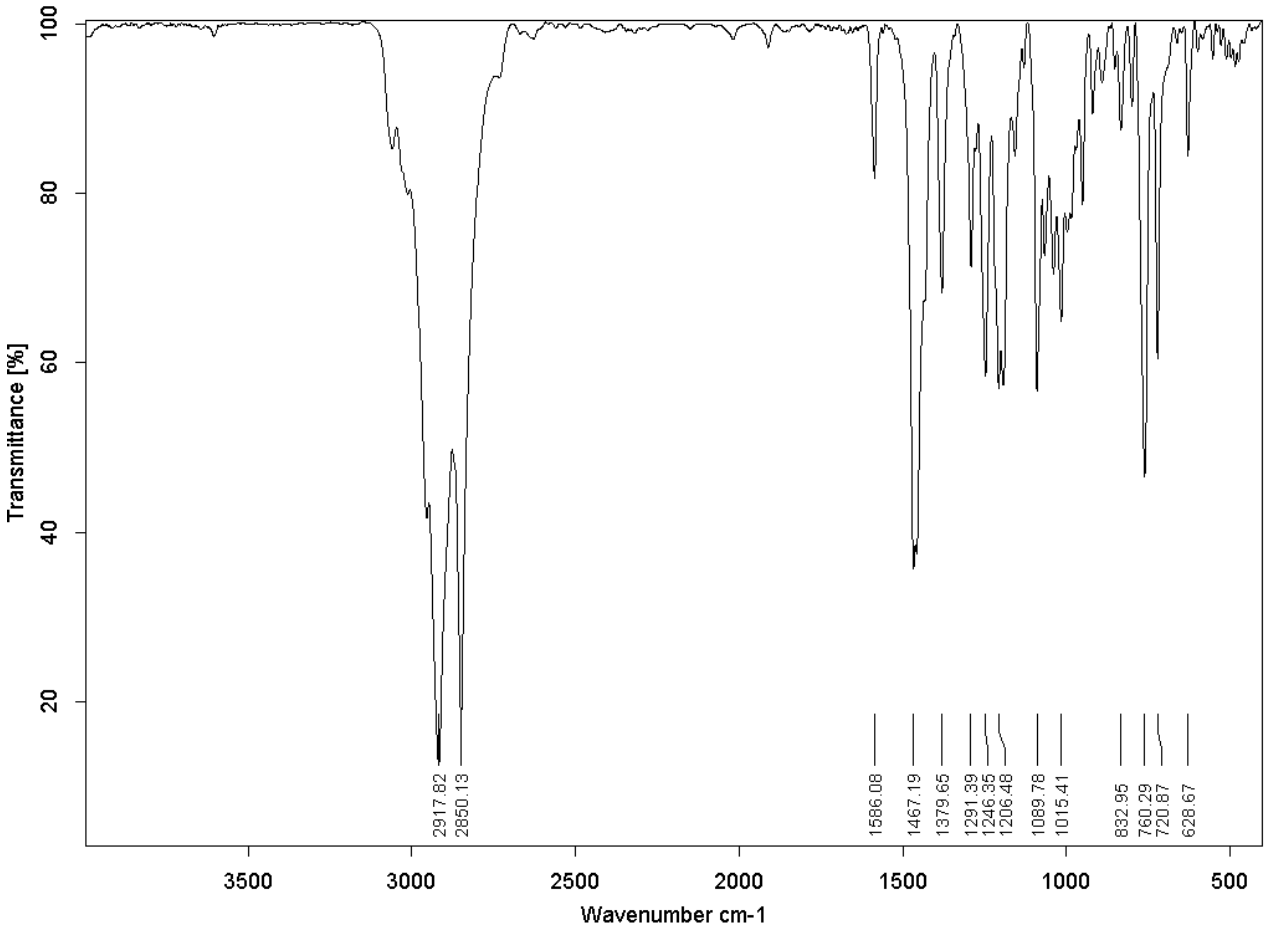
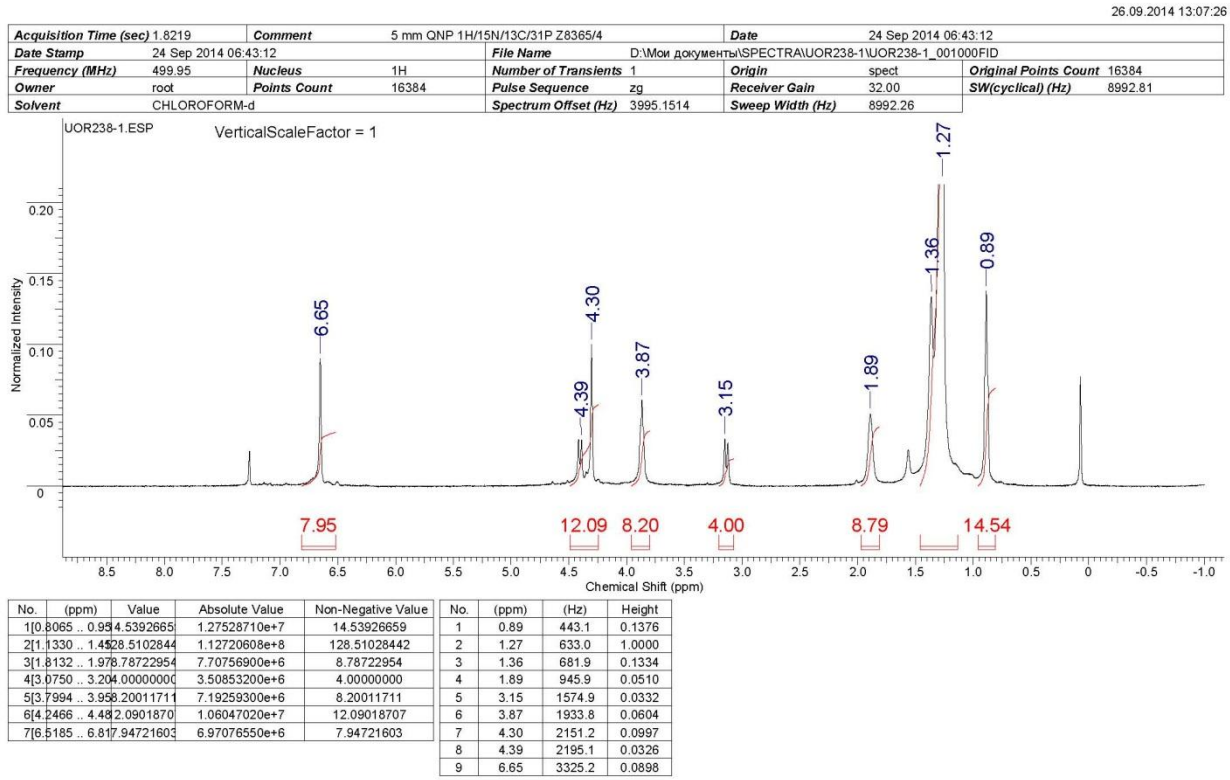


Fig. S12. FT-IR of compound **10**.



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8065 .. 0.95	4.53926659	1.27528710e+7	14.53926659
2	[1.1330 .. 1.45	28.51028442	1.12720608e+8	128.51028442
3	[1.8132 .. 1.97	8.78722954	7.70756900e+6	8.78722954
4	[3.0750 .. 3.20	4.00000000	3.50853200e+6	4.00000000
5	[3.7994 .. 3.95	8.20011711	7.19259300e+6	8.20011711
6	[4.2466 .. 4.48	2.09018707	1.06047020e+7	12.09018707
7	[6.5185 .. 6.81	7.94721603	6.97076550e+6	7.94721603

No.	(ppm)	(Hz)	Height
1	0.89	443.1	0.1376
2	1.27	633.0	1.0000
3	1.36	681.9	0.1334
4	1.89	945.9	0.0510
5	3.15	1574.9	0.0332
6	3.87	1933.8	0.0604
7	4.30	2151.2	0.0997
8	4.39	2195.1	0.0326
9	6.65	3325.2	0.0898

Fig. S13. ^{1}H NMR of compound **11**.

26.09.2014 13:12:09

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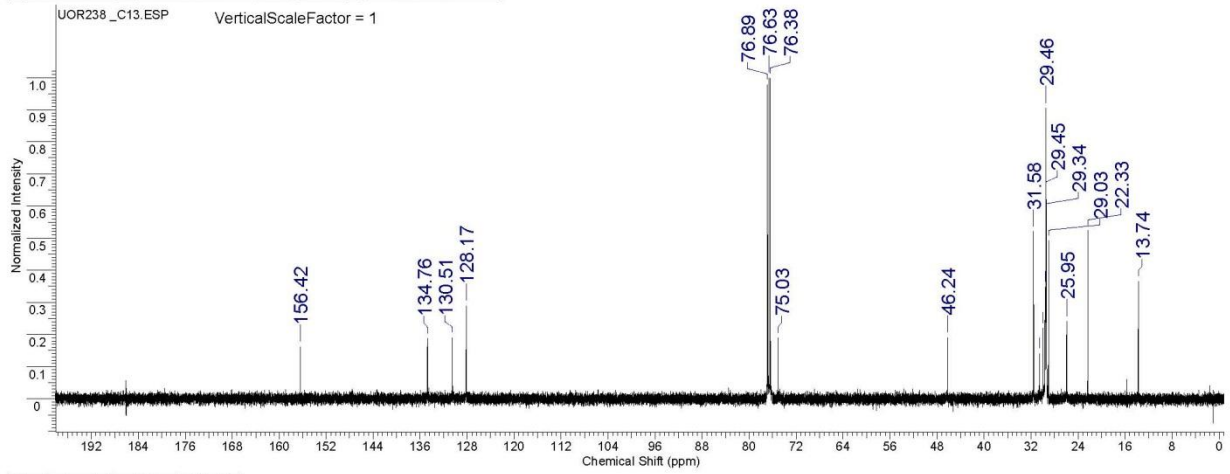
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	1203	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	14952.5186	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	13.74	1727.0	0.3652
2	22.33	2807.6	0.5236
3	25.95	3262.3	0.2414
4	29.03	3649.8	0.4915
5	29.34	3689.2	0.5744
6	29.41	3697.2	0.5881
7	29.42	3699.2	0.6199
8	29.45	3702.2	0.6414
9	29.46	3704.1	0.9047
10	29.49	3707.6	0.5139
11	29.58	3718.6	0.3350

No.	(ppm)	(Hz)	Height
12	29.62	3724.6	0.3479
13	29.92	3761.5	0.2201
14	30.54	3839.3	0.1411
15	31.58	3970.4	0.5207
16	46.24	5813.5	0.1905
17	75.03	9433.7	0.1895
18	76.38	9603.2	0.9976
19	76.63	9634.6	1.0000
20	76.89	9667.0	0.9782
21	128.17	16114.6	0.2896
22	130.51	16408.8	0.1900
23	134.76	16943.4	0.1886
24	156.42	19666.5	0.1627

Fig. S14. ^{13}C NMR of compound **11**.

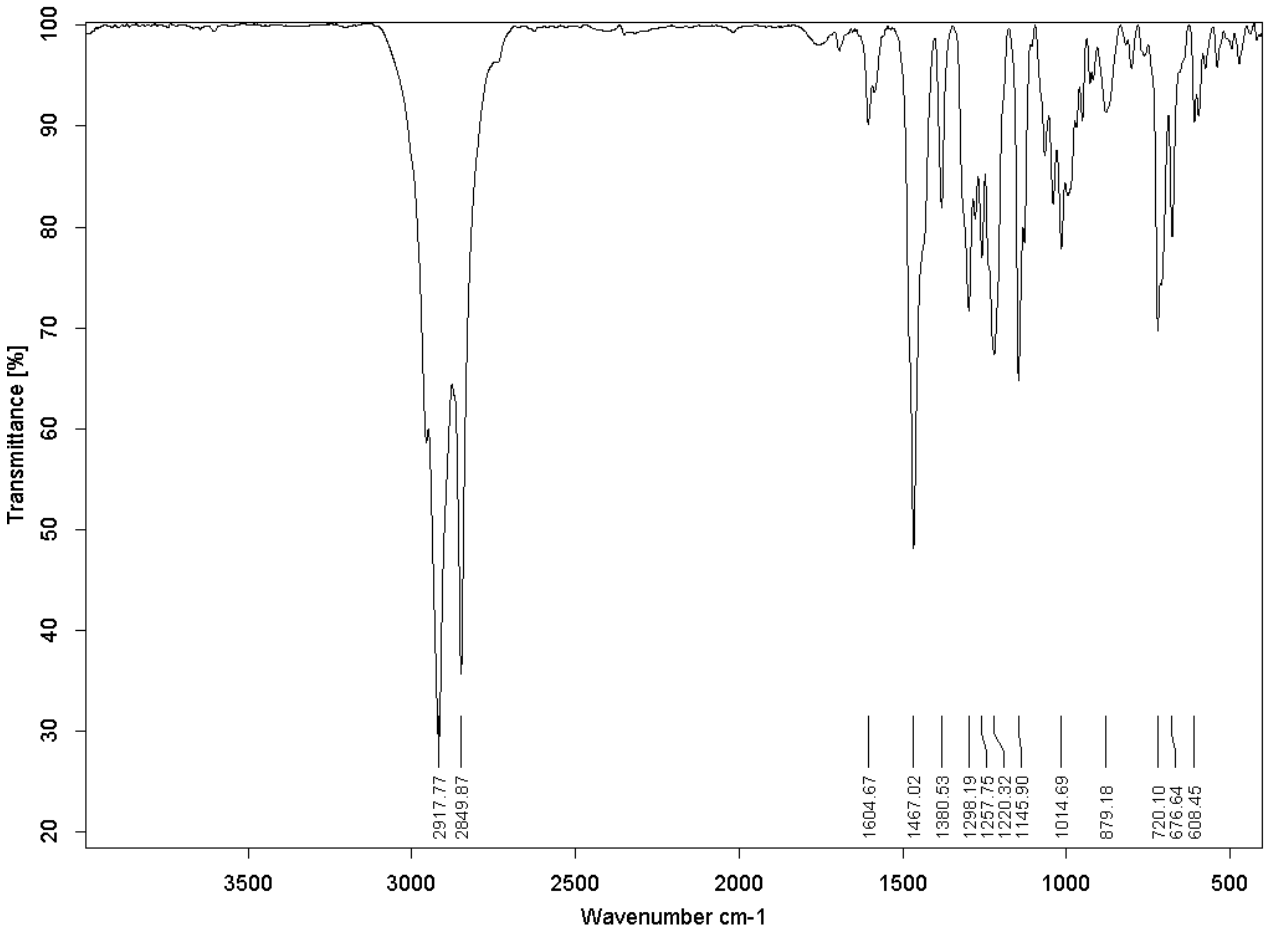


Fig. S15. FT-IR of compound **11**.

29.09.2014 11:02:16

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Frequency (MHz)	499.95	***Nucleus***	1H	***Number of Transients***	1	***Origin***	spect	***Original Points Count***	16384
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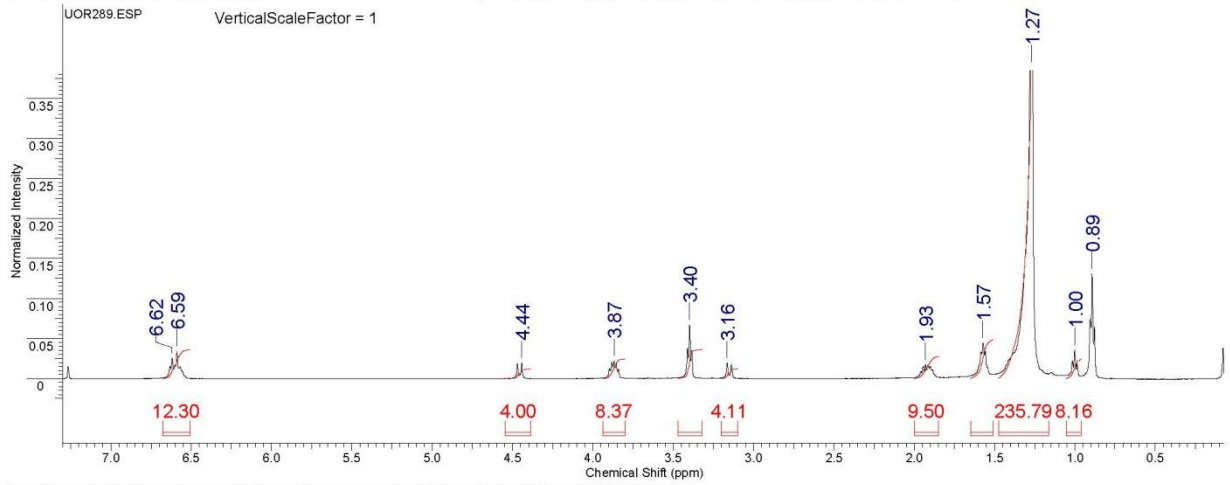
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	3995.1514	***Sweep Width (Hz)***	8992.26		



No.	(ppm)	Value	Absolute Value	Non-Negative Value
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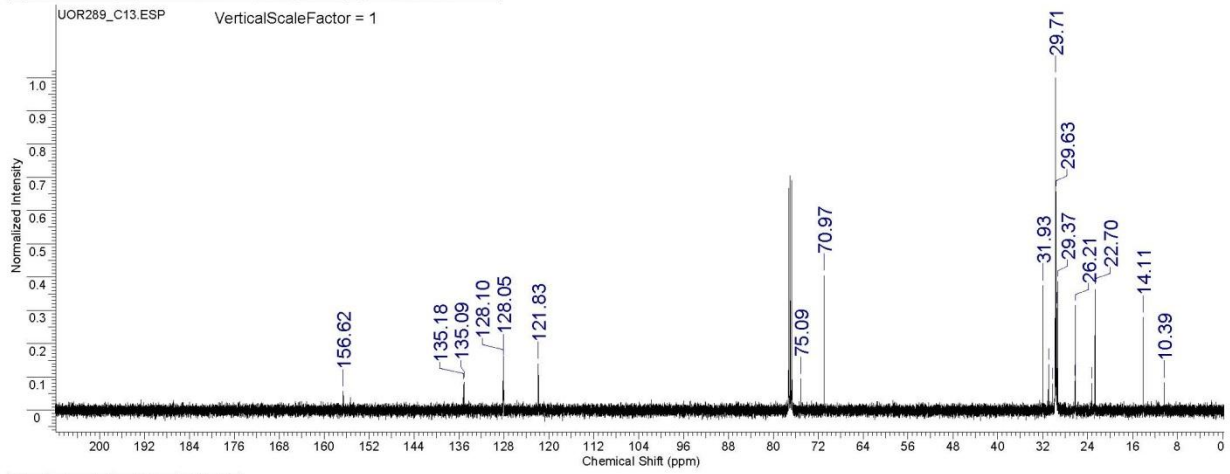
2	[1.1612 .. 1.427	35.78677736	2.53713200e+8	235.78677368
3	[1.5110 .. 1.646	16.68405151	1.79525080e+7	16.68405151
4	[1.8494 .. 1.999	9.49699306	1.02190320e+7	9.49699306
5	[3.0996 .. 3.204	4.11074972	4.42328250e+6	4.11074972
6	[3.3233 .. 3.471	12.40588093	1.33490770e+7	12.40588093
7	[3.7993 .. 3.938	8.36552238	9.00153700e+6	8.36552238
8	[4.3870 .. 4.544	4.00000000	4.30411250e+6	4.00000000
9	[6.5062 .. 6.671	12.29749584	1.32324510e+7	12.29749584

No.	(ppm)	(Hz)	Height
1	0.89	446.4	0.1308
2	1.00	500.2	0.0358
3	1.27	634.1	1.0000
4	1.57	785.6	0.0447
5	1.93	965.1	0.0173
6	3.16	1582.0	0.0195
7	3.40	1698.9	0.0672
8	3.87	1934.4	0.0220
9	4.44	2221.5	0.0192
10	6.59	3294.0	0.0339
11	6.62	3308.8	0.0256

Fig. S16. ^{1}H NMR of compound **13**.

29.09.2014 11:04:19

Acquisition Time (sec)	1.5667	***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	12 Sep 2014 19:33:20
Date Stamp	12 Sep 2014 19:33:20			***File Name***	D:\Мои документы\SPECTRA\UOR289 C13\UOR289 C13_001000FID		
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	455	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	14998.9053	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	10.39	1306.1	0.0829
2	14.11	1773.9	0.2784
3	22.70	2853.5	0.3631
4	23.29	2928.3	0.0800
5	26.21	3295.8	0.3157
6	26.26	3301.7	0.0886
7	29.37	3692.7	0.3863
8	29.52	3711.1	0.3060
9	29.63	3725.1	0.6573
10	29.71	3735.1	1.0000
11	29.73	3738.1	0.5725

No.	(ppm)	(Hz)	Height
12	29.79	3746.0	0.3666
13	29.85	3753.5	0.1113
14	30.25	3803.4	0.0792
15	31.00	3897.1	0.1370
16	31.93	4014.8	0.3742
17	70.97	8922.6	0.4038
18	75.09	9440.7	0.0943
19	121.83	15317.8	0.1394
20	128.05	16099.7	0.1630
21	128.10	16106.2	0.1498
22	135.09	16984.8	0.0832
23	135.18	16995.8	0.0776
24	156.56	19684.0	0.0442
25	156.62	19692.0	0.0569

Fig. S17. ^{13}C NMR of compound **13**.

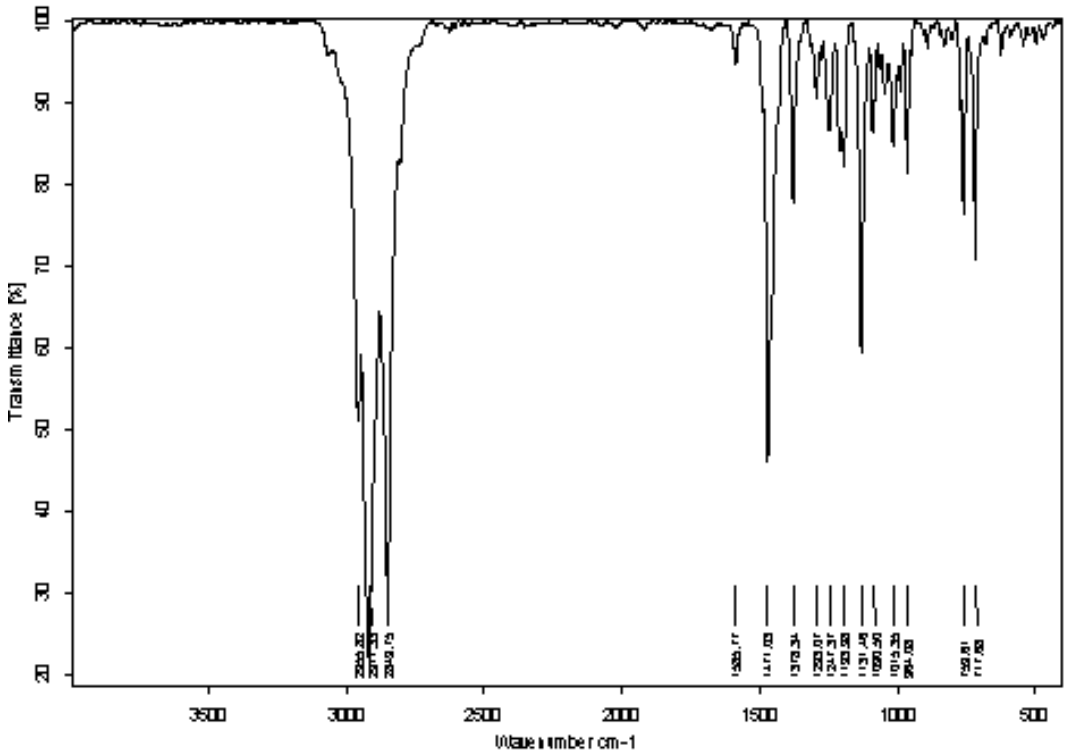
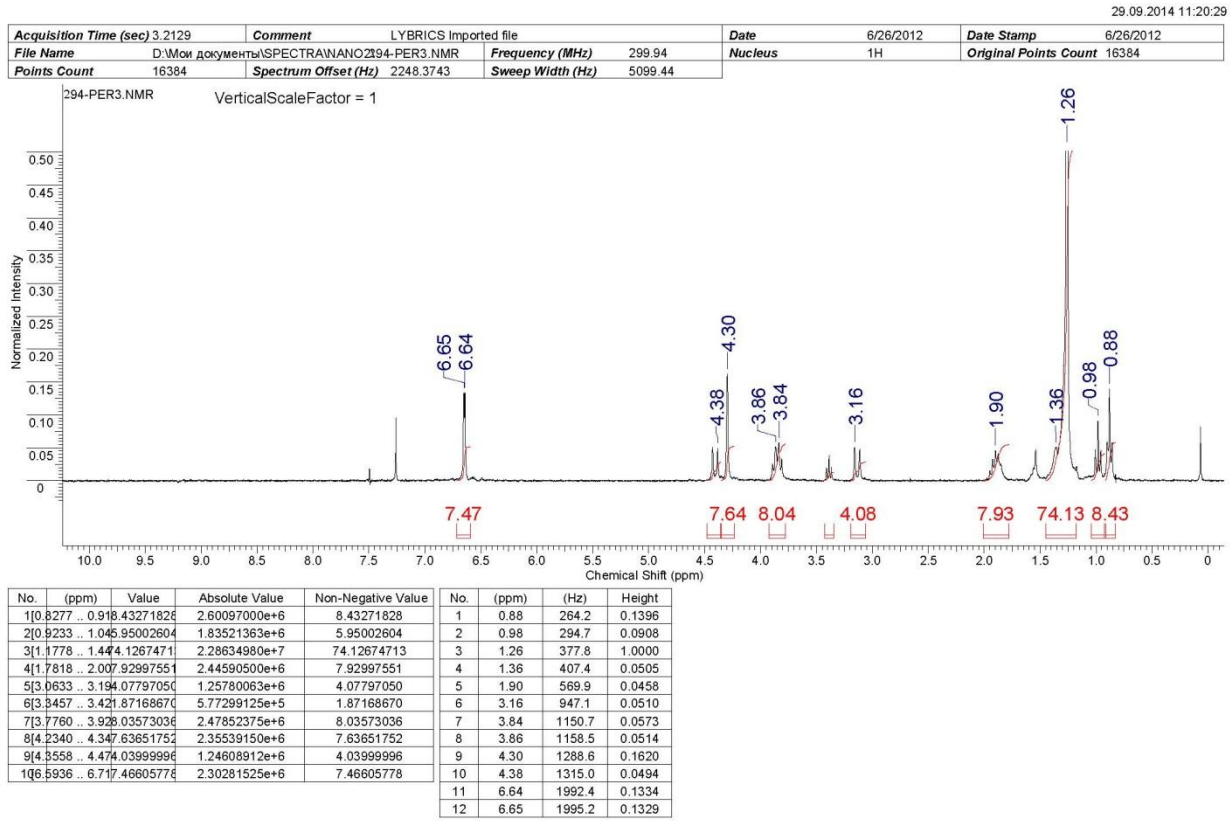


Fig. S18. FT-IR of compound **13**.



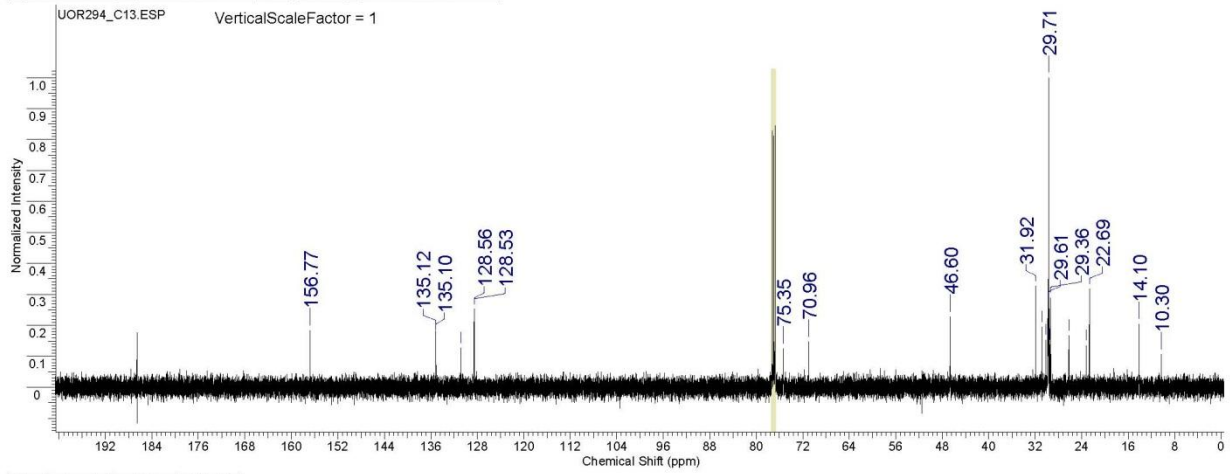
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8277 .. 0.918	.43271828	2.60097000e+6	8.43271828
2	[0.9233 .. 1.045	.95002604	1.83521363e+6	5.95002604
3	[1.1778 .. 1.447	4.1267471	2.28634980e+7	74.12674713
4	[1.7818 .. 2.007	.92997551	2.44590500e+6	7.92997551
5	[3.0633 .. 3.194	.07797050	1.25780063e+6	4.07797050
6	[3.3457 .. 3.421	.87168670	5.77299125e+5	1.87168670
7	[3.7760 .. 3.928	.03573036	2.47852375e+6	8.03573036
8	[4.2340 .. 4.347	.63651752	2.35539150e+6	7.63651752
9	[4.3558 .. 4.474	.03999996	1.24608912e+6	4.03999996
10	[6.5936 .. 6.717	.46605778	2.30281525e+6	7.46605778

No.	(ppm)	(Hz)	Height
1	0.88	264.2	0.1396
2	0.98	294.7	0.0908
3	1.26	377.8	1.0000
4	1.36	407.4	0.0505
5	1.90	569.9	0.0458
6	3.16	947.1	0.0510
7	3.84	1150.7	0.0573
8	3.86	1158.5	0.0514
9	4.30	1288.6	0.1620
10	4.38	1315.0	0.0494
11	6.64	1992.4	0.1334
12	6.65	1995.2	0.1329

Fig. S19. ^{1}H NMR of compound **14**.

29.09.2014 11:27:38

Acquisition Time (sec)	1.5667	***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	16 Sep 2014 19:46:08
Date Stamp	16 Sep 2014 19:46:08			***File Name***	D:\Мои документы\SPECTRA\UOR294_C13\UOR294_C13_001000FID		
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	204	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	14998.4082	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	10.30	1295.2	0.1063
2	14.10	1772.4	0.2044
3	22.69	2852.5	0.3176
4	23.23	2921.3	0.1345
5	26.18	3291.8	0.1562
6	26.20	3294.3	0.1667
7	29.36	3691.2	0.2890
8	29.51	3709.6	0.1370
9	29.61	3723.1	0.2742
10	29.66	3729.6	0.4194
11	29.71	3735.6	1.0000

No.	(ppm)	(Hz)	Height
12	29.76	3742.1	0.2580
13	29.78	3744.6	0.2394
14	29.82	3749.0	0.2235
15	30.16	3792.4	0.1527
16	30.89	3884.2	0.1946
17	31.92	4013.3	0.3264
18	46.60	5858.3	0.2280
19	70.96	8921.1	0.1475
20	75.35	9474.1	0.1246
21	128.53	16159.5	0.2513
22	128.56	16163.0	0.2533
23	130.86	16453.2	0.1263
24	130.89	16456.7	0.1190
25	135.10	16985.8	0.1694
26	135.12	16988.3	0.1819
27	156.76	19708.4	0.0594
28	156.77	19709.9	0.1841

Fig. S20. ^{13}C NMR of compound **14**.

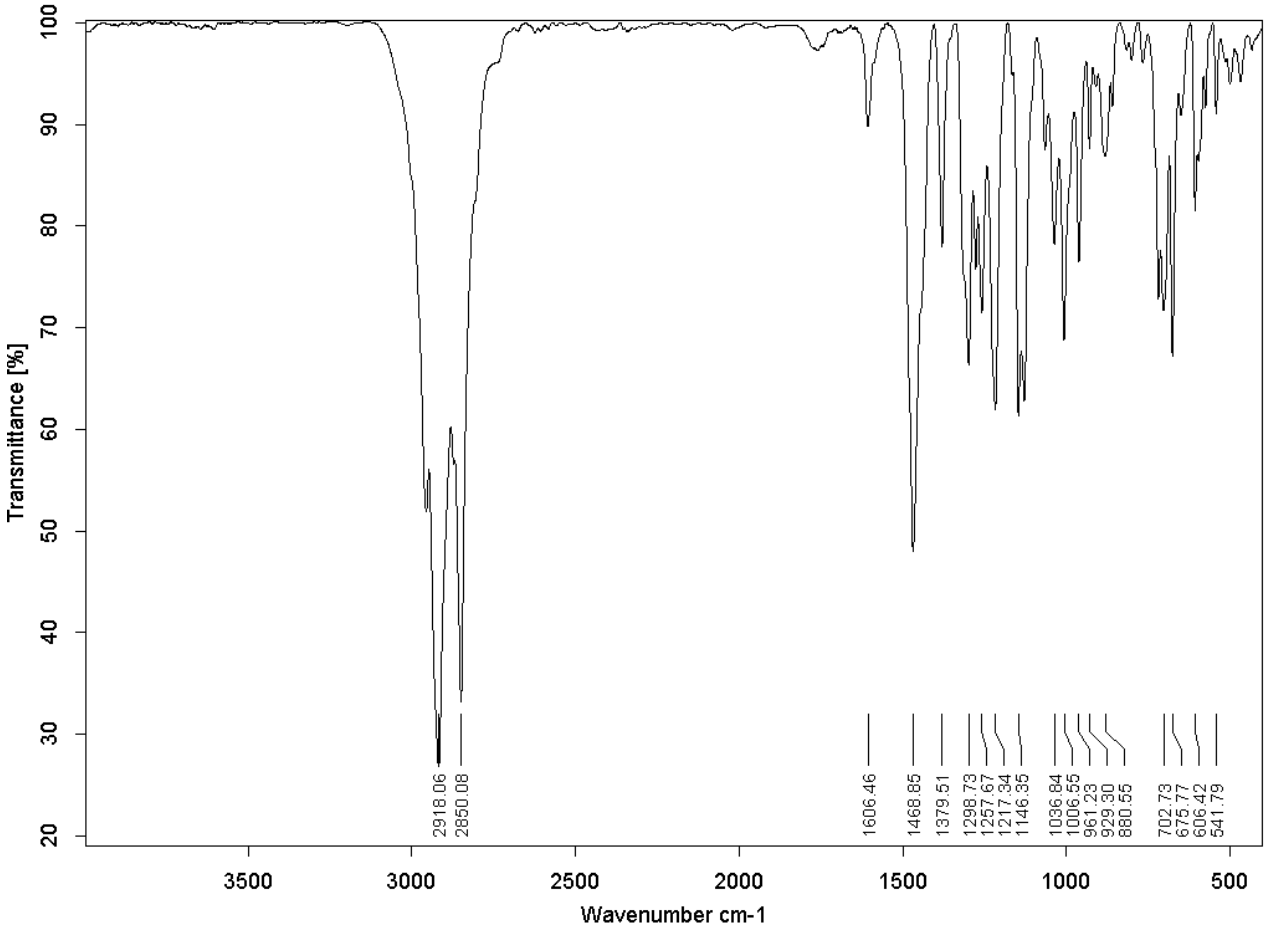
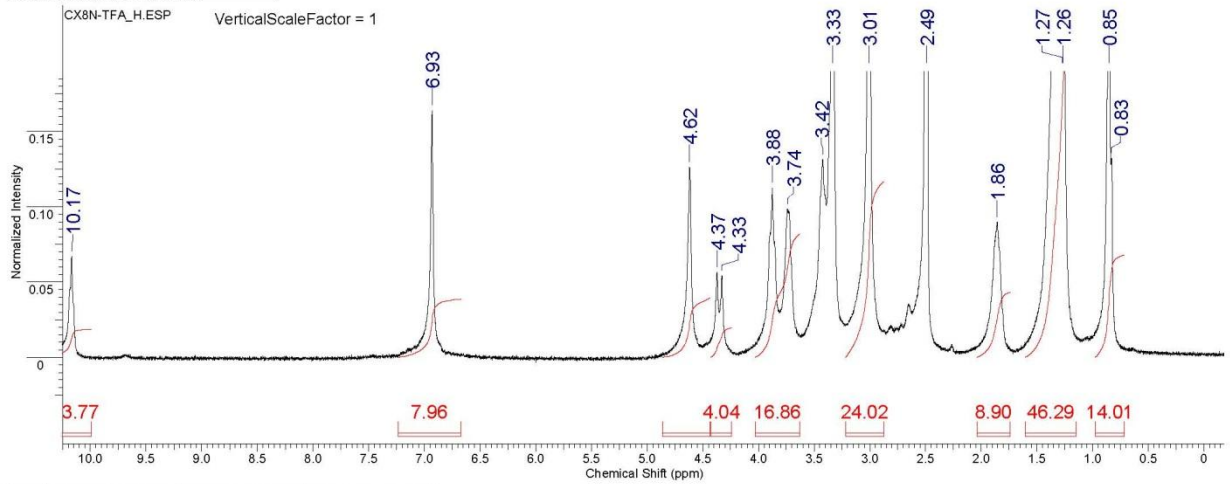


Fig. S21. FT-IR of compound **14**.

29.09.2014 12:44:36

Acquisition Time (sec)	3.2047	***Comment***	Imported from UXNMR.			***Date***	08 Oct 2010 15:00:16
File Name	C:\Documents and Settings\Admin\Мои документы\FluorescenceRodik\nmr\Rodik-081010\Rodik-081010_002000fid					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	16	***Original Points Count***	16384	***Points Count***	16384
Pulse Sequence	zg30	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1850.8000	***Sweep Width (Hz)***	5112.47
Temperature (degree C)	27.000						



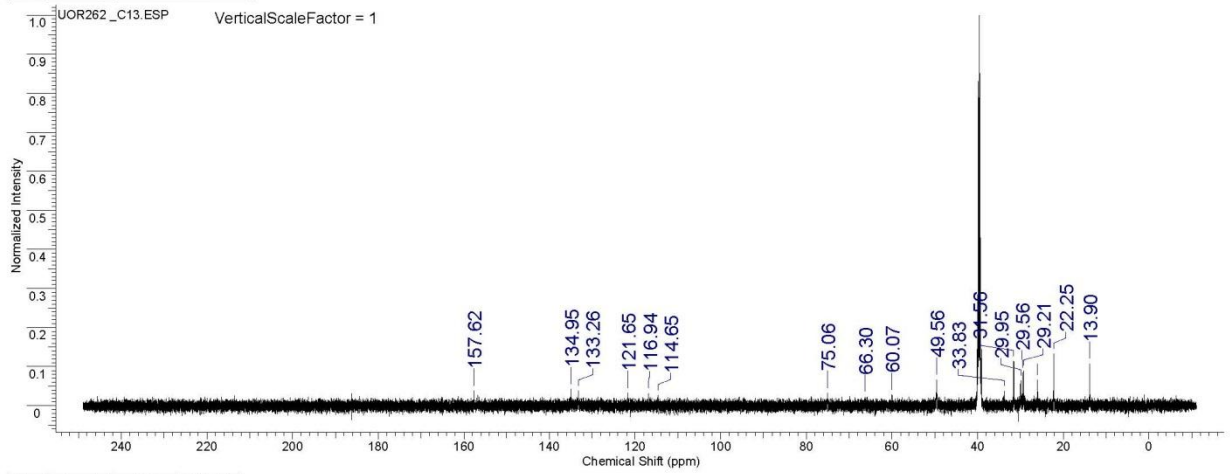
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.7147 .. 0.974	4.0131979	3.96301152e+8	14.01319790
2	[1.1474 .. 1.604	6.2896690	1.30909798e+9	46.28966904
3	[1.7387 .. 2.038	8.90087414	2.51721744e+8	8.90087414
4	[2.8769 .. 3.212	4.0210628	6.79329216e+8	24.02106285
5	[3.6299 .. 4.021	6.8600006	4.76810336e+8	16.86000061
6	[4.2422 .. 4.424	4.03999996	1.14253480e+8	4.03999996
7	[4.4363 .. 4.868	3.12843609	2.29876768e+8	8.12843609
8	[6.6705 .. 7.237	7.96018887	2.25118624e+8	7.96018887
9	[9.9910 .. 10.43	3.76589775	1.06501712e+8	3.76589775

No.	(ppm)	(Hz)	Height
1	0.83	248.8	0.1323
2	0.85	255.4	0.3175
3	1.26	379.6	0.3675
4	1.27	380.8	0.3658
5	1.86	557.5	0.0897
6	2.49	748.1	0.7582
7	3.01	902.6	0.4160
8	3.33	1000.0	1.0000
9	3.42	1027.1	0.1312
10	3.74	1122.0	0.0985
11	3.88	1163.5	0.1126
12	4.33	1299.2	0.0542
13	4.37	1312.0	0.0563
14	4.62	1386.0	0.1263
15	6.93	2080.3	0.1639
16	10.17	3051.8	0.0670

Fig. S22. ^{1}H NMR of compound **15**.

29.09.2014 12:52:40

Acquisition Time (sec)	1.5667	***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	18 Sep 2014 00:21:20
Date Stamp	18 Sep 2014 00:21:20			***File Name***	D:\Мои документы\SPECTRA\UOR262 C13\UOR262 C13_001000FID		
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	570	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	14952.5186
Sweep Width (Hz)	32679.24						



No.	(ppm)	(Hz)	Height
1	13.90	1747.4	0.1070
2	22.25	2797.6	0.1328
3	26.01	3269.8	0.0651
4	29.21	3672.2	0.0897
5	29.56	3717.1	0.0851
6	29.95	3766.0	0.0640
7	31.56	3967.9	0.1137
8	33.83	4253.7	0.0371
9	49.56	6231.3	0.0667
10	60.07	7552.8	0.0274
11	66.30	8335.6	0.0229

No.	(ppm)	(Hz)	Height
12	156.77	19710.9	0.2910

Fig. S23. ^{13}C NMR of compound **15**.

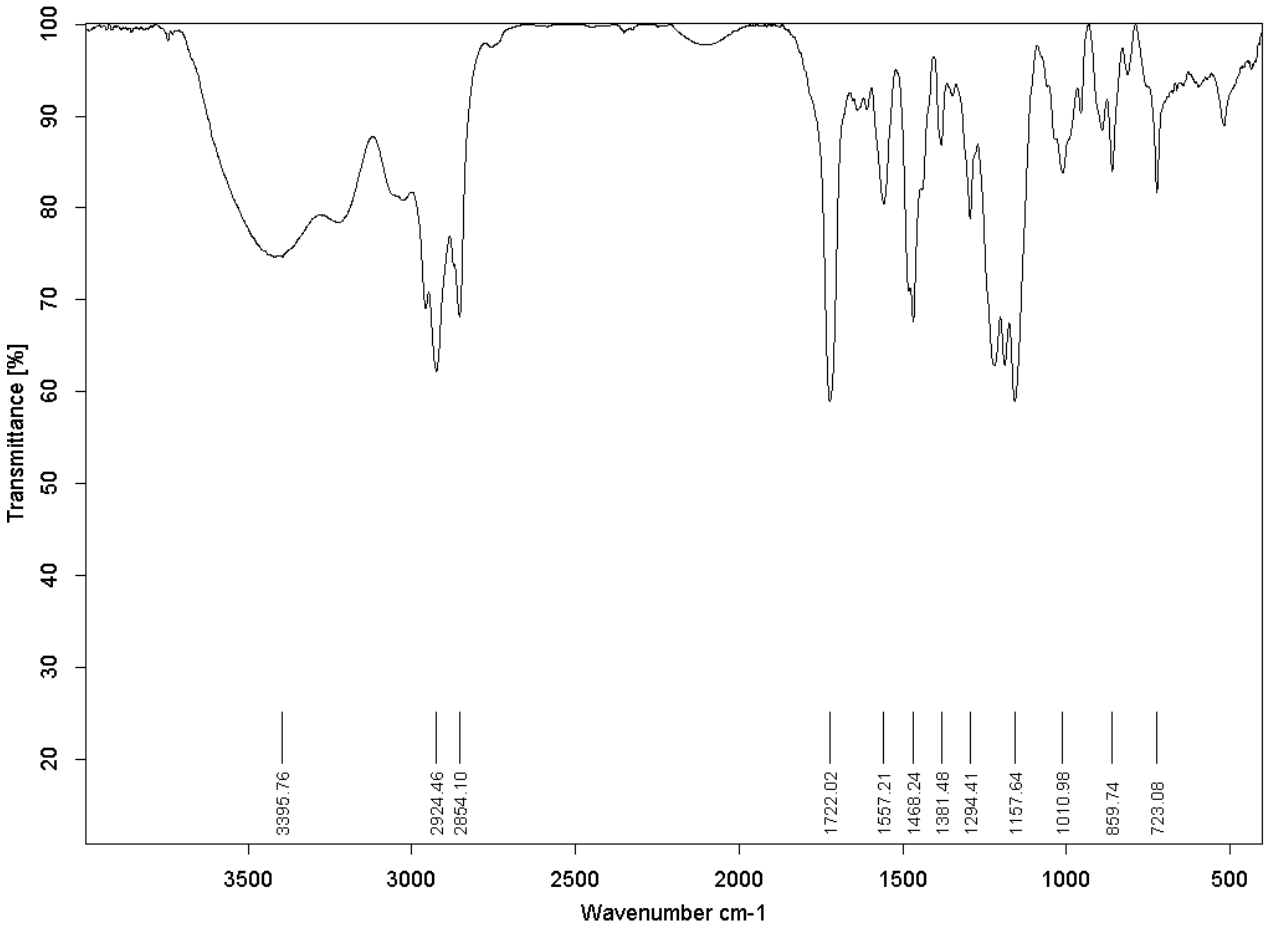
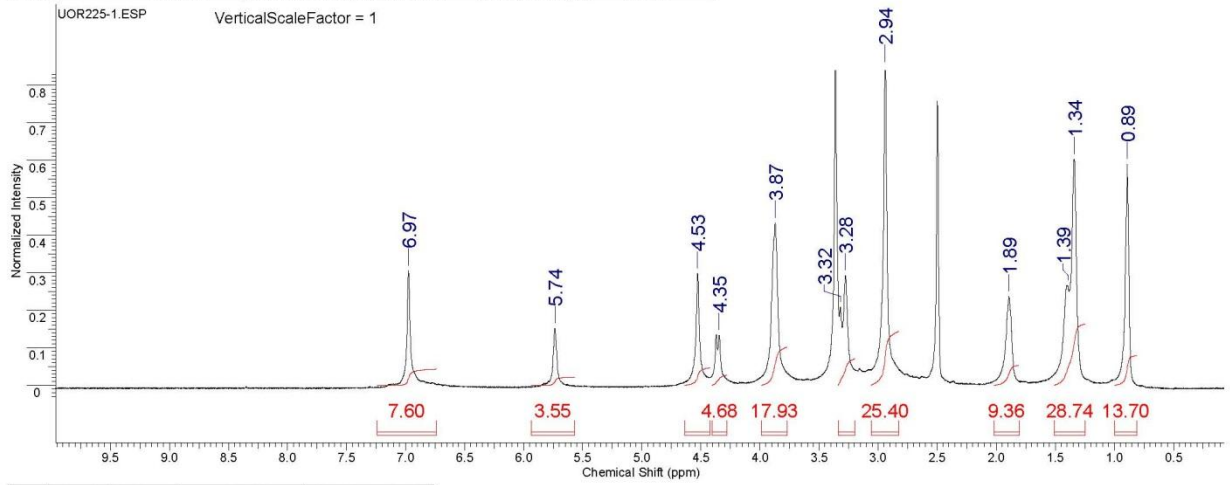


Fig. S24. FT-IR of compound **15**.

26.09.2014 13:25:01

Acquisition Time (sec)	1.8219	**Comment**	5 mm QNP 1H/15N/13C/31P Z8365/4			**Date**	24 Sep 2014 06:38:56	
Date Stamp	24 Sep 2014 06:38:56			**File Name**	D:\Мои документы\SPECTRA\UOR225-1\UOR225-1_001000FID			
Frequency (MHz)	499.95	**Nucleus**	1H	**Number of Transients**	1	**Origin**	spect	**Original Points Count** 16384
Owner	root	**Points Count**	16384	**Pulse Sequence**	zg	**Receiver Gain**	32.00	**SW(cyclical) (Hz)** 8992.81
Solvent	DMSO-d6	**Spectrum Offset (Hz)**	3995.1514	**Sweep Width (Hz)**	8992.26			



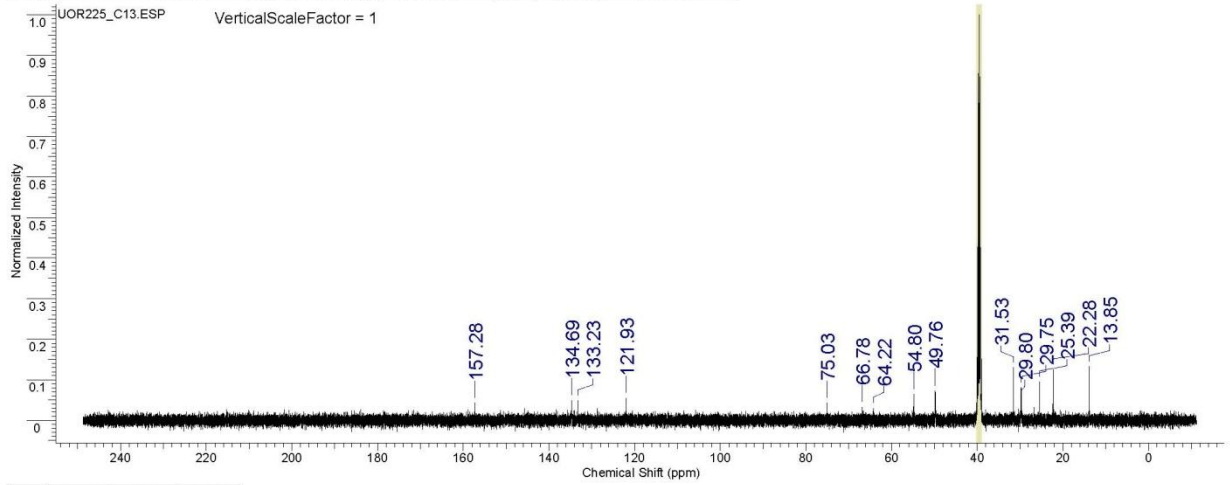
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8087 .. 0.99	13.7046527	1.68726860e+7	13.70465279
2	[1.2485 .. 1.50	28.7393283	3.53828480e+7	28.73932838
3	[1.8089 .. 2.01	9.36168289	1.15257740e+7	9.36168289
4	[2.8255 .. 3.05	25.4041156	3.12766540e+7	25.40411568
5	[3.1966 .. 3.33	12.4615240	1.53421900e+7	12.46152401
6	[3.7710 .. 3.98	17.9279842	2.20723020e+7	17.92798424
7	[4.2805 .. 4.40	4.68298340	5.76552450e+6	4.68298340
8	[4.4253 .. 4.63	8.26171494	1.01715330e+7	8.26171494
9	[5.5703 .. 5.93	3.54999995	4.37063500e+6	3.54999995
10	[6.7399 .. 7.24	7.60357332	9.36125200e+6	7.60357332

No.	(ppm)	(Hz)	Height
1	0.89	445.8	0.5895
2	1.34	670.3	0.6027
3	1.39	697.2	0.2648
4	1.89	945.3	0.2369
5	2.94	1470.0	0.9161
6	3.28	1638.0	0.2920
7	3.32	1659.4	0.2087
8	3.87	1935.5	0.4335
9	4.35	2172.6	0.1331
10	4.53	2263.7	0.2970
11	5.74	2868.0	0.1515
12	6.97	3487.2	0.3054

Fig. S25. ^{1}H NMR of compound **CX6**.

26.09.2014 13:15:16

Acquisition Time (sec) 1.5667		***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	16 Sep 2014 19:31:12		
Date Stamp	16 Sep 2014 19:31:12			***File Name***	D:\Мои документы\SPECTRA\UOR225_C13\UOR225_C13_001000FID				
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	412	***Origin***	spect	***Original Points Count***	51200
Owner	root	***Points Count***	65536	***Pulse Sequence***	zgpg	***Receiver Gain***	51200.00	***SW(cyclical) (Hz)***	32679.74
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	14936.8184	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	13.85	1740.7	0.1331
2	22.28	2801.3	0.1247
3	25.39	3192.3	0.0949
4	29.75	3740.3	0.0810
5	29.80	3747.3	0.0451
6	31.53	3964.2	0.1300
7	49.76	6256.0	0.0732
8	54.80	6889.8	0.0639
9	64.22	8074.1	0.0295
10	66.78	8396.2	0.0325
11	75.03	9433.4	0.0424
12	121.93	15330.5	0.0548

No.	(ppm)	(Hz)	Height
13	133.23	16750.7	0.0484
14	134.69	16934.7	0.0489
15	157.28	19774.5	0.0432

Fig. S26. ^{13}C NMR of compound **CX6**.

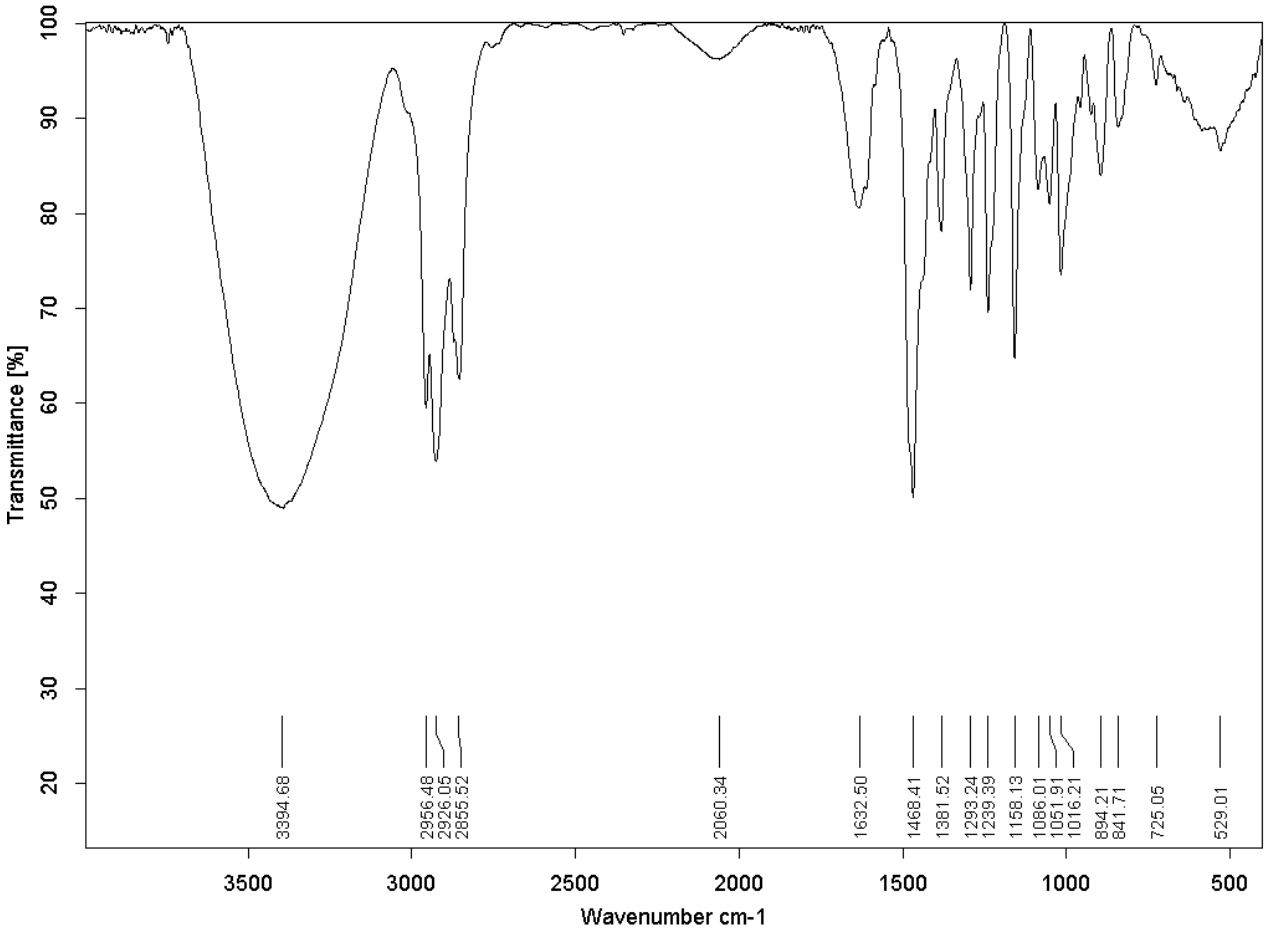
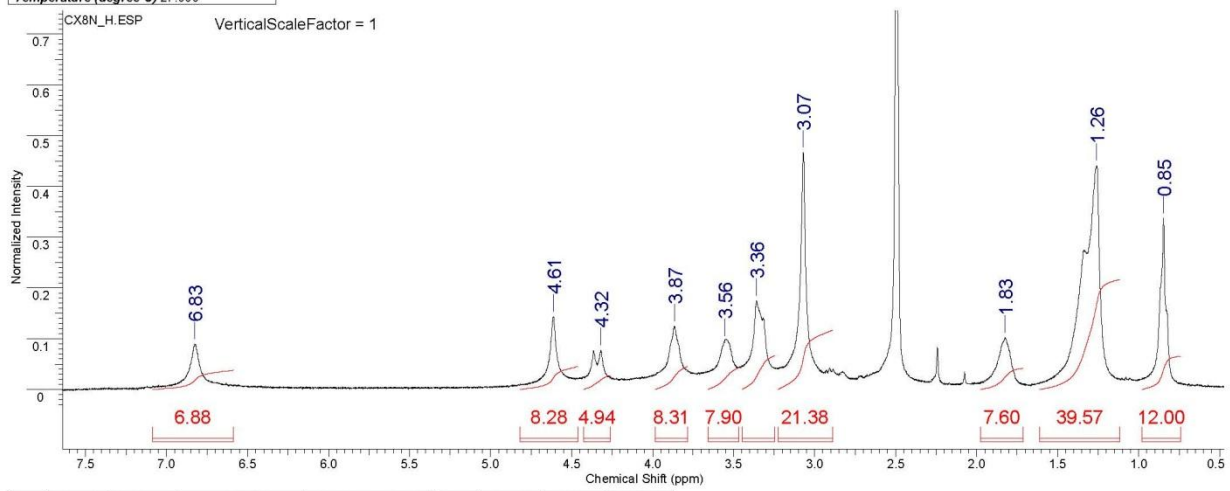


Fig. S27. FT-IR of compound **CX6**.

29.09.2014 12:12:09

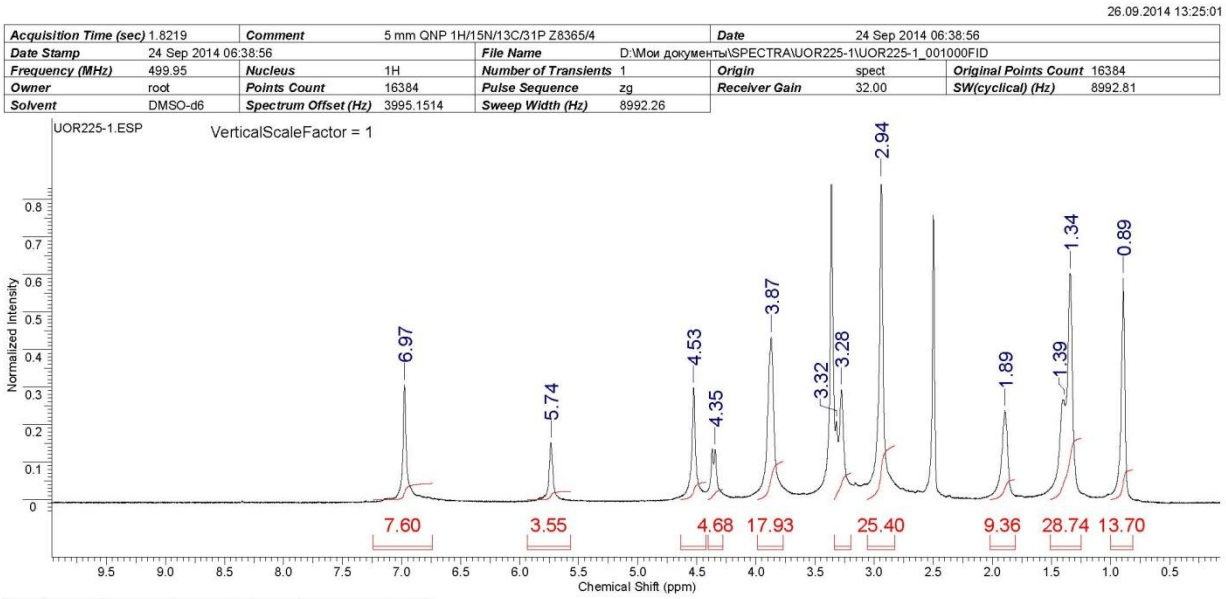
Acquisition Time (sec)	3.2047	***Comment***	Imported from UXNMR.			***Date***	14 Oct 2010 12:18:08
File Name	C:\Documents and Settings\Admin\Мои документы\FluorescenceRodik\nmr\Rodik-141010\Rodik-141010_001000fid					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	16	***Original Points Count***	16384	***Points Count***	16384
Pulse Sequence	zg30	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1850.8000	***Sweep Width (Hz)***	5112.47
Temperature (degree C)	27.000						



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	0.7397 .. 0.97	12.00148296	3.46253504e+8	12.00148296
2	1.1158 .. 1.61	39.56575012	1.14150720e+9	39.56575012
3	1.7129 .. 1.97	7.59613419	2.19155248e+8	7.59613419
4	2.8901 .. 3.22	21.37549591	6.16702144e+8	21.37549591
5	3.2483 .. 3.44	12.14904308	3.50510720e+8	12.14904308
6	3.4669 .. 3.65	7.90329885	2.28017216e+8	7.90329885
7	3.7829 .. 3.98	8.31374073	2.39858848e+8	8.31374073
8	4.2606 .. 4.42	4.93999290	1.42523200e+8	4.93999290
9	4.4599 .. 4.81	8.27556610	2.38757456e+8	8.27556610
10	6.5865 .. 7.08	6.87571192	1.98370416e+8	6.87571192

No.	(ppm)	(Hz)	Height
1	0.85	254.1	0.3368
2	1.26	377.7	0.4407
3	1.83	547.8	0.1020
4	3.07	921.3	0.4672
5	3.36	1008.1	0.1744
6	3.56	1067.4	0.0954
7	3.87	1160.4	0.1243
8	4.32	1296.4	0.0771
9	4.61	1384.1	0.1429
10	6.83	2048.5	0.0891

Fig. S28. ^{1}H NMR of compound **CX8N**.



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8087 .. 0.99	13.7046527	1.68726860e+7	13.70465279
2	[1.2485 .. 1.50	28.7393283	3.53828480e+7	28.73932838
3	[1.8089 .. 2.01	9.36168289	1.15257740e+7	9.36168289
4	[2.8255 .. 3.05	25.4041156	3.12766540e+7	25.40411568
5	[3.1966 .. 3.33	12.4615240	1.53421900e+7	12.46152401
6	[3.7710 .. 3.98	17.9279842	2.20723020e+7	17.92798424
7	[4.2805 .. 4.40	4.68298340	5.76552450e+6	4.68298340
8	[4.4253 .. 4.63	8.26171494	1.01715330e+7	8.26171494
9	[5.5703 .. 5.93	3.54999995	4.37063500e+6	3.54999995
10	[6.7399 .. 7.24	7.60357332	9.36125200e+6	7.60357332

No.	(ppm)	(Hz)	Height
12	70.79	8899.7	0.0141
13	77.05	9687.0	0.0195
14	122.35	15383.2	0.0150
15	134.98	16970.9	0.0214
16	137.32	17265.1	0.0139
17	160.23	20144.8	0.0135
18	163.02	20496.3	0.0143

Fig. S29. ^{13}C NMR of compound **CX8N**.

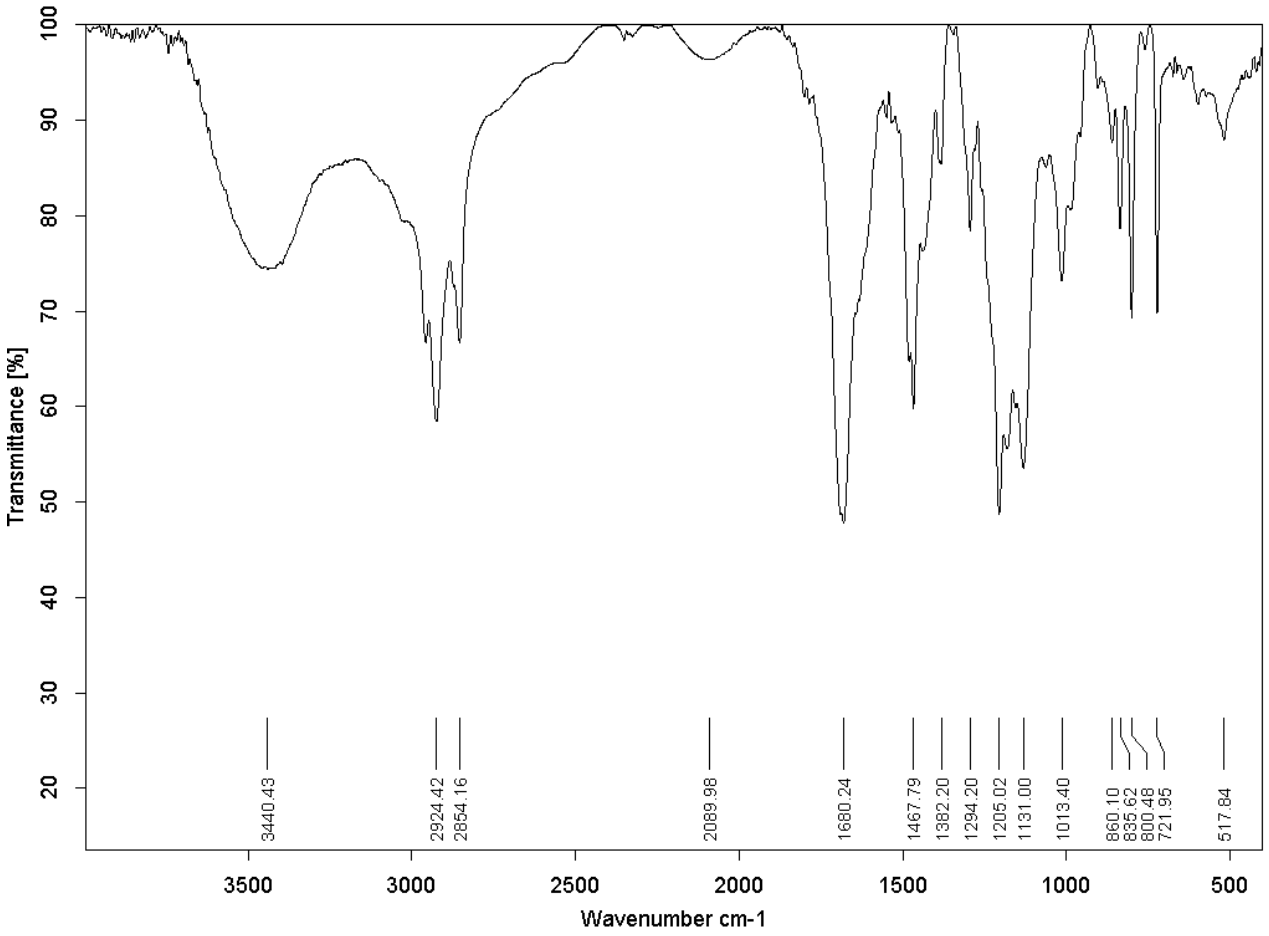
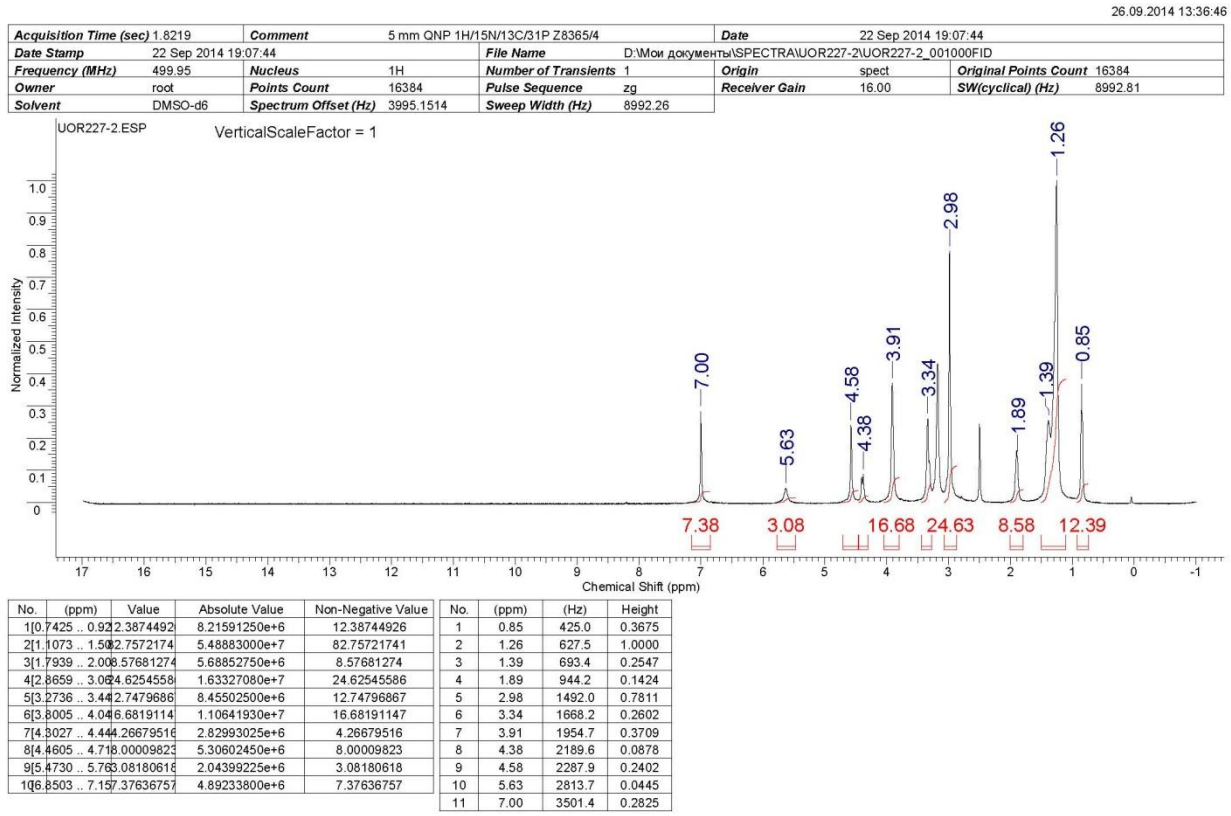


Fig. S30. FT-IR of compound **CX8N**.



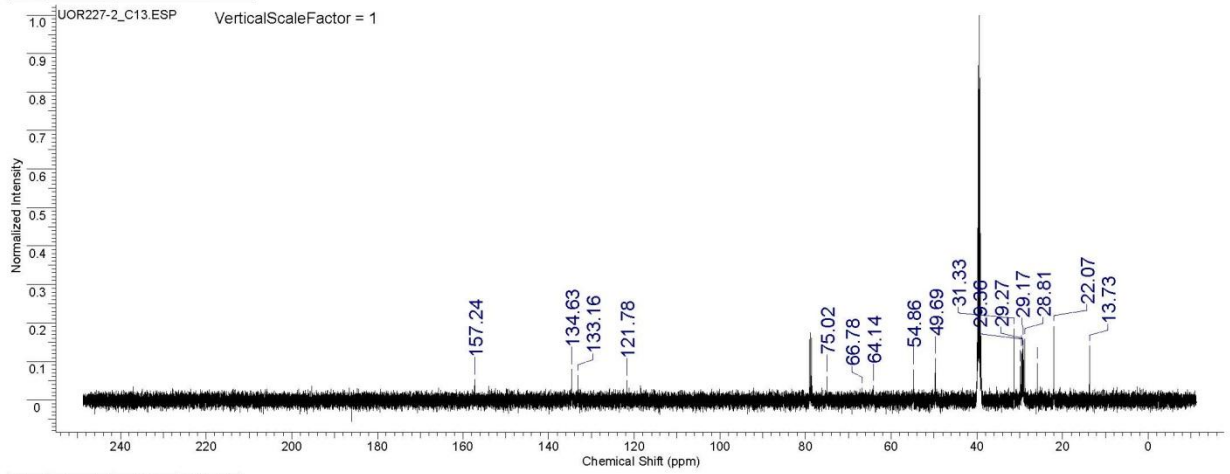
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.7425 .. 0.92	12.38744926	8.21591250e+6	12.38744926
2	[1.1073 .. 1.50	82.75721741	5.48883000e+7	82.75721741
3	[1.7939 .. 2.00	8.57681274	5.68852750e+6	8.57681274
4	[2.8659 .. 3.06	24.62545586	1.63327080e+7	24.62545586
5	[3.2736 .. 3.44	12.74796867	8.45502500e+6	12.74796867
6	[3.8005 .. 4.04	16.68191147	1.10641930e+7	16.68191147
7	[4.3027 .. 4.44	4.26679516	2.82993025e+6	4.26679516
8	[4.4605 .. 4.71	8.00009823	5.30602450e+6	8.00009823
9	[5.4730 .. 5.76	3.08180618	2.04399225e+6	3.08180618
10	[6.8503 .. 7.15	7.37636757	4.89233800e+6	7.37636757

No.	(ppm)	(Hz)	Height
1	0.85	425.0	0.3675
2	1.26	627.5	1.0000
3	1.39	693.4	0.2547
4	1.89	944.2	0.1424
5	2.98	1492.0	0.7811
6	3.34	1668.2	0.2602
7	3.91	1954.7	0.3709
8	4.38	2189.6	0.0878
9	4.58	2287.9	0.2402
10	5.63	2813.7	0.0445
11	7.00	3501.4	0.2825

Fig. S31. ^{1}H NMR of compound **CX12**.

26.09.2014 13:31:19

Acquisition Time (sec)	1.5667	***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	22 Sep 2014 19:14:08
Date Stamp	22 Sep 2014 19:14:08			***File Name***	D:\Мои документы\SPECTRA\UOR227-2_C13\UOR227-2_C13_001000FID		
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	494	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	14929.8379
Sweep Width (Hz)	32679.24						



No.	(ppm)	(Hz)	Height
1	13.73	1726.7	0.1405
2	22.07	2774.4	0.1914
3	25.89	3255.1	0.0944
4	28.81	3621.6	0.1580
5	29.17	3667.0	0.1563
6	29.27	3680.0	0.1327
7	29.36	3690.9	0.1302
8	29.52	3711.9	0.1268
9	29.55	3715.9	0.1243
10	29.79	3745.3	0.0460
11	29.82	3749.8	0.0772

No.	(ppm)	(Hz)	Height
12	29.85	3752.8	0.0873
13	31.33	3938.8	0.1846
14	49.69	6247.0	0.1075
15	54.86	6897.8	0.0788
16	64.14	8063.6	0.0370
17	66.78	8395.7	0.0310
18	75.02	9432.4	0.0600
19	121.78	15310.6	0.0505
20	133.16	16742.2	0.0631
21	134.63	16926.2	0.0804
22	157.24	19769.5	0.0532

Fig. S32. ^{13}C NMR of compound **CX12**.

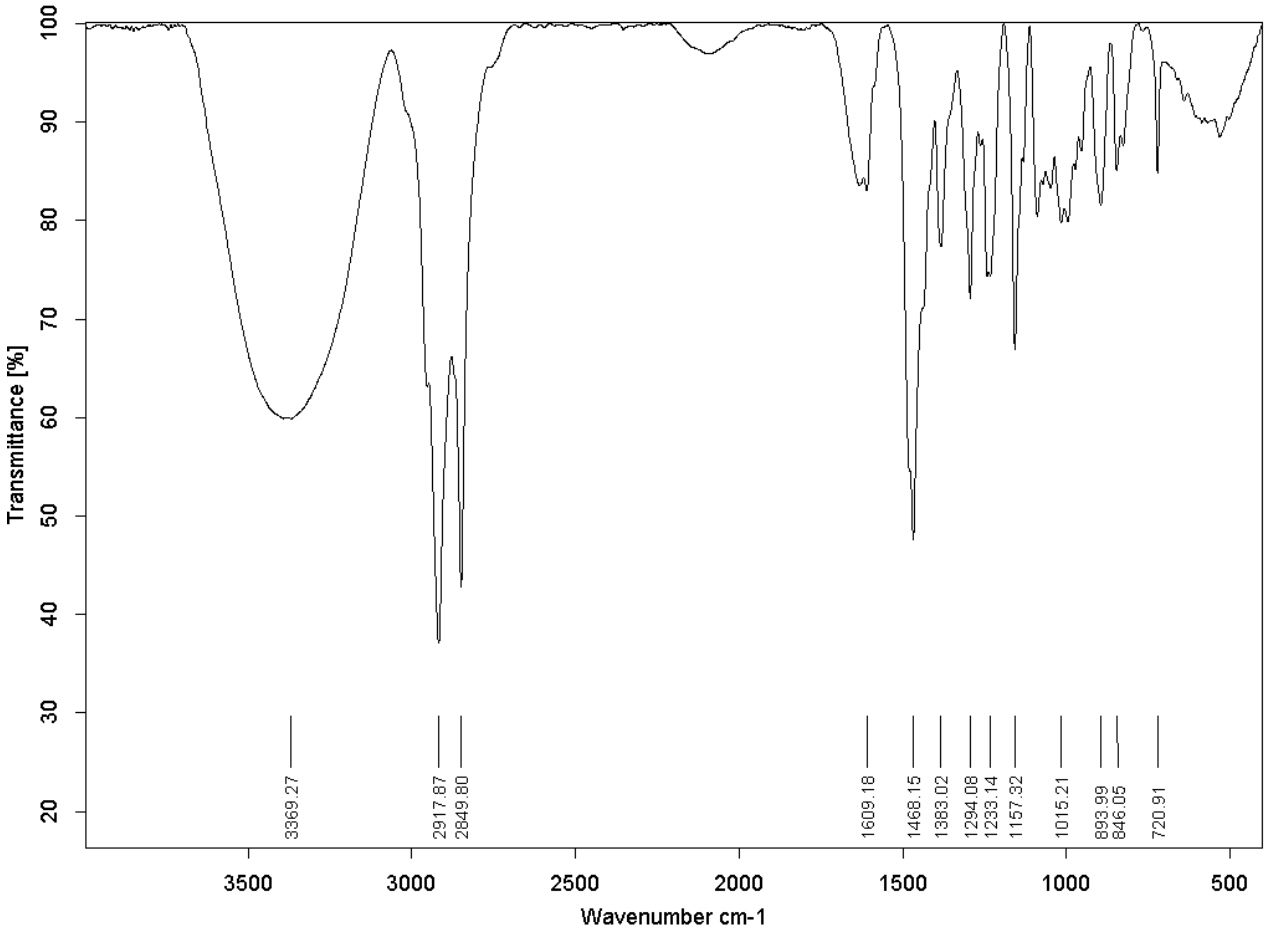
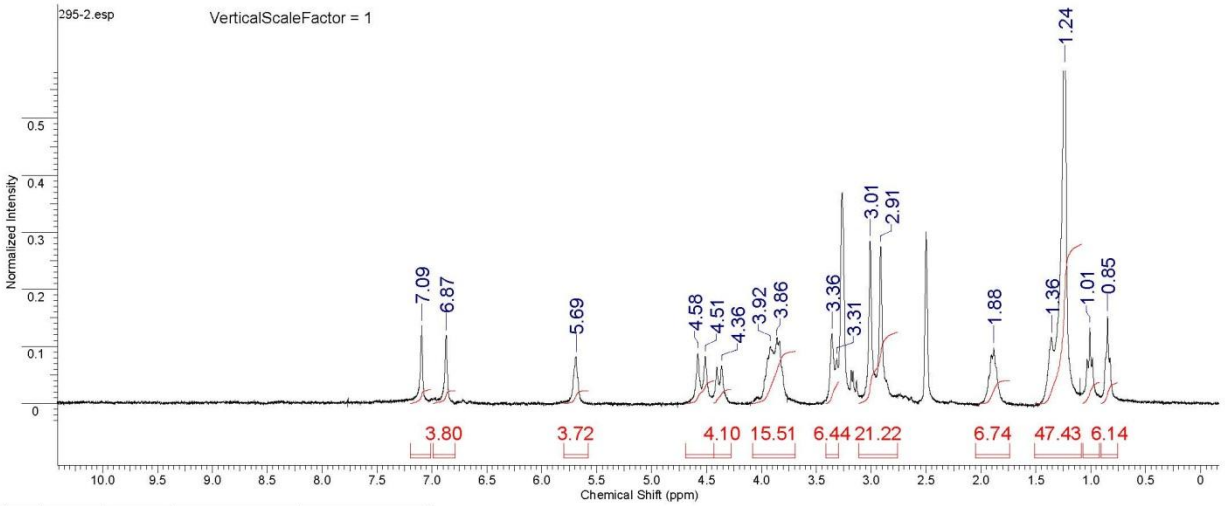


Fig. S33. FT-IR of compound **CX12**.

29.09.2014 11:48:13

Acquisition Time (sec) 3.2129	***Comment***	LYBRICS Imported file			***Date***	7/24/2012	***Date Stamp*** 7/24/2012
File Name	D:\Мои документы\SPECTRA\NANO2	295-2.NMR	***Frequency (MHz)***	299.95	***Nucleus***	1H	***Original Points Count*** 16384
Points Count 16384	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2329.0605	***Sweep Width (Hz)***	5099.44	



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.7528 .. 0.90	6.14427137	2.68380325e+6	6.14427137
2	[0.9226 .. 1.07	6.30272007	2.75301325e+6	6.30272007
3	[1.0836 .. 1.51	47.4324607	2.07183880e+7	47.43246078
4	[1.7415 .. 2.04	6.74063444	2.94429325e+6	6.74063444
5	[2.7585 .. 3.11	21.2176666	9.26782700e+6	21.21766663
6	[3.2981 .. 3.41	6.44143963	2.81360575e+6	6.44143963
7	[3.6926 .. 4.07	15.5064535	6.77318250e+6	15.50645351
8	[4.2788 .. 4.43	4.10043430	1.79106013e+6	4.10043430
9	[4.4352 .. 4.69	6.74768877	2.94737450e+6	6.74768877
10	[5.5777 .. 5.80	3.71947527	1.62465800e+6	3.71947527
11	[6.7877 .. 6.99	3.79698300	1.65851325e+6	3.79698300
12	[7.0095 .. 7.19	4.10303164	1.79219463e+6	4.10303164

No.	(ppm)	(Hz)	Height
1	0.85	254.0	0.1523
2	1.01	302.9	0.1330
3	1.24	371.4	1.0000
4	1.36	407.2	0.1152
5	1.88	565.0	0.0976
6	2.91	874.1	0.2748
7	3.01	902.4	0.2843
8	3.31	993.6	0.0786
9	3.36	1007.0	0.1218
10	3.86	1158.2	0.1101
11	3.92	1175.7	0.1000
12	4.36	1308.6	0.0661
13	4.51	1353.1	0.0830
14	4.58	1373.3	0.0882
15	5.69	1706.4	0.0813
16	6.87	2061.5	0.1196
17	7.09	2127.5	0.1360

Fig. S34. ^{1}H NMR of compound **CX3-16**.

26.09.2014 13:31:19

Acquisition Time (sec)	1.5667	***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	22 Sep 2014 19:14:08
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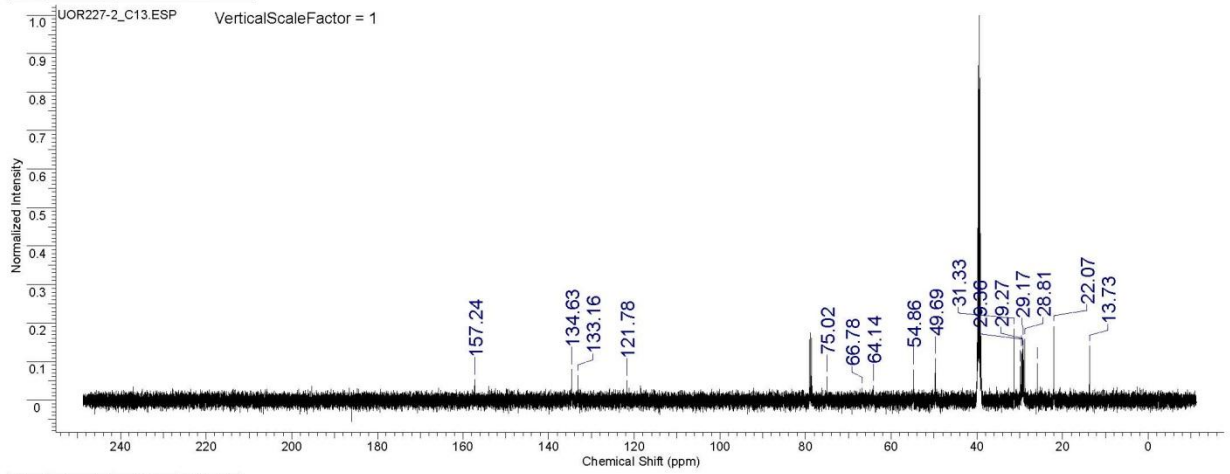
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	494	***Origin***	spect
Original Points Count	51200	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	51200.00	***SW(cyclical) (Hz)***	32679.74	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	14929.8379
Sweep Width (Hz)	32679.24						



No.	(ppm)	(Hz)	Height
1	13.73	1726.7	0.1405
2	22.07	2774.4	0.1914
3	25.89	3255.1	0.0944
4	28.81	3621.6	0.1580
5	29.17	3667.0	0.1563
6	29.27	3680.0	0.1327
7	29.36	3690.9	0.1302
8	29.52	3711.9	0.1268
9	29.55	3715.9	0.1243
10	29.79	3745.3	0.0460
11	29.82	3749.8	0.0772

No.	(ppm)	(Hz)	Height
12	29.85	3752.8	0.0873
13	31.33	3938.8	0.1846
14	49.69	6247.0	0.1075
15	54.86	6897.8	0.0788
16	64.14	8063.6	0.0370
17	66.78	8395.7	0.0310
18	75.02	9432.4	0.0600
19	121.78	15310.6	0.0505
20	133.16	16742.2	0.0631
21	134.63	16926.2	0.0804
22	157.24	19769.5	0.0532

Fig. S35. ^{13}C NMR of compound **CX3-16**.

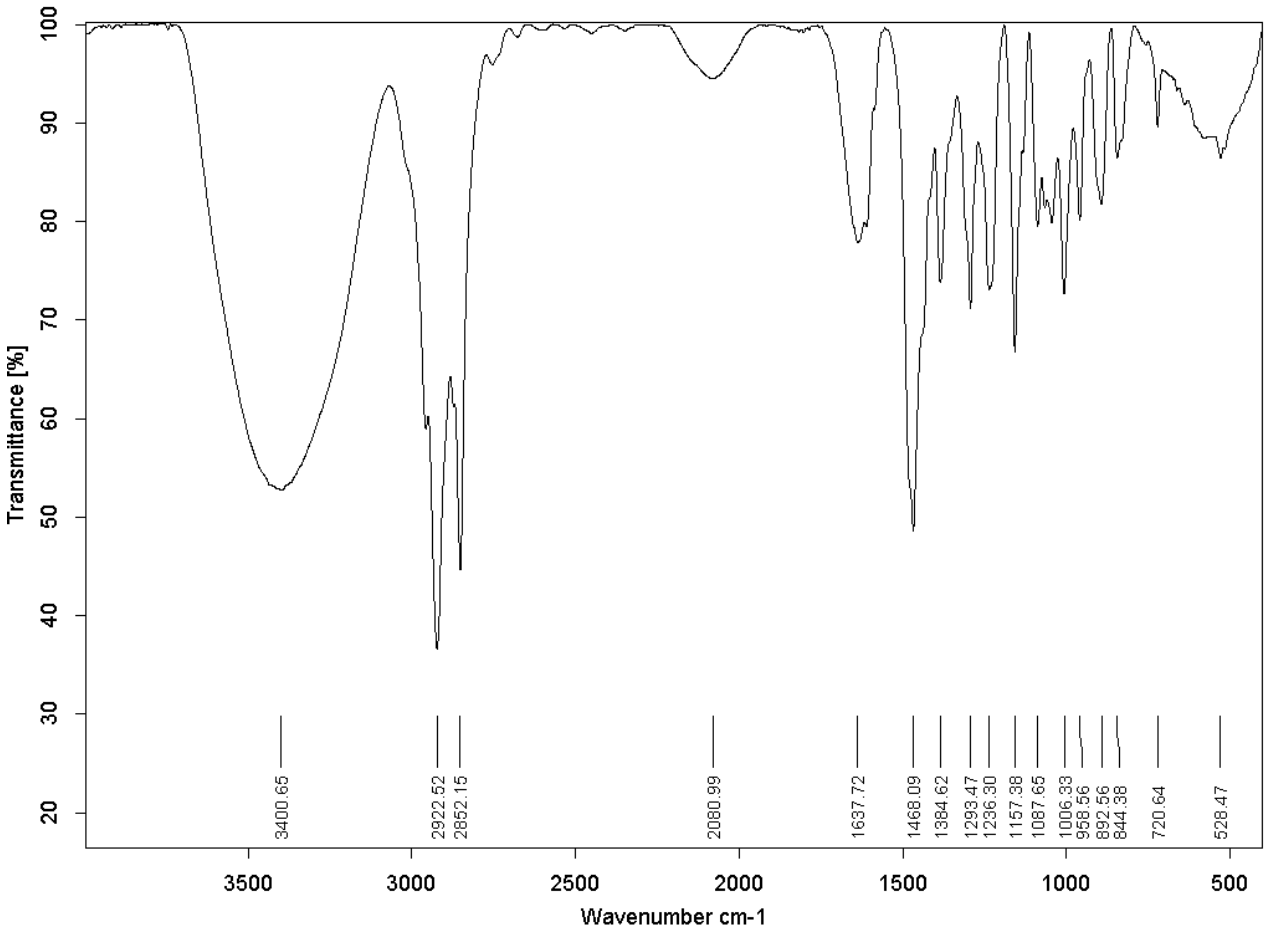
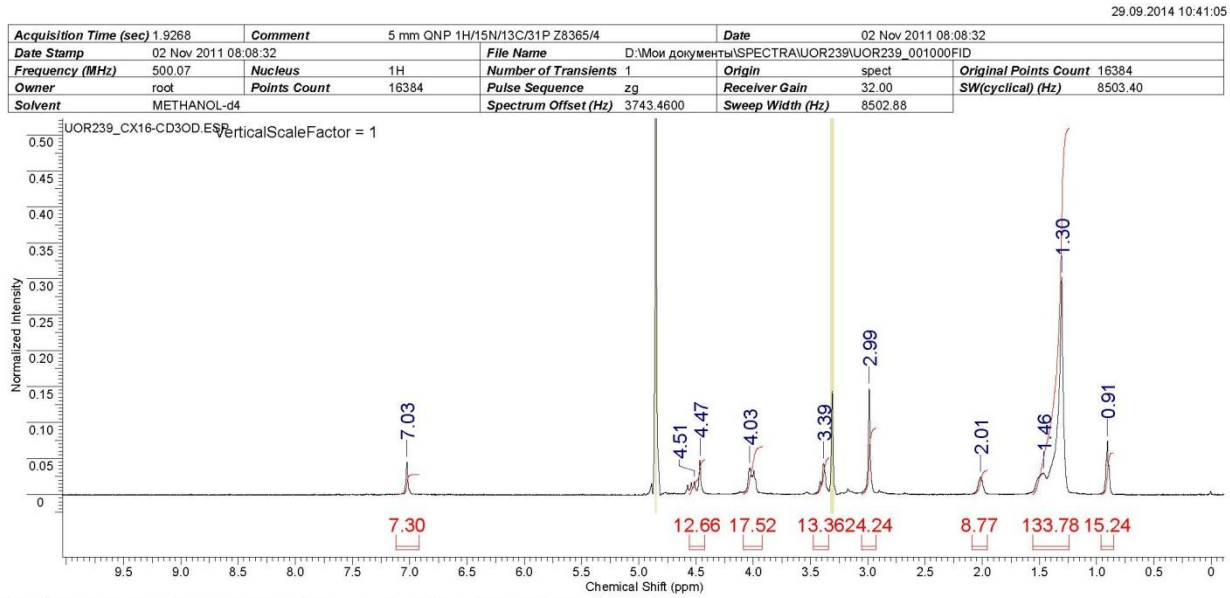


Fig. S36. FT-IR of compound **CX3-16**.



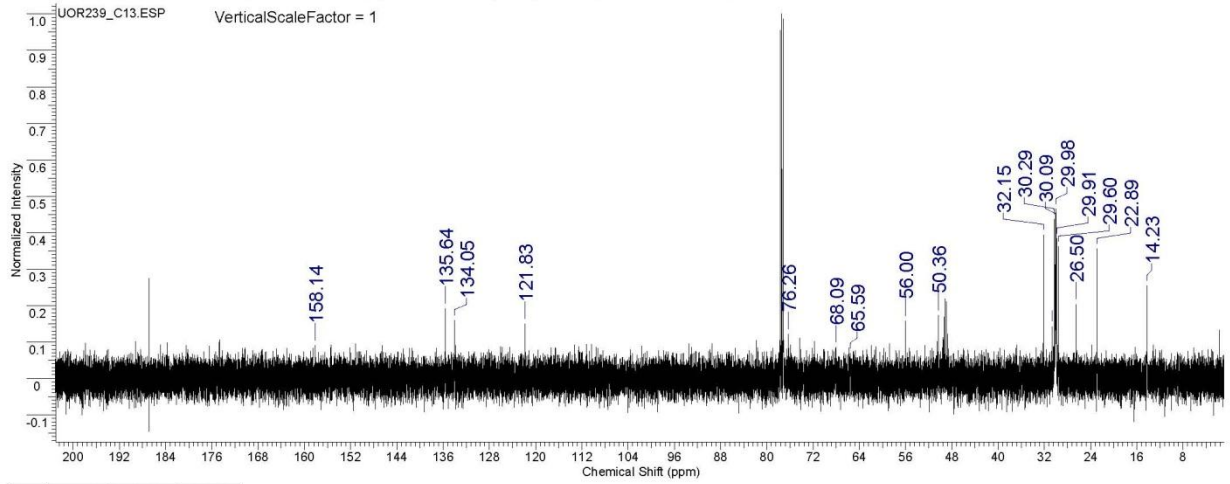
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.8553 .. 0.95	15.2367563	5.79010500e+6	15.23675632
2	[1.2425 .. 1.55	133.7841491	5.08391880e+7	133.78414917
3	[1.9548 .. 2.09	8.77058506	3.33290125e+6	8.77058506
4	[2.9284 .. 3.05	24.2419891	9.21217500e+6	24.24198914
5	[3.3418 .. 3.47	13.3627481	5.07796500e+6	13.36274815
6	[3.9227 .. 4.08	17.5245914	6.65950300e+6	17.52459145
7	[4.4251 .. 4.55	12.6572876	4.80988350e+6	12.65728760
8	[6.9191 .. 7.12	7.30000019	2.77406600e+6	7.30000019

No.	(ppm)	(Hz)	Height
1	0.91	453.2	0.0742
2	1.30	652.5	0.3020
3	1.46	731.4	0.0296
4	2.01	1007.5	0.0245
5	2.99	1493.3	0.1469
6	3.39	1693.6	0.0432
7	4.03	2015.4	0.0366
8	4.47	2232.9	0.0471
9	4.51	2257.8	0.0180
10	7.03	3513.3	0.0453

Fig. S37. ^{1}H NMR of compound **CX16**.

29.09.2014 10:57:15

Acquisition Time (sec) 1.5667		***Comment***	5 mm QNP 1H/15N/13C/31P Z8365/4			***Date***	18 Sep 2014 21:11:28		
Date Stamp	18 Sep 2014 21:11:28			***File Name***	D:\Мои документы\SPECTRA\UOR239_C13\UOR239_C13_001000FID				
Frequency (MHz)	125.73	***Nucleus***	13C	***Number of Transients***	171	***Origin***	spect	***Original Points Count***	51200
Owner	root	***Points Count***	65536	***Pulse Sequence***	zgpg	***Receiver Gain***	51200.00	***SW(cyclical) (Hz)***	32679.74
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	15041.8223	***Sweep Width (Hz)***	32679.24				



No.	(ppm)	(Hz)	Height
1	14.23	1788.9	0.2534
2	22.89	2877.4	0.3552
3	26.50	3331.2	0.2031
4	29.60	3721.1	0.3610
5	29.91	3760.5	0.3828
6	29.92	3761.5	0.3626
7	29.98	3769.5	0.4645
8	30.01	3773.5	0.4540
9	30.03	3775.5	0.4217
10	30.05	3778.0	0.2852
11	30.07	3781.0	0.4107
12	30.08	3782.0	0.4160

No.	(ppm)	(Hz)	Height
13	30.09	3783.5	0.4227
14	30.14	3789.0	0.3112
15	30.29	3808.4	0.4363
16	30.69	3858.8	0.1424
17	32.15	4041.8	0.3938
18	50.36	6331.6	0.1724
19	56.00	7040.7	0.1567
20	65.59	8245.9	0.0677
21	68.09	8560.6	0.0852
22	76.26	9587.8	0.1210
23	121.83	15317.3	0.1496
24	134.05	16854.2	0.1591
25	135.64	17053.6	0.1914
26	158.14	19882.0	0.0908

Fig. S38. ^{13}C NMR of compound **CX16**.

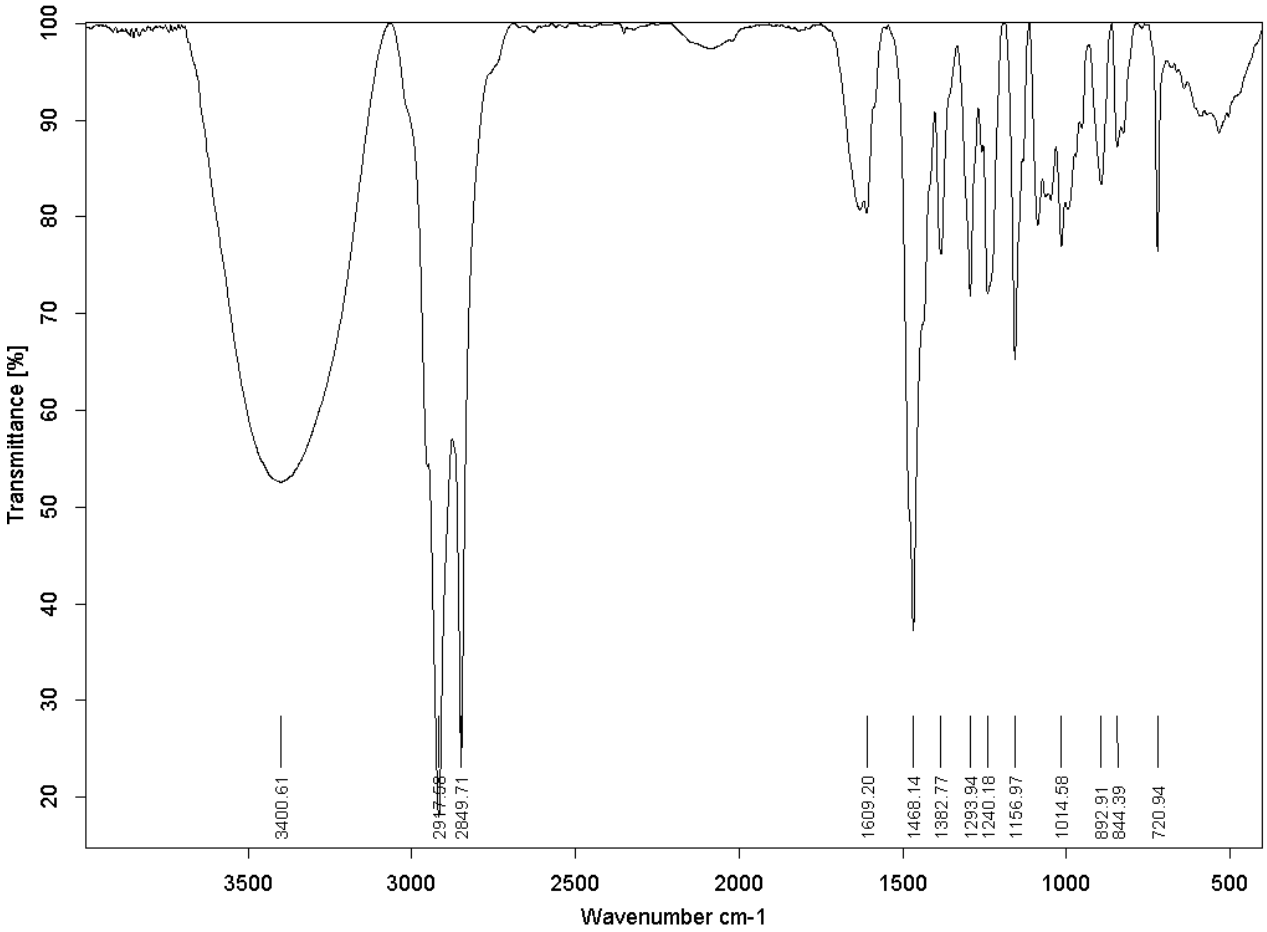


Fig. S39. FT-IR of compound **CX16**.