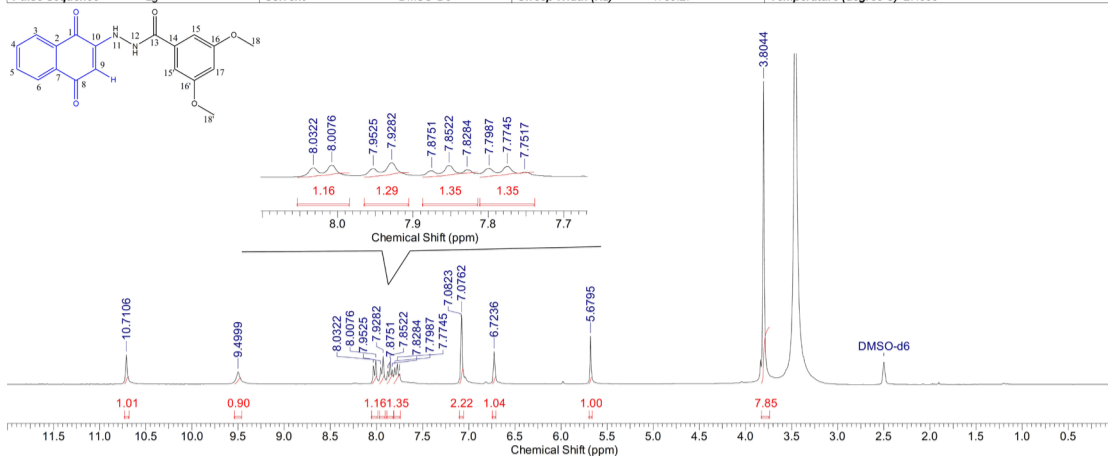
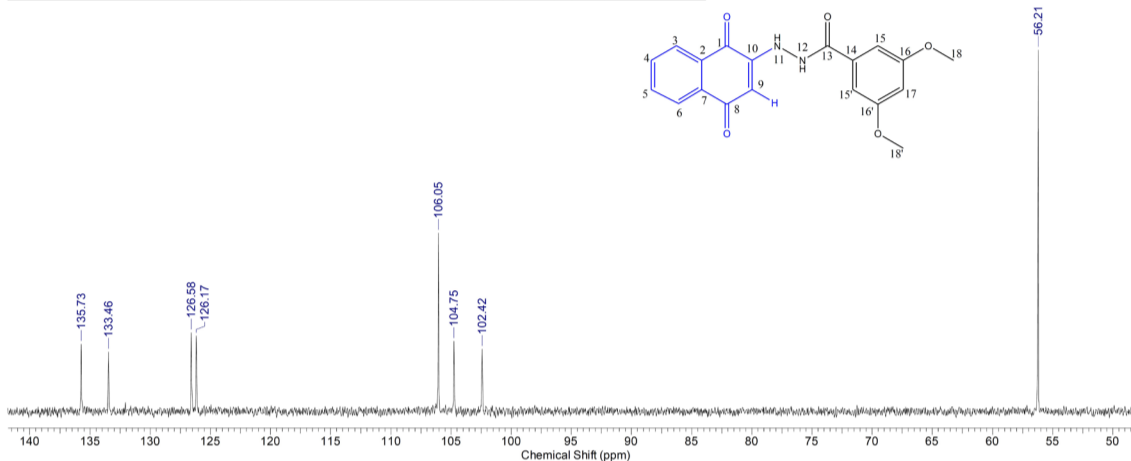


SUPPLEMENTARY MATERIAL

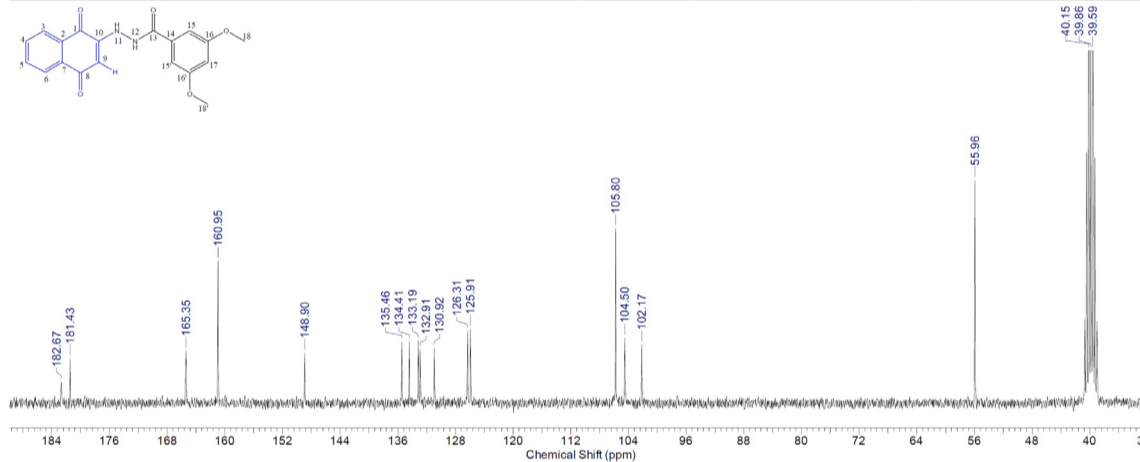
Acquisition Time (sec)	6.8420	Comment	1H -DMSO - RDC-022- DPL - Rosane	Date	10 Nov 2016 09:11:44
File Name	C:\Users\Brasil\Desktop\Qualificação Rosane\Espectros\Espectros Não processados\RDC-022 - correto_001001r	Frequency (MHz)	300.13	Nucleus	1H
Nucleus	1H	Number of Transients	8	Original Points Count	32768
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	4789.27
				Temperature (degree C)	27.000



Acquisition Time (sec)	1.7400	Comment	DEPT 135 -DMSO - RDC-022- DPL - Rosane	Date	16 Nov 2016 13:54:36
File Name	C:\Users\Brasil\Desktop\RDC-022_002001r	Frequency (MHz)	75.47	Nucleus	13C
Number of Transients	320	Original Points Count	32768	Points Count	32768
Solvent	DMSO-D6	Sweep Width (Hz)	18832.39	Temperature (degree C)	27.000
				Pulse Sequence	dept135



Acquisition Time (sec)	0.8700	Comment	13C -DMSO - RDC-022- DPL - Rosane	Date	10 Nov 2016 09:38:52
File Name	C:\Users\Brasil\Desktop\Qualificação Rosane\Espectros\RDC-022 - correto_333001r	Frequency (MHz)	75.47	Nucleus	13C
Nucleus	13C	Number of Transients	1412	Original Points Count	16384
Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	18832.39
				Temperature (degree C)	27.000



Title	cial do Brasil (GMT-3:00)	Comment	Amostra 032 por Iscm data quarta-feira, maio 17 2017
Origin	cial do Brasil (GMT-3:00)	File Name	C:\USERS\ROSANGELA\DESKTOP\ROSANE\DISSERTAÇÃO\OINFRAVERMELHO\RDC_022_1.SP
Date Stamp	wed may 17 14:03:23 2017 Hora oficial do Brasil (GMT-3:00)	Date	wed may 17 14:03:49 2017 Hora oficial do Brasil (GMT-3:00)
Technique	Infrared	Instrument	Frontier FT-IR
X Axis	Wavenumber (cm-1)	Y Axis	Arbitrary
Points Count	3601	Data Spacing	1.0000
		Spectral Region	IR
		Spectrum Range	400.0000 - 4000.0000

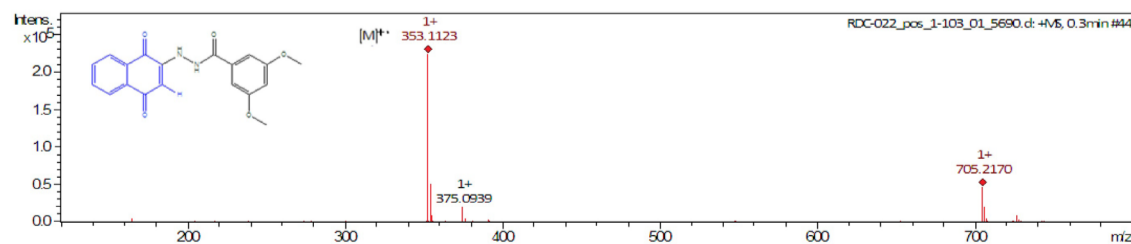
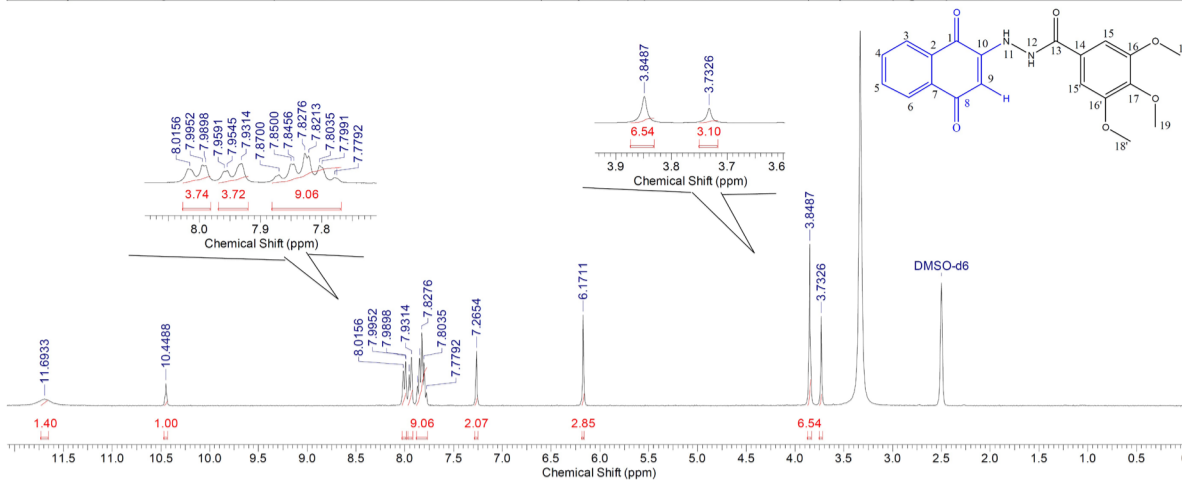
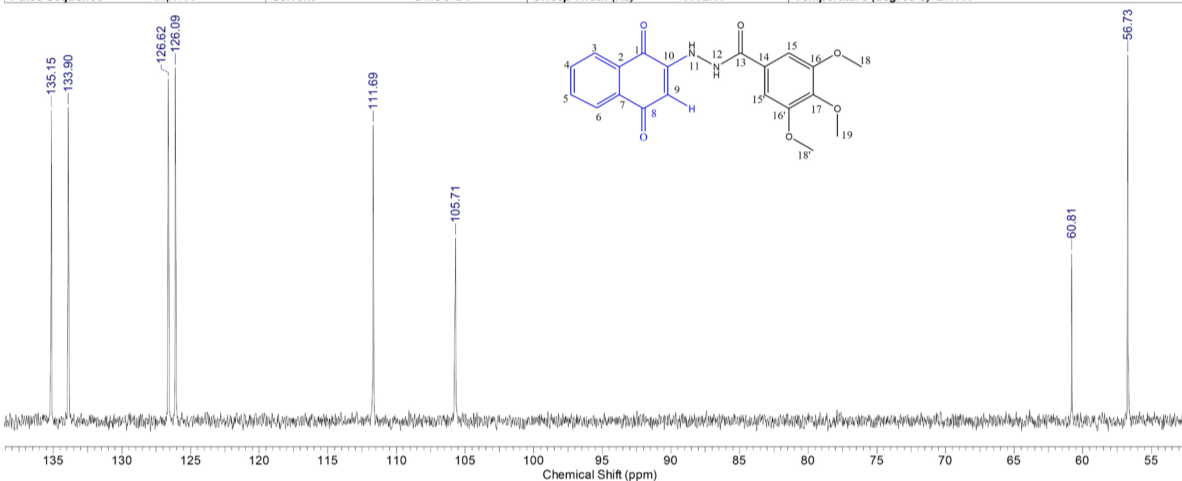


Figure S1. Structural elucidation of *N'*-(1,4-Dioxo-1,4-dihydronaphthalen-2-yl)-3,5-dimethoxybenzohydrazide (13).

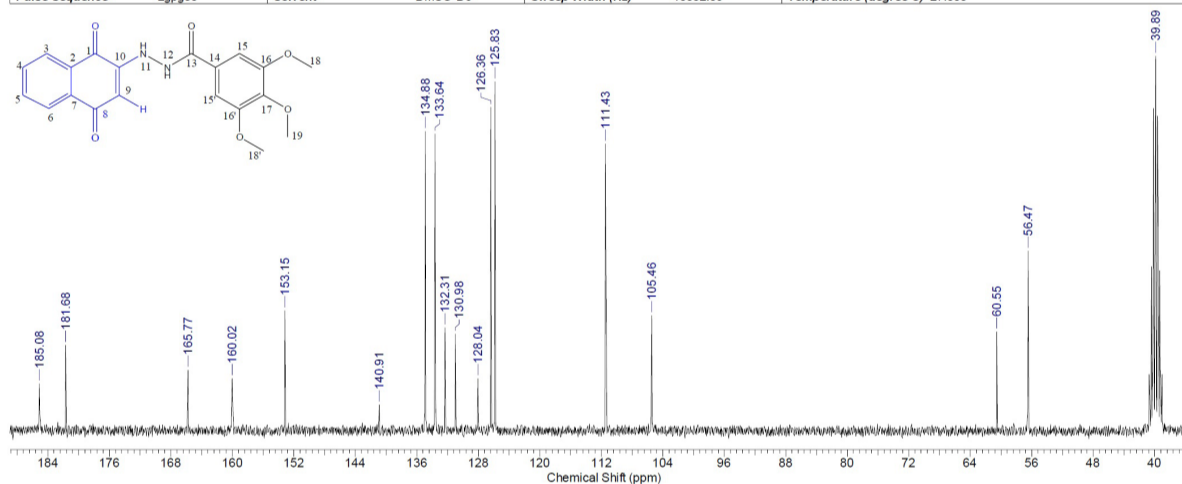
Acquisition Time (sec)	6.8420	Comment	1H - DMSO - RDC 030E - DPL - ROSANE	Date	17 May 2016 10:35:18
File Name	C:\Users\Brasil\Desktop\Qualificação Rosane\Espectros\Espectros Não processados\RDC 030E_001001r			Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	8	Original Points Count	32768
Pulse Sequence	zg	Solvent	DMSO-D6	Sweep Width (Hz)	4789.27
				Points Count	65536
				Temperature (degree C)	27.000



Acquisition Time (sec)	1.7400	Comment	DEPT 135 - DMSO - RDC 030 - DPL - ROSANE	Date	16 Nov 2016 15:18:00
File Name	C:\Users\Brasil\Desktop\Qualificação Rosane\Espectros\RDC 030_002001r			Frequency (MHz)	75.47
Nucleus	13C	Number of Transients	200	Original Points Count	32768
Pulse Sequence	dept135	Solvent	DMSO-D6	Sweep Width (Hz)	18832.39
				Points Count	32768
				Temperature (degree C)	27.000



Acquisition Time (sec)	0.8700	Comment	13C - DMSO - RDC 030 - DPL - ROSANE	Date	16 Nov 2016 15:03:32
File Name	C:\Users\Brasil\Desktop\Qualificação Rosane\Espectros\RDC 030_003001r			Frequency (MHz)	75.47
Nucleus	13C	Number of Transients	972	Original Points Count	16384
Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	18832.39
				Points Count	32768
				Temperature (degree C)	27.000



Title	cial do Brasil (GMT-3:00)	Comment	Amostra 020 por Iscm data quarta-feira, maio 10 2017	Origin	cial do Brasil (GMT-3:00)
File Name	C:\USERS\USUARIO\DESKTOP\RDC_30E_1.SP			Date Stamp	wed may 10 16:58:02 2017 Hora oficial do Brasil (GMT-3:00)
Date	wed may 10 16:58:50 2017 Hora oficial do Brasil (GMT-3:00)			Technique	Infrared
Spectral Region	IR	X Axis	Wavenumber (cm-1)	Y Axis	%Transmittance
Points Count	3601	Data Spacing	1.0000		Spectrum Range 400.0000 - 4000.0000

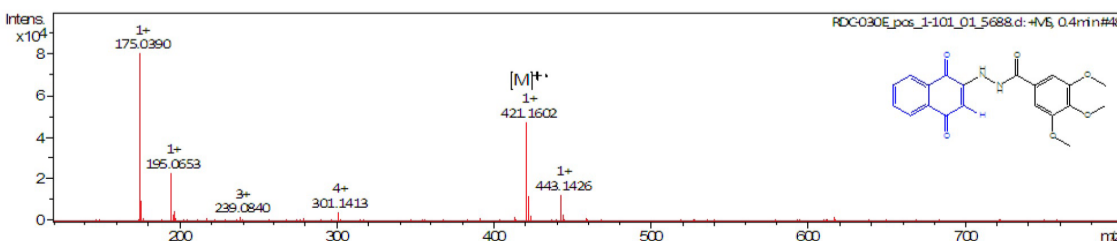
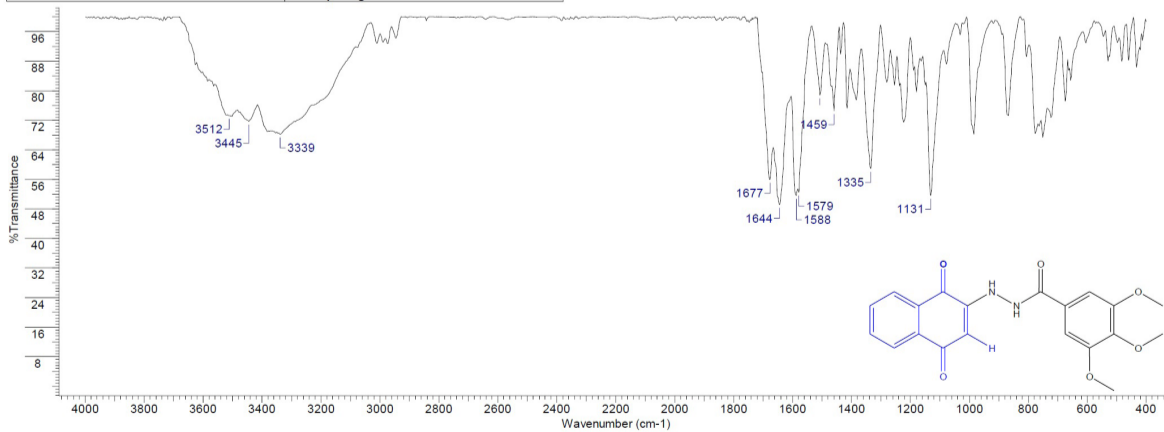
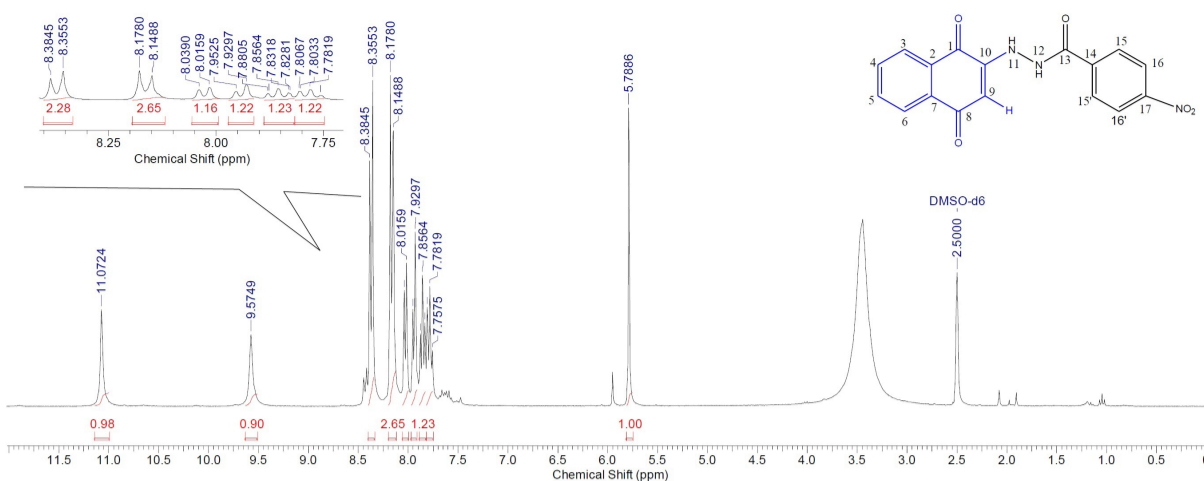
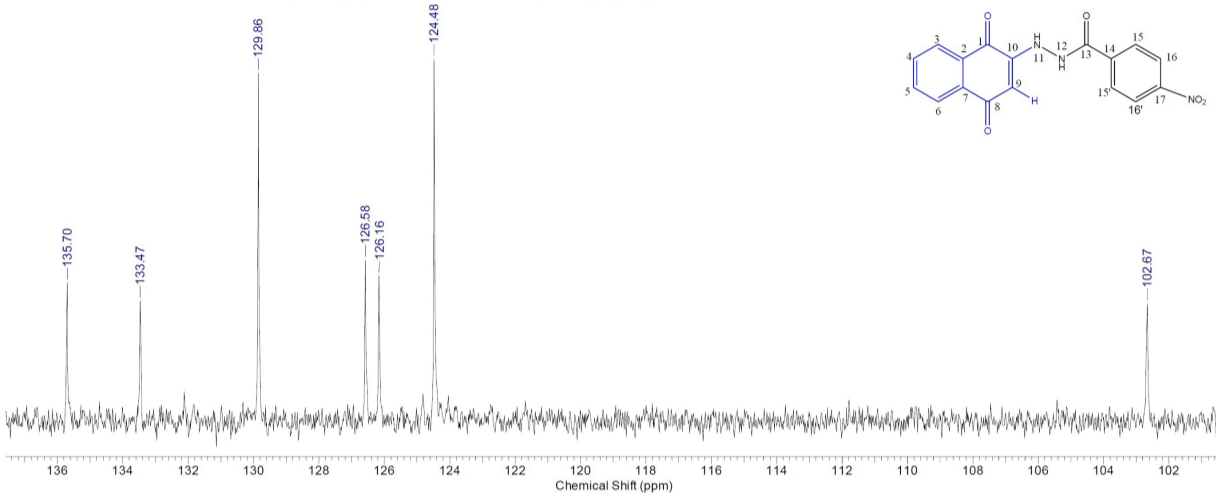


Figure S2. Structural elucidation of *N'*-(1,4-Dioxo-1,4-dihydronaphthalen-2-yl)-3,4,5-trimethoxybenzohydrazide (14).

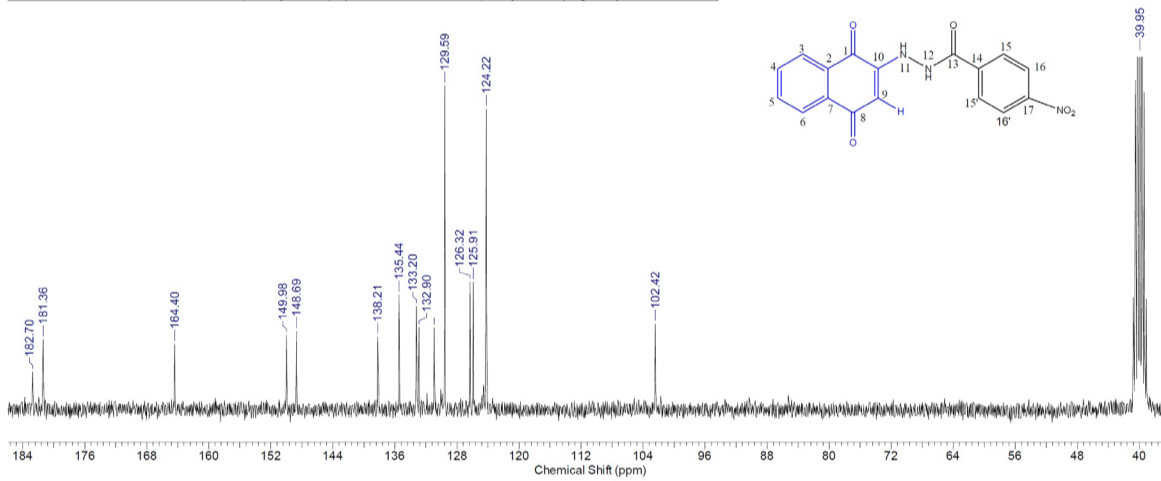
Acquisition Time (sec)	6.8420	Comment	1H-DMSO - RDC N1-2- DPL - Rosane	Date	16 Nov 2016 14:00:18
File Name	C:\Users\Brasil\Desktop\RDC N1-2_001001r	Frequency (MHz)	300.13	Nucleus	1H
Original Points Count	32768	Points Count	65536	Pulse Sequence	zg
Temperature (degree C)	27.000	Solvent	DMSO-D6	Sweep Width (Hz)	4789.27



Acquisition Time (sec)	1.7400	Comment	DEPT 135 -DMSO - RDC N1-2- DPL - Rosane	Date	10 Nov 2016 10:31:52
File Name	C:\Users\Brasil\Desktop\RDC N1-2_002001r	Frequency (MHz)	75.47	Nucleus	13C
Number of Transients	160	Original Points Count	32768	Points Count	32768
Solvent	DMSO-D6	Sweep Width (Hz)	18832.39	Pulse Sequence	dept135
		Temperature (degree C)	27.000		



Acquisition Time (sec)	0.8700	Comment	13C-DMSO - RDC N1-2- DPL - Rosane	Date	10 Nov 2016 10:16:14
File Name	C:\Users\Brasil\Desktop\RDC N1-2_003001r	Frequency (MHz)	75.47	Nucleus	13C
Number of Transients	1219	Original Points Count	16384	Points Count	32768
Solvent	DMSO-D6	Sweep Width (Hz)	18832.39	Pulse Sequence	zgpg30
		Temperature (degree C)	27.000		



Title	ciado Brasil (GMT-3.00)	Comment	Amostra 021 por Iscm_data quarta-feira, maio 10 2017	Origin	ciado Brasil (GMT-3.00)
File Name	C:\USERS\BRASIL\DESKTOP\RDC-N1-1.SP	Date Stamp	wed may 10 17:06:21 2017 Hora oficial do Brasil (GMT-3.00)		
Date	wed may 10 17:06:46 2017 Hora oficial do Brasil (GMT-3.00)	Technique	Infrared	Experiment	Fractor ET-III
Spectral Region	IR	X Axis	Wavenumber (cm-1)	Y Axis	% Transmittance
Points Count	3601	Data Spacing	1.0000	Spectrum Range	400.0000 -4000.0000

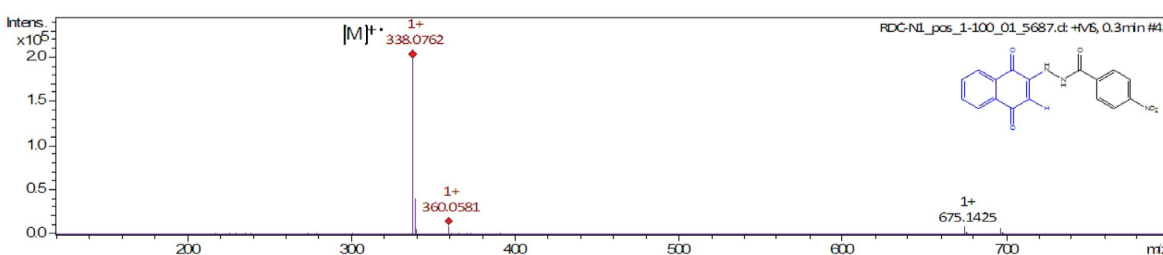
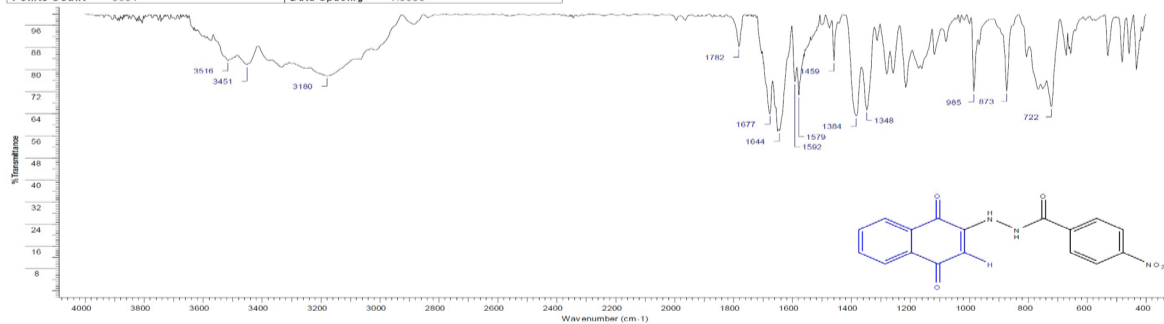


Figure S3. Structural elucidation of *N'*-(1,4-Dioxo-1,4-dihydronaphthalen-2-yl)-4-nitrobenzohydrazide (15).

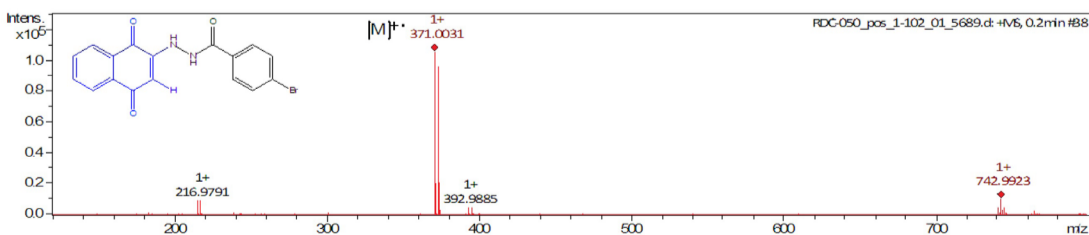
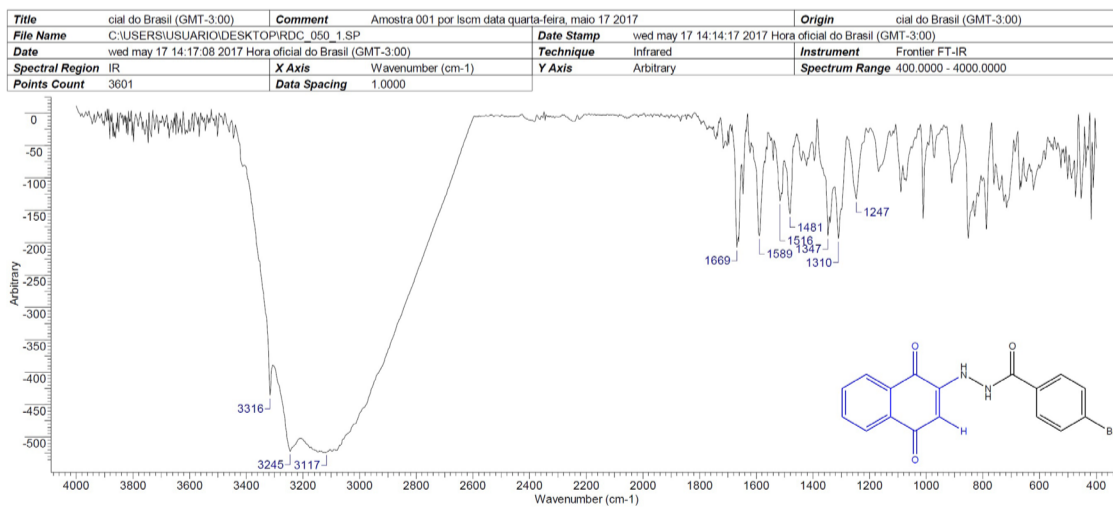
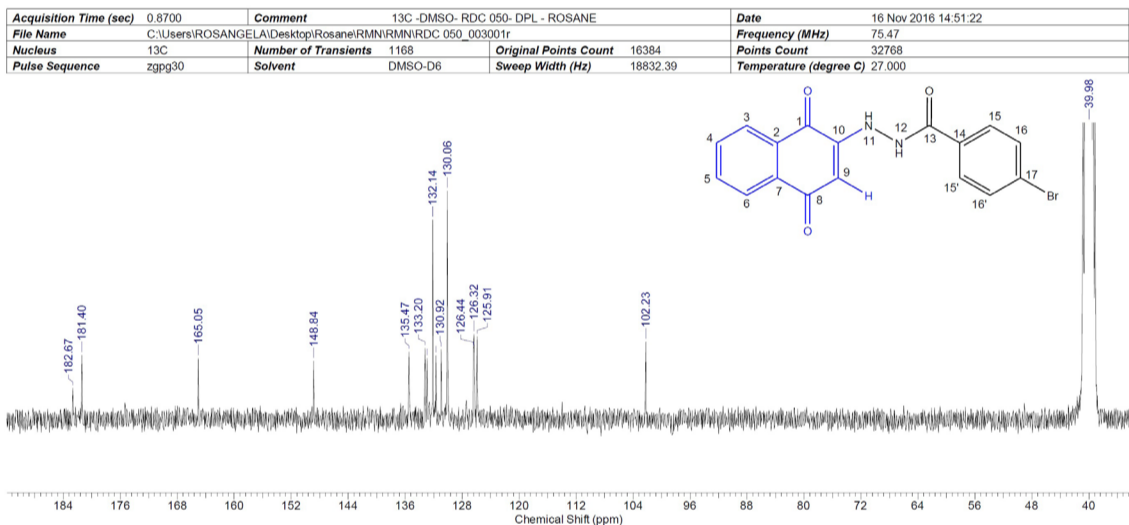
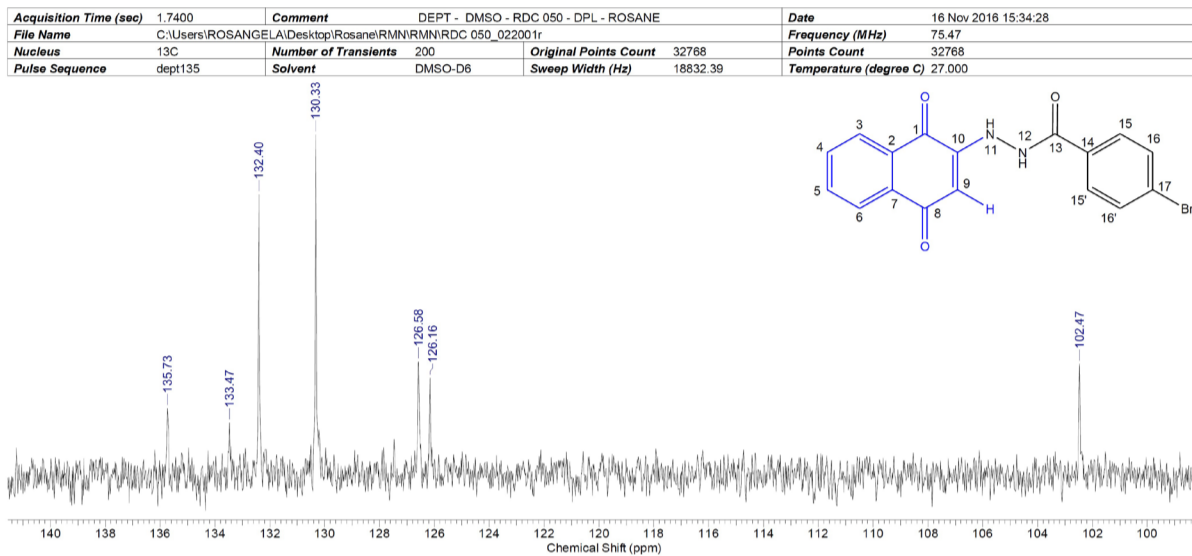
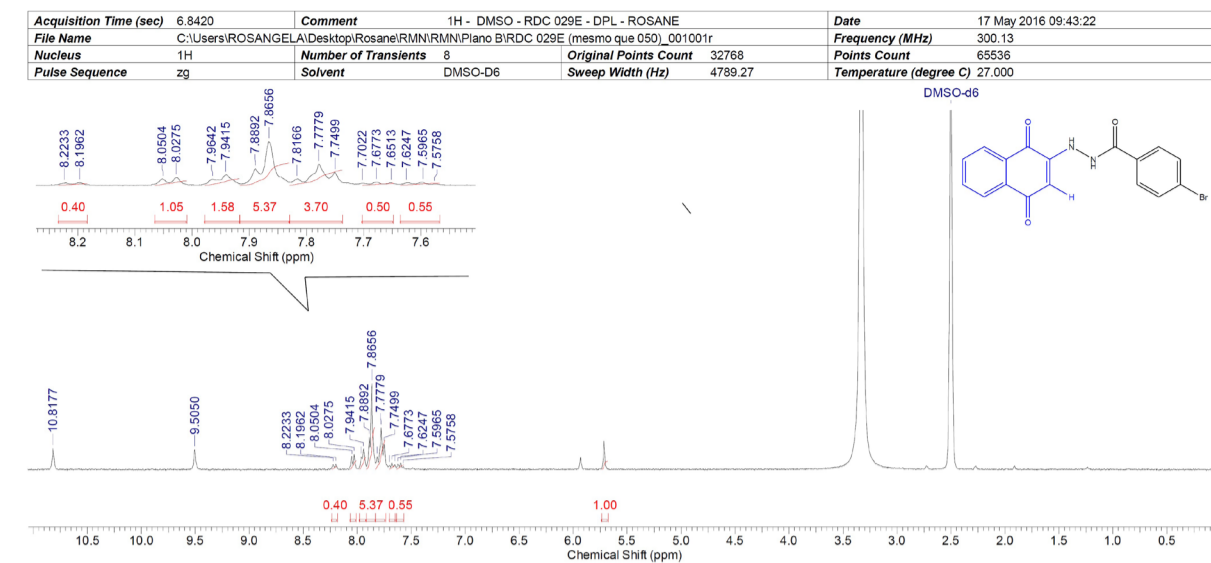


Figure S4. Structural elucidation of 4-Bromo-N'-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzohydrazide (16).

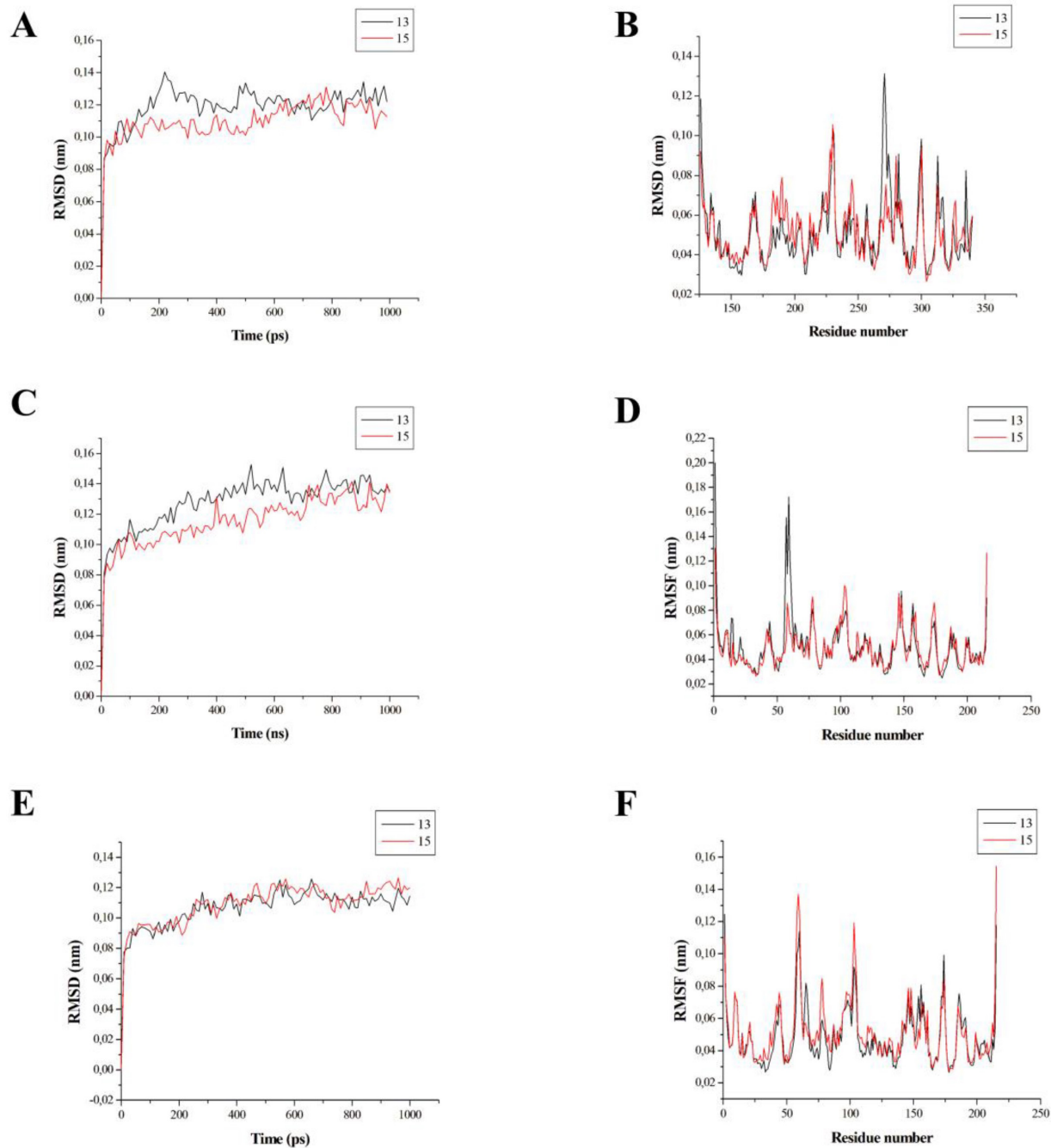


Figure S5. Graphical representation of RMSD and RMSF of all systems submitted to molecular dynamics simulations.