Electronic Supplementary Information (ESI)

3D QSAR-based design and liquid phase combinatorial synthesis of 1,2-disubstituted benzimidazole-5-carboxylic acid and 3-substituted-5H-benzimidazo[1,2-d][1,4]benzodiazepin-6 (7H)-one derivatives as anti-mycobacterial agents

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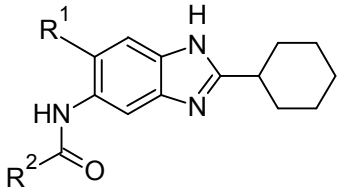
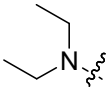
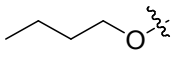
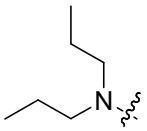
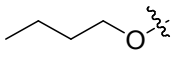
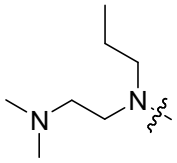
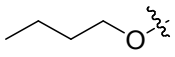
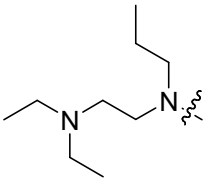
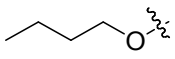
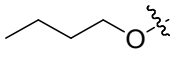
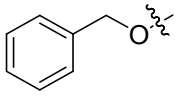
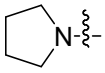
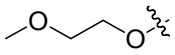
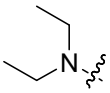
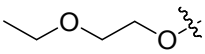
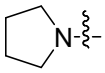
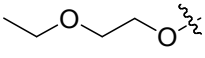
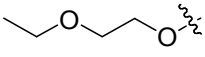
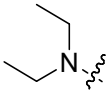
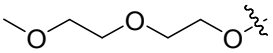
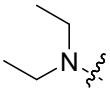
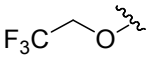
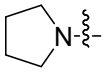
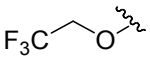
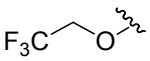
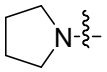
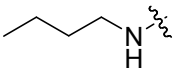
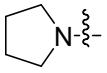
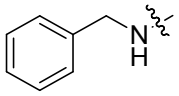
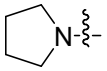
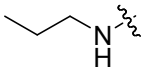
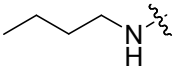
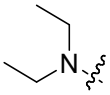
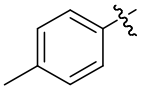
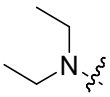
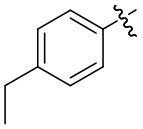
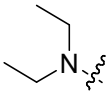
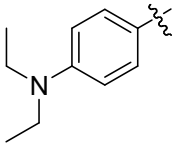
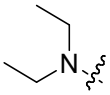
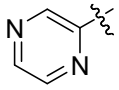
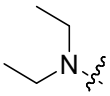
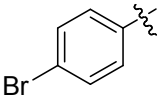
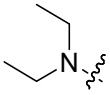
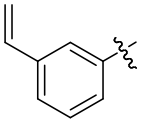
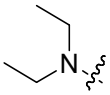
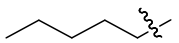
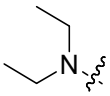
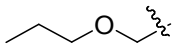
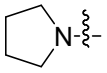
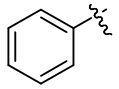
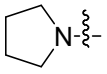
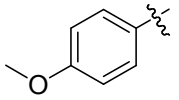
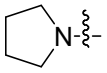
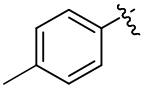
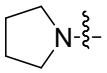
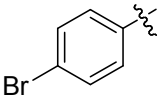
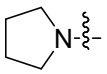
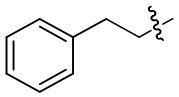
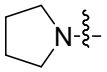
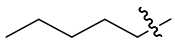
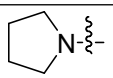
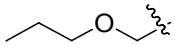
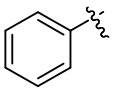
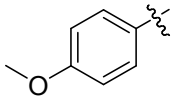
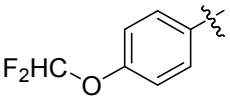
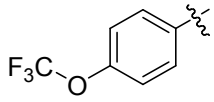
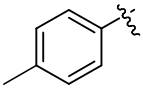
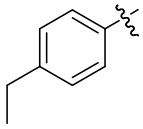
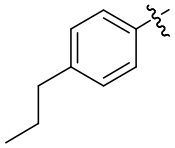
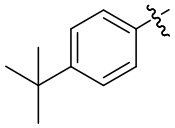
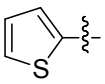
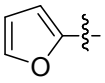
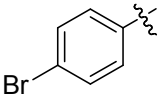
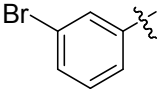
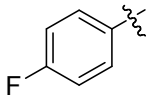
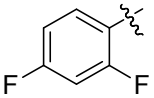
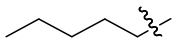
[c] Tuberculosis Research Laboratory, Vaccine and Infectious Disease Research Centre, Translational Health Science and Technology Institute, Faridabad-Gurugram Expressway, Haryana, India.

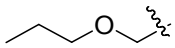
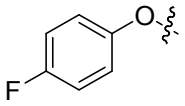
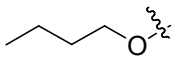
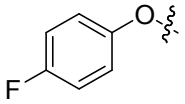
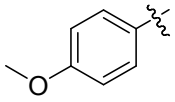
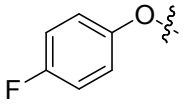
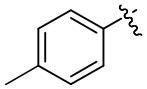
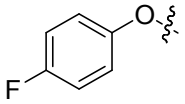
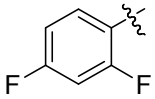
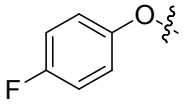
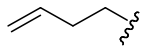
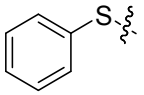
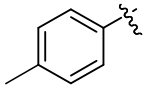
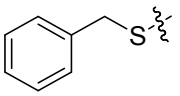
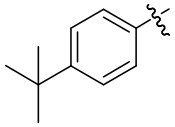
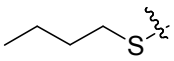
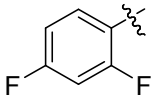
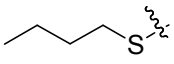
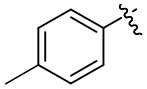
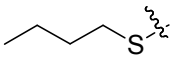
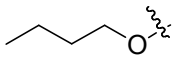
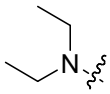
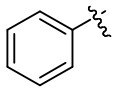
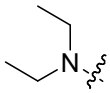
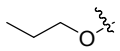
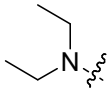
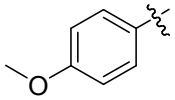
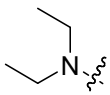
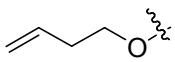
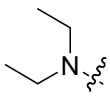
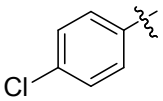
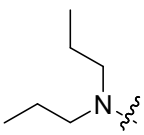
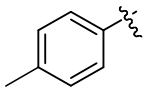
Table-S1. Structure of the compounds with MIC and pMIC value used for 3D QSAR analysis

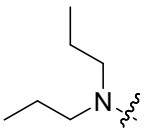
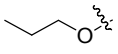
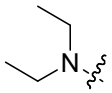
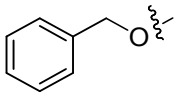
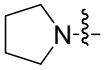
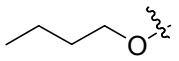
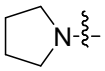
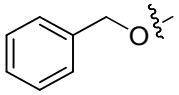
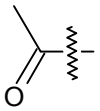
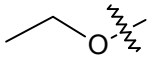


Sr No.	R^1	R^2	MIC(μM)	pMIC
Tr1			0.63	6.2000
Tr2			6.25	5.2040
Tr3			100	4.0000
Tr4			50	4.3010
Tr5			0.06	7.2218
Tr6			0.16	6.7958
Tr7			3.13	5.5040
Tr8			1.56	5.8060
Tr9			1.56	5.8060
Tr10			0.31	6.5086
Ts11*			12.5	4.9030
Ts12*			1.56	5.8060
Tr13			0.31	6.5080

Ts14*			0.63	6.2000
Tr15			25	4.6020
Tr16			25	4.6020
Tr17			100	4.0000
Ts18*			6.25	5.2041
Tr19*			12.5	4.9030
Tr20			1.56	5.8060
Tr21			12.5	4.9030
Tr22			10.0	5.0000
Tr23			100	4.0000
Tr24			25	4.6020
Tr25			12.5	4.9030
Tr26			25	4.6020
Tr27			6.25	5.2041
Tr28			6.25	5.2041
Tr29			3.13	5.5040
Ts30*			1.56	5.8068
Ts31*			12.5	4.9030

Tr32			6.25	5.2041
Ts33*			12.5	4.9030
Ts34*			1.56	5.8068
Tr35			0.31	6.5086
Tr36			0.31	6.5086
Tr37			0.16	6.7950
Tr38			0.31	6.5086
Tr39			0.16	6.7950
Tr40			0.63	6.2000
Tr41			1.56	5.8068
Ts42*			5.0	5.3010
Ts43*			6.25	5.2041
Tr44			0.31	6.5086
Ts45*			3.13	5.4800
Tr46			0.63	6.2000
Tr47			0.31	6.5086
Tr48			1.25	5.9030

Tr49*			6.25	5.2041
Tr50			0.63	6.2000
Tr51			3.13	5.4800
Tr52			1.56	5.8068
Tr53			12.5	4.9030
Ts54*			12.5	4.9030
Tr55			6.25	5.2041
Tr56			12.5	4.9030
Ts57*			1.25	5.9030
Ts58*			1.25	5.9030
Ts59*			1.25	5.9030
Tr60			7.9	5.1023
Ts61*			4.3	5.3660
Ts62*			7.4	5.1300
Ts63*			4.2	5.3767
Ts64*			14.1	4.8500
Ts65*			15.1	4.8210

Ts66*			2.0	5.6989
Ts67*			3.8	5.4202
Tr68			1.0	6
Tr69			3.7	5.4317
Ts70*			2.3	5.6382

* Test set molecules (Ts) Training set molecules (Tr)

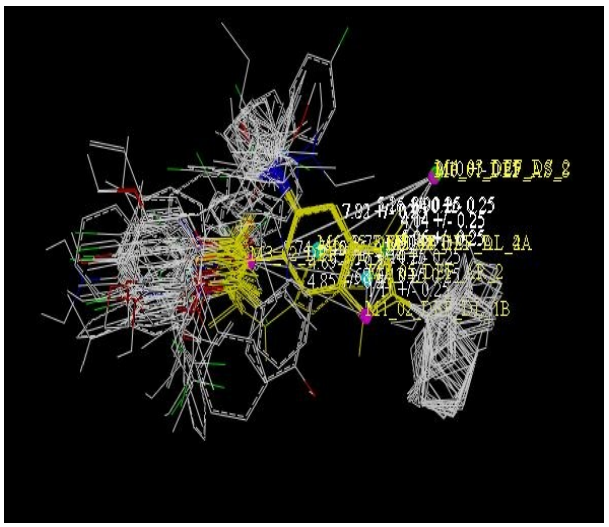


Fig.-S1. Pharmacophore based-alignment of training and test set compounds

Table-S2. Statistical data of PLS analysis

Statistical Parameters	CoMFA	CoMSIA
q^2	0.727	0.640
r^2_{ncv}	0.962	0.978
r^2_{cv}	0.721	0.620
r^2_{bs}	0.962	0.975
N	6	6
F_{test}	161	132
SEE	0.176	0.152
R^2_{Pred}	0.714	0.748
Field contribution		
Steric	0.525	0.290
Electrostatic	0.475	0.092
Hydrophobic	-	0.203
H-bond donor	-	0.265
H-bond acceptor	-	0.150

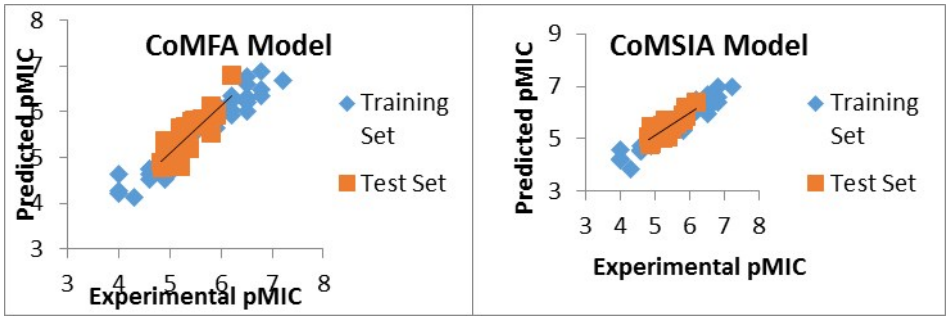
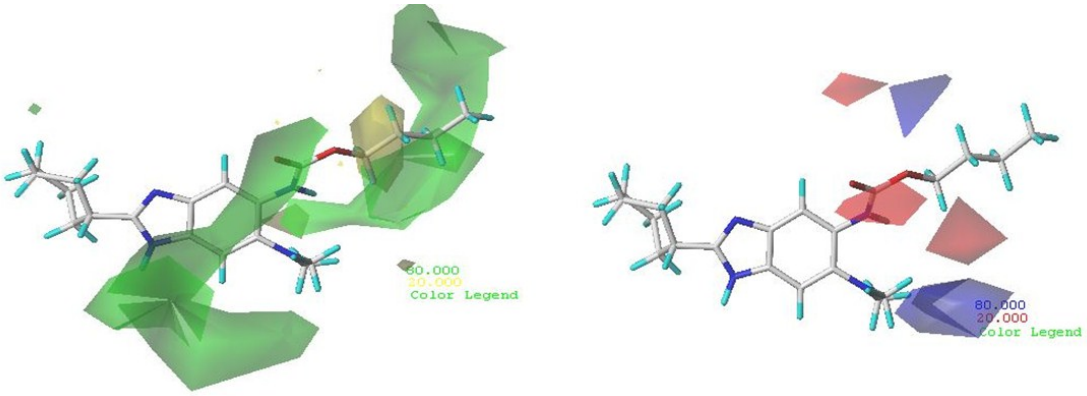


Fig.-S2. Plots of experimental pMIC and predicted pMIC using CoMFA and CoMSIA models



(A) **(B)**

Fig.-S3. CoMFA contour maps with compound **Tr5** inside the maps. (A) Steric fields- favourable (green 80% contribution) and unfavourable (yellow *20%* contribution). (B) Electrostatic fields- favourable (blue 80% contribution) and unfavourable (red *20%* contribution).

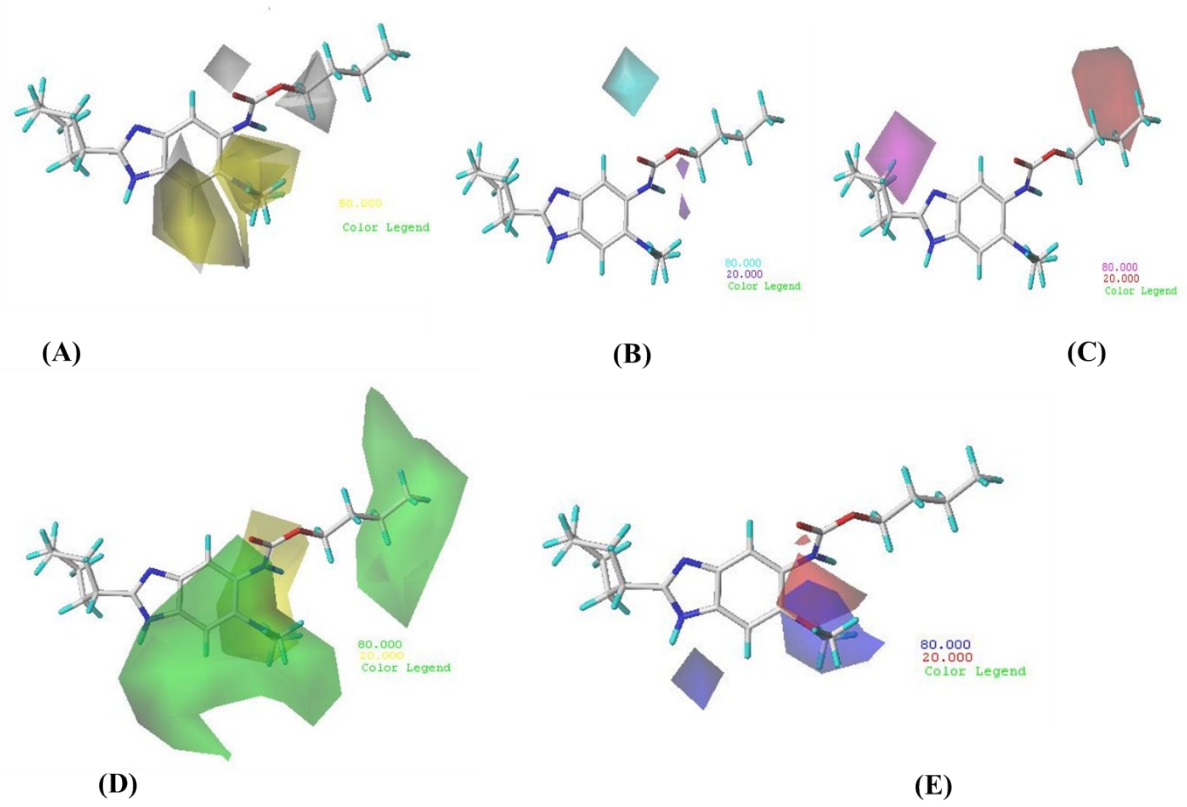
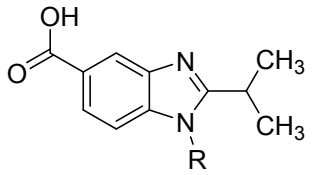
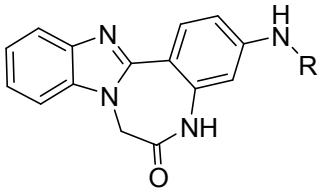


Fig.-S4. CoMSIA contour maps. Compound **Tr5** was overlaid in each map. Favourable and unfavourable field regions were 80% and 20%, respectively (A) Hydrophobic fields- favourable (*yellow*) and unfavourable (*grey*) (B) H-bond donor fields- favourable (*cyan*) and unfavourable (*purple*) fields. (C) H-bond acceptor fields- favourable (*magenta*) and unfavourable (*red*). (D) Steric fields- favourable (*green*) and unfavourable (*yellow*). (E) Electrostatic fields- favourable (*blue*) and unfavourable (*red*).

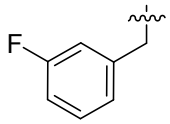
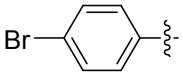
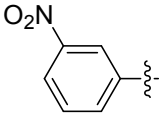
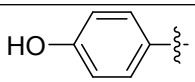
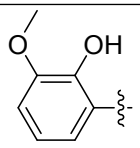
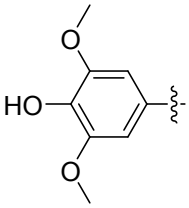
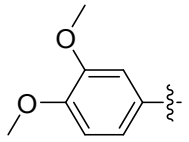
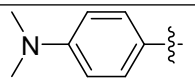
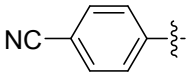
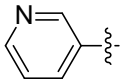
Table-S3. Predicted pMIC based on generated CoMFA and CoMSIA models along with designed molecules.

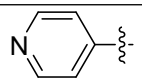
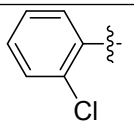
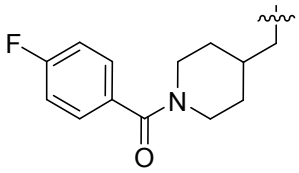
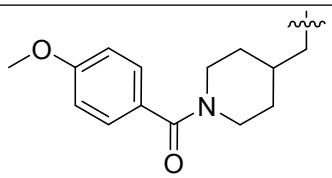
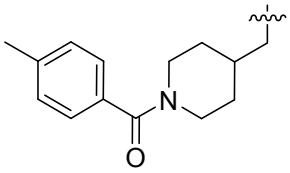
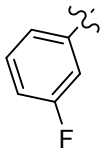
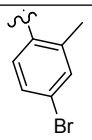
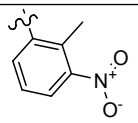
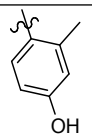
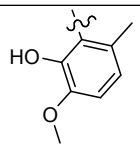
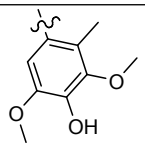


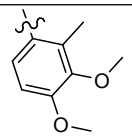
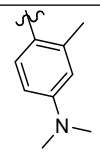
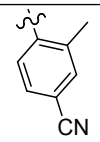
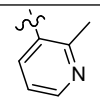
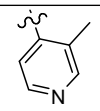
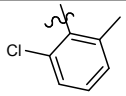
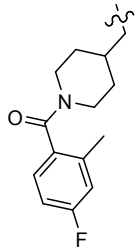
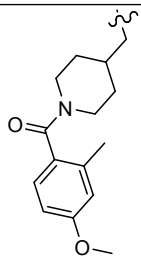
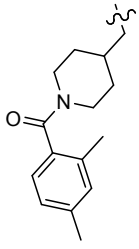
(D1 to D30)

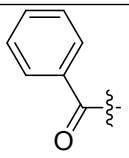
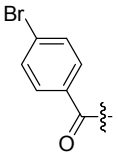
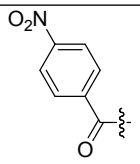
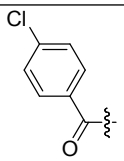
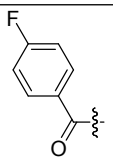
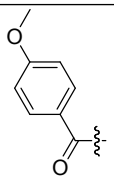
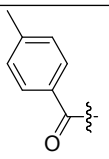
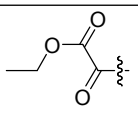
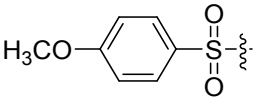


(D31 to D52)

Designed Compound number	R	CoMFA Predicted pMIC	CoMSIA Predicted pMIC	Synthesised compound number
D1		7.352	7.523	**7a**
D2		7.753	7.521	**7b**
D3		7.451	7.329	**7c**
D4		7.983	7.017	**7d**
D5		7.326	7.419	**7e**
D6		7.451	6.946	**7f**
D7		7.345	7.451	**7g**
D8		6.981	6.819	**7h**
D9		6.318	6.417	**7i**
D10		6.989	6.861	**7j**

D11		6.993	6.843	**7k**
D12		6.872	6.792	**7l**
D13		6.913	6.852	**7m**
D14		6.912	6.854	**7n**
D15		6.985	6.891	**7o**
D16		5.014	4.923	----------
D17		3.865	3.726	----------
D18		4.167	3.972	----------
D19		4.235	4.186	----------
D20		3.768	3.762	----------
D21		4.461	4.185	----------

D22		3.386	3.293	----------
D23		3.591	3.481	----------
D24		3.612	3.619	----------
D25		4.193	4.156	----------
D26		3.981	3.825	----------
D27		3.382	3.646	----------
D28		3.656	3.291	----------
D29		3.492	3.167	----------
D30		3.678	3.651	----------

D31		7.966	7.815	**16**
D32		7.405	7.304	**17a**
D33		7.502	7.618	**17b**
D34		7.210	7.834	**17c**
D35		6.321	6.983	**17d**
D36		5.947	6.017	**17e**
D37		7.046	6.993	**17f**
D38		7.263	7.184	**17g**
D39		7.776	7.861	**17h**
D40		7.439	7.327	**17i**

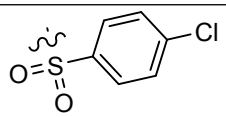
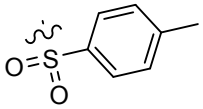
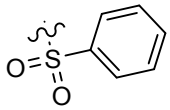
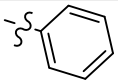
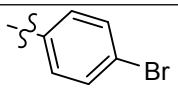
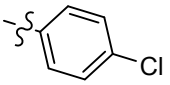
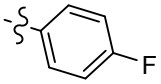
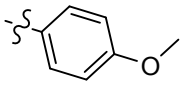
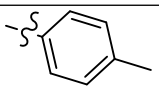
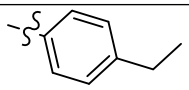
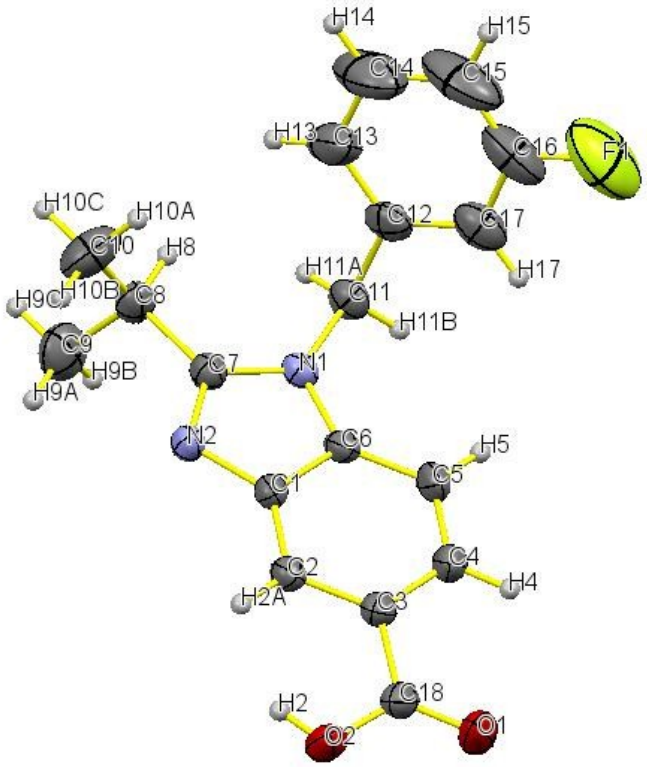
D41		4.892	4.521	----------
D42		4.321	4.322	----------
D43		4.181	4.224	----------
D44		3.932	3.712	----------
D45	$-CH_3$	3.165	3.217	----------
D46		3.182	3.271	----------
D47		3.561	3.213	----------
D48		3.256	3.167	----------
D49		3.651	3.514	----------
D50		3.134	3.092	----------
D51		3.571	3.431	----------
D52		3.276	3.241	----------

Fig.-S5. Determination of structure of compound **7a** by X-ray crystallographic studies.



Experimental details of crystal data of 7a

Empirical Formula	$C_{18}H_{17}FN_2O_2$
Formula Weight	312.34
Crystal Color, Habit	orange, block
Crystal Dimensions	0.700 X 0.590 X 0.330 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 10.0539(9) Å b = 10.653(1) Å c = 14.944(2) Å V = 1600.5(3) $Å^3$

Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.296 g/cm^3
F_{000}	656.00
m(MoKa)	0.932 cm^{-1}

Compounds characterization data of synthesised compounds 7a-o (series-1)

1-(3-Fluorobenzyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7a**)

Compound **7a** was synthesized as off-white amorphous solid in yield of 18%, mp – 205-207 ^oC; ESI-MS m/z: 313 (M+1); ^1H NMR (400 MHz, DMSO-d6) δ 1.26 (d, 6H, *J*=6.8Hz), 3.28 (m, 1H), 5.63 (s, 2H), 6.83 (d, 1H, *J*=8.0Hz), 6.95 (d, 1H, *J*=10.0Hz), 7.11 (td, 1H, J_{12}=1.6Hz, J_{13}=8.4Hz), 7.35 (q, 1H, *J*=8.0Hz), 7.55 (d, 1H, *J*=8.4Hz), 7.83 (d, 1H, *J*=8.4Hz), 8.23 (s, 1H), 12.81 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 22.0, 26.2, 45.9, 110.5, 113.6, 114.7, 120.8, 122.6, 123.8, 124.9, 131.3, 138.8, 140.3, 142.3, 161.5, 162.3, 168.4. HPLC: 98.86%. Single crystal XRD confirms structure.

1-(4-Bromophenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7b**)

Compound **7b** was synthesized as white amorphous solid in yield of 22%, mp – 210-211 ^oC; ESI-MS m/z: 359 (M+1) and 361 (M+3); ^1H NMR (400 MHz, DMSO-d6) δ 1.56 (d, 6H, *J*=6.8Hz), 4.64 (m, 1H), 7.62 (d, 2H, *J*=8.0Hz), 7.68 (d, 1H, *J*=8.4Hz), 7.76 (d, 2H, *J*=8.0Hz), 8.01 (d, 1H, *J*=8.4Hz), 8.33 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.9, 48.5, 110.9, 120.8, 123.2, 124.3, 130.0, 131.4, 131.6, 133.5, 134.3, 142.8, 152.2, 170.8. HPLC: 100%.

2-Isopropyl-1-(3-nitrophenyl)-1H-benzo[d]imidazole-5-carboxylic acid (**7c**)

Compound **7c** was synthesized as yellow amorphous solid in yield of 14%, mp – 195-198 ^oC; ESI-MS m/z: 326 (M+1); ^1H NMR (400 MHz, DMSO-d6) δ 1.64 (d, 6H, *J*=7.2Hz), 4.73 (m, 1H), 7.89 (m, 2H), 7.97 (d, 1H, *J*=8.8Hz), 8.16 (d, 1H, *J*=8.0Hz), 8.31 (s, 1H), 8.43 (dd, 1H, J_{12}=1.6Hz, J_{13}=8.0Hz), 8.51 (s, 1H), 12.89 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.8, 49.1, 112.8, 121.8, 123.7, 124.3, 124.6, 124.7, 130.4, 131.6, 135.7, 136.5, 142.8, 147.8, 152.6, 167.6. HPLC: 97.59%.

1-(4-Hydroxyphenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7d**)

Compound **7d** was synthesized as off-white amorphous solid in yield of 20%, mp – 212-214 ^{o}C; ESI-MS m/z: 297 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.59 (d, 6H, *J*=6.8Hz), 4.73 (m, 1H), 6.98 (d, 2H, *J*=8.4Hz), 7.52 (d, 2H, *J*=8.4Hz), 7.89 (s, 2H), 8.26 (s, 1H), 10.14 (bs, 1H), 12.79 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 48.6, 112.3, 115.4, 120.6, 120.8, 123.0, 124.1, 130.9, 136.4, 142.8, 155.2, 158.9, 167.8. HPLC: 100%.

1-(2-Hydroxy-3-methoxyphenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7e**)

Compound **7e** was synthesized as off-white amorphous solid in yield of 27%, mp – 210-211 ^{o}C; ESI-MS m/z: 327 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.53 (d, 6H, *J*=6.8Hz), 3.88 (s, 3H), 4.39 (m, 1H), 6.92 (m, 2H), 7.15 (d, 1H, *J*=7.2Hz), 7.88 (s, 2H), 8.26 (s, 1H), 9.88 (bs, 1H), 12.36 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.5, 48.9, 55.8, 112.0, 113.2, 117.8, 119.2, 120.9, 122.7, 123.0, 123.9, 136.0, 142.9, 145.1, 147.6, 153.0, 167.8. HPLC: 98.45%.

1-(3,5-Dimethoxyphenyl-4-hydroxy)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7f**)

Compound **7f** was synthesized as off-white amorphous solid in yield of 24%, mp – 218-220 ^{o}C; ESI-MS m/z: 357 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.62 (d, 6H, *J*=6.4Hz), 3.87 (s, 6H), 4.87 (m, 1H), 6.94 (s, 2H), 7.89 (s, 2H), 8.29 (s, 1H), 9.01 (bs, 1H), 12.81 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 48.7, 56.0, 106.9, 112.3, 119.7, 120.8, 123.0, 124.2, 136.5, 137.2, 142.8, 147.8, 155.4, 167.8. HPLC: 98.77%.

1-(3,4-Dimethoxyphenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7g**)

Compound **7g** was synthesized as off-white amorphous solid in yield of 27%, mp – 207-209 ^{o}C; ESI-MS m/z: 341 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.61 (d, 6H, *J*=6.8Hz), 3.86 (s, 3H), 3.87 (s, 3H), 4.79 (m, 1H), 7.14 (d, 1H, *J*=8.0Hz), 7.21 (m, 2H), 7.90 (s, 2H), 8.28 (s, 1H), 12.84 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 48.7, 55.5, 55.5, 111.5, 112.3, 112.7, 120.9, 121.9, 122.3, 123.1, 124.2, 136.5, 142.8, 148.6, 150.0, 154.9, 167.8. HPLC: 100%.

1-(4-(Dimethylamino)phenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7h**)

Compound **7h** was synthesized as off-white amorphous solid in yield of 22%, mp – 191-192 ^{o}C; ESI-MS m/z: 323 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.58 (d, 6H, *J*=6.8Hz), 3.00 (s, 6H), 4.78 (m, 1H), 6.84 (d, 2H, *J*=8.4Hz), 7.49 (d, 2H, *J*=8.8Hz), 7.86 (s, 2H), 8.25 (s, 1H),

12.76 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 29.3, 48.6, 111.1, 111.6, 112.1, 116.7, 120.5, 120.6, 122.7, 123.3, 123.9, 124.0, 130.2, 136.6, 143.0, 151.0, 155.7, 167.9. HPLC: 92.88%.

1-(4-Cyanophenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7i**)

Compound **7i** was synthesized as off-white amorphous solid in yield of 25%, mp – 198-200 ^{o}C; ESI-MS m/z: 306 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.62 (d, 6H, *J*=6.8Hz), 4.70 (m, 1H), 7.85 (m, 4H), 8.07 (d, 2H, *J*=7.6Hz), 8.31 (s, 1H), 12.86 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.8, 49.1, 112.5, 118.3, 121.4, 123.6, 124.6, 129.4, 129.9, 130.4, 132.6, 134.6, 136.5, 142.8, 153.1, 167.6. HPLC: 93.25%.

2-Isopropyl-1-(pyridin-3-yl)-1H-benzo[d]imidazole-5-carboxylic acid (**7j**)

Compound **7j** was synthesized as off-white amorphous solid in yield of 21%, mp – 208-211 ^{o}C; ESI-MS m/z: 282 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.60 (d, 6H, *J*=6.8Hz), 4.65 (m, 1H), 7.61 (m, 1H), 7.85 (q, 2H, *J*=8.8Hz), 8.11 (m, 1H), 8.25 (s, 1H), 8.77 (dd, 1H, J_{12}=1.6Hz, J_{13}=8.8Hz), 8.88 (d, 1H, *J*=1.6Hz); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 49.0, 112.0, 121.1, 123.6, 126.6, 128.0, 135.6, 137.0, 142.9, 148.0, 149.6, 150.6, 151.6, 169.0. HPLC: 95.80%.

2-Isopropyl-1-(pyridin-4-yl)-1H-benzo[d]imidazole-5-carboxylic acid (**7k**)

Compound **7k** was synthesized as off-white amorphous solid in yield of 17%, mp – 207-209 ^{o}C; ESI-MS m/z: 282 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.59 (d, 6H, *J*=6.8Hz), 4.72 (m, 1H), 7.13 (d, 2H, *J*=8.4Hz), 7.62 (d, 2H, *J*=8.4Hz), 7.90 (s, 2H), 8.28 (s, 1H), 12.86 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 48.7, 112.3, 114.1, 120.9, 122.3, 123.1, 124.2, 130.8, 136.4, 142.9, 154.8, 160.4, 167.8. HPLC: 100%.

1-(2-Chlorophenyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7l**)

Compound **7l** was synthesized as off-white amorphous solid in yield of 29%, mp – 212-213 ^{o}C; ESI-MS m/z: 315 (M+1) and 317 (M+3); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.47 (d, 6H, *J*=6.8Hz), 4.25 (m, 1H), 7.55 (m, 1H), 7.64 (m, 2H), 7.71 (d, 1H, *J*=8.0Hz), 7.95 (s, 2H), 8.32 (s, 1H), 12.87 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.7, 49.0, 112.3, 121.3, 123.5, 124.4, 127.4, 129.5, 129.9, 132.0, 133.1, 135.7, 142.8, 151.8, 167.7. HPLC: 100%.

1-((1-(4-Fluorobenzoyl)piperidin-4-yl)methyl)-2-isopropyl-1H-benzo[d]imidazole-5-carboxylic acid (**7m**)

Compound **7m** was synthesized as off-white amorphous solid in yield of 19%, mp – 178-181 ^{o}C; ESI-MS m/z: 424 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.22 (m, 1H), 1.34 (d, 6H, *J*=6.4Hz), 1.35 (m, 1H), 1.50 (m, 2H), 2.12 (m, 1H), 2.67 (m, 1H), 2.99 (m, 1H), 3.31 (m, 1H), 3.57 (m, 1H), 4.19 (d, 2H, *J*=7.2Hz), 4.48 (m, 1H), 7.27 (m, 2H), 7.44 (m, 2H), 7.68 (d, 1H, *J*=8.4Hz), 7.84 (d, 1H, *J*=8.4Hz), 8.18 (s, 1H), 12.76 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 13.9, 21.8, 25.5, 28.8, 29.4, 36.6, 41.3, 46.9, 47.7, 110.3, 115.4, 120.1, 122.9, 123.9, 127.3, 127.3, 129.1, 132.0, 132.6, 138.4, 141.7, 161.1, 162.0, 163.6, 166.3, 167.9. HPLC: 99.14%.

2-Isopropyl-1-((1-(4-methoxybenzoyl)piperidin-4-yl)methyl)-1H-benzo[d]imidazole-5-carboxylic acid (**7n**)

Compound **7n** was synthesized as off-white amorphous solid in yield of 15%, mp – 183-184 ^{o}C; ESI-MS m/z: 436 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.33 (d, 6H, *J*=6.8Hz), 1.35 (m, 2H), 1.48 (m, 2H), 2.10 (m, 1H), 2.69 (m, 1H), 2.92 (m, 1H), 3.31 (m, 1H), 3.80 (s, 3H), 3.85 (m, 1H), 4.18 (d, 2H, *J*=6.8Hz), 4.45 (m, 1H), 6.98 (d, 2H, *J*=8.4Hz), 7.34 (d, 2H, *J*=8.4Hz), 7.68 (d, 1H, *J*=8.4Hz), 7.84 (d, 1H, *J*=8.0Hz), 8.18 (s, 1H), 12.75 (bs, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 21.8, 25.5, 29.2, 36.7, 47.8, 55.1, 64.8, 110.3, 113.5, 120.1, 122.9, 123.9, 128.1, 128.7, 131.3, 138.4, 141.7, 160.0, 162.0, 167.9, 168.8. HPLC: 96.49%.

2-Isopropyl-1-((1-(4-methylbenzoyl)piperidin-4-yl)methyl)-1H-benzo[d]imidazole-5-carboxylic acid (**7o**)

Compound **7o** was synthesized as off-white amorphous solid in yield of 18%, mp – 177-178 ^{o}C; ESI-MS m/z: 420 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.34 (d, 8H, *J*=6.0Hz), 1.49 (m, 2H), 2.11 (m, 1H), 2.33 (s, 3H), 2.64 (m, 1H), 2.96 (m, 1H), 3.28 (m, 2H), 4.19 (d, 2H, *J*=6.8Hz), 4.49 (m, 1H), 7.23 (q, 4H, *J*=8.0Hz), 7.68 (d, 1H, *J*=8.4Hz), 7.85 (d, 1H, *J*=8.0Hz), 8.19 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 20.8, 21.0, 22.0, 25.5, 28.9, 29.5, 36.6, 41.2, 46.8, 47.7, 60.1, 69.7, 72.3, 110.3, 120.1, 122.9, 124.0, 126.7, 128.8, 133.3, 138.3, 138.9, 141.7, 162.0, 168.0, 168.9. HPLC: 98.70%.

Compounds characterization data of synthesised compounds 16, 17a-i (series-2)

*3-Amino-5H-benzimidazo[1,2-D][1,4]benzodiazepin-6(7H)-one (**16**)*

Compound **16** was synthesized as yellow amorphous solid in yield of 25%, mp – 163-165^{o}C; ESI-MS m/z: 265 (M+1); ^{1}H-NMR (400 MHz, DMSO-d6) δ 4.82 (s, 2H), 5.89 (s, 2H), 6.38 (d, 1H, *J*=1.6Hz), 6.53 (dd, 1H, J_{12}=2Hz, J_{13}=8.8Hz), 7.20 (m, 2H), 7.62 (m, 1H), 7.71 (m, 2H), 10.39 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.7, 104.7, 107.9, 109.5, 111.1, 118.4, 121.6, 122.0, 131.2, 134.4, 137.5, 143.0, 151.7, 151.8, 167.6. HPLC: 98.06%

*N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide (**17a**)*

Compound **17a** was synthesized as off-white amorphous solid in yield of 38%, mp – 185-187 ^{o}C; ESI-MS m/z: 369 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 4.87 (s, 2H), 7.30 (d, 2H, *J*=7.2Hz), 7.37 (s, 4H), 7.58 (m, 2H), 8.02 (m, 3H), 8.27 (m, 1H), 10.36 (s, 1H), 10.70 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.9, 101.5, 109.7, 116.5, 119.1, 120.7, 122.0, 124.6, 127.6, 128.3, 129.9, 131.2, 134.4, 135.1, 136.1, 139.9, 143.1, 150.9, 165.4, 167.9. HPLC: 99.69 %

*4-Bromo-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide **(17b)***

Compound **17b** was synthesized as off-white amorphous solid in yield of 29%, mp – 189-193 ^{o}C; ESI-MS m/z: 447 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 4.87 (s, 2H), 7.30 (d, 2H, *J*=7.2Hz), 7.37 (m, 5H), 7.58 (m, 2H), 7.98 (s, 2H), 8.11 (s, 1H), 8.26 (m, 1H), 10.42 (s, 1H), 10.70 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.9, 101.6, 109.8, 110.9, 116.9, 119.1, 120.7, 122.0, 124.6, 125.3, 129.3, 129.9, 131.2, 134.4, 136.1, 140.0, 143.1, 150.6, 151.0, 164.4, 167.8. HPLC: 100 %

*4-Nitro-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide **(17c)***

Compound **17c** was synthesized as yellow amorphous solid in yield of 39%, mp – 181-184 ^{o}C; ESI-MS m/z: 414 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 4.88 (s, 2H), 7.30 (d, 1H, *J*=7.2Hz), 7.36 (d, 1H, *J*=7.6Hz), 7.57 (m, 2H), 7.70 (m, 2H), 8.09 (m, 1H), 8.23 (m, 3H), 8.38 (m, 3H), 10.66 (s, 1H), 10.71 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.9, 101.7, 109.9, 110.9, 116.8, 119.2, 120.6, 122.0, 123.5, 124.6, 129.1, 129.9, 130.1, 131.2, 131.7, 133.9, 134.4, 136.1, 140.2, 143.1, 149.0, 150.7, 151.1, 163.6, 167.8. HPLC: 97.898 %

4-Chloro-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide ***(17d)***

Compound **17d** was synthesized as off-white amorphous solid in yield of 30%, mp – 188-191 ^{o}C; ESI-MS m/z: 403 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 4.88 (s, 2H), 7.32 (m, 2H), 7.37 (s, 3H), 8.05 (m, 4H), 8.26 (m, 2H), 10.43 (s, 1H), 10.71 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.9, 101.6, 109.8, 110.8, 116.9, 119.1, 120.7, 122.0, 124.6, 128.4, 129.5, 130.1, 131.2, 133.5, 134.1, 136.1, 136.3, 140.0, 143.1, 150.6, 151.0, 164.2, 167.9. HPLC: 100 %

4-Fluoro-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide ***(17e)***

Compound **17e** was synthesized as off-white amorphous solid in yield of 34%, mp – 184-186 ^{o}C; ESI-MS m/z: 387 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 4.98 (s, 2H), 7.31 (s, 2H), 7.40 (t, 2H, *J*=8.4Hz), 7.57 (d, 2H, *J*=6.8Hz), 7.83 (d, 1H, *J*=7.2Hz), 7.95 (s, 1H), 8.09 (d, 3H, *J*=8.0Hz), 10.68 (s, 1H), 10.79 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.8, 109.9, 112.6, 115.2, 116.1, 116.6, 119.0, 122.3, 130.5, 132.1, 134.6, 136.7, 141.7, 143.1, 150.4, 162.9, 164.8, 165.4, 166.3, 167.8. HPLC: 95.7 %

4-Methoxy-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide ***(17f)***

Compound **17f** was synthesized as off-white amorphous solid in yield of 28%, mp – 191-193 ^{o}C; ESI-MS m/z: 399 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 3.83 (s, 3H), 4.96 (s, 2H), 7.09 (s, 2H), 7.11 (s, 2H), 7.29 (t, 1H, *J*=5.6Hz), 7.72 (d, 1H, *J*=7.6Hz), 7.82 (d, 1H, *J*=7.2Hz), 7.93 (s, 1H), 8.00 (m, 1H), 10.48 (s, 1H), 10.73 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 46.8, 55.4, 110.0, 112.5, 113.6, 115.6, 116.5, 118.8, 122.4, 126.5, 129.8, 130.4, 134.5, 136.7, 142.0, 142.9, 150.5, 162.1, 165.2, 167.8. HPLC: 95.8 %

4-Methyl-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzamide ***(17g)***

Compound **17g** was synthesized as off-white amorphous solid in yield of 26%, mp – 176-178 ^{o}C; ESI-MS m/z: 383 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 3.36 (s, 3H), 4.95 (s, 2H), 7.28 (d, 2H, *J*=5.6Hz), 7.31 (m, 2H), 7.72 (m, 2H), 7.82 (d, 1H, *J*=7.2Hz), 7.90 (d, 1H, *J*=8.0Hz), 8.05 (d, 1H, *J*=8.4Hz), 10.55 (s, 1H), 10.72 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 21.0, 46.8, 109.9, 112.6, 115.9, 116.6, 119.0, 122.3, 127.8, 128.9, 130.4, 131.6, 134.6, 136.7, 141.8, 141.9, 143.2, 150.5, 165.7, 167.8. HPLC: 98.33 %

Ethyl-2-oxo-2-((6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)amino)acetate ***(17h)***

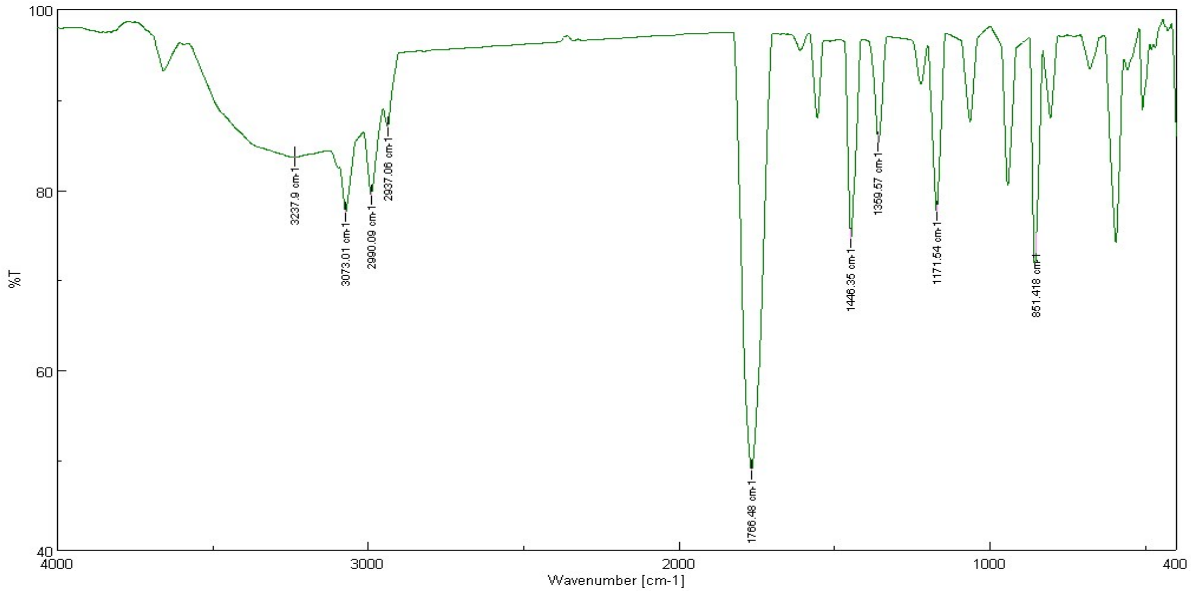
Compound **17h** was synthesized as off-white amorphous solid in yield of 33%, mp – 175-177 ^{o}C; ESI-MS m/z: 364 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 1.34 (s, 3H), 4.34 (s, 2H), 4.97 (s, 2H), 7.31 (m, 2H), 7.59 (m, 3H), 8.10 (m, 2H), 10.71 (s, 1H), 10.97 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 13.8, 46.8, 62.3, 101.8, 110.0, 116.6, 116.7, 119.3, 120.5, 122.0, 124.6, 129.9, 130.1, 131.3, 132.0, 132.8, 134.3, 136.1, 140.5, 142.9, 151.0, 151.3, 155.3, 160.7, 167.9. HPLC: 100 %

4-Methoxy-N-(6-oxo-6,7-dihydro-5H-benzimidazo[1,2-d][1,4]benzodiazepin-3-yl)benzenesulfonamide ***(17i)***

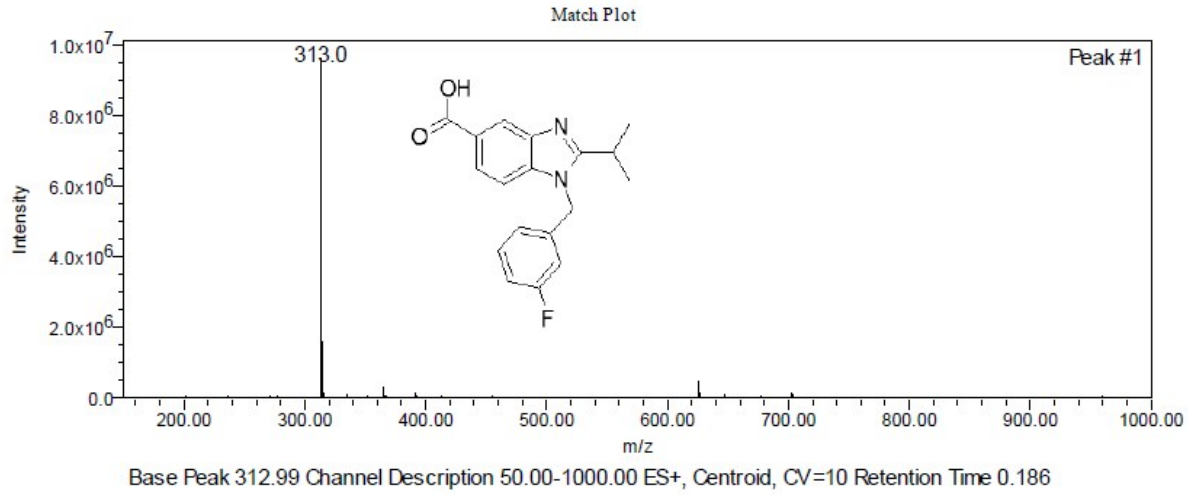
Compound **17i** was synthesized as yellow amorphous solid in yield of 31%, mp – 203-204 ^{o}C; ESI-MS m/z: 435 (M+1); ^{1}H NMR (400 MHz, DMSO-d6) δ 2.34 (s, 3H), 4.92 (s, 2H), 7.06 (dd, 1H, J_{12}=2.0Hz, J_{13}= 8.8Hz), 7.10 (s, 1H), 7.14 (m, 2H), 7.32 (m, 2H), 7.79 (m, 2H), 7.90 (d, 1H, J=8.8Hz), 10.72 (s, 1H), 10.84 (s, 1H). HPLC: 94.5 %

Spectral Data for Series 1

FTIR spectra of 7a



MASS Analysis of synthesized compound: 7a M+1: 313



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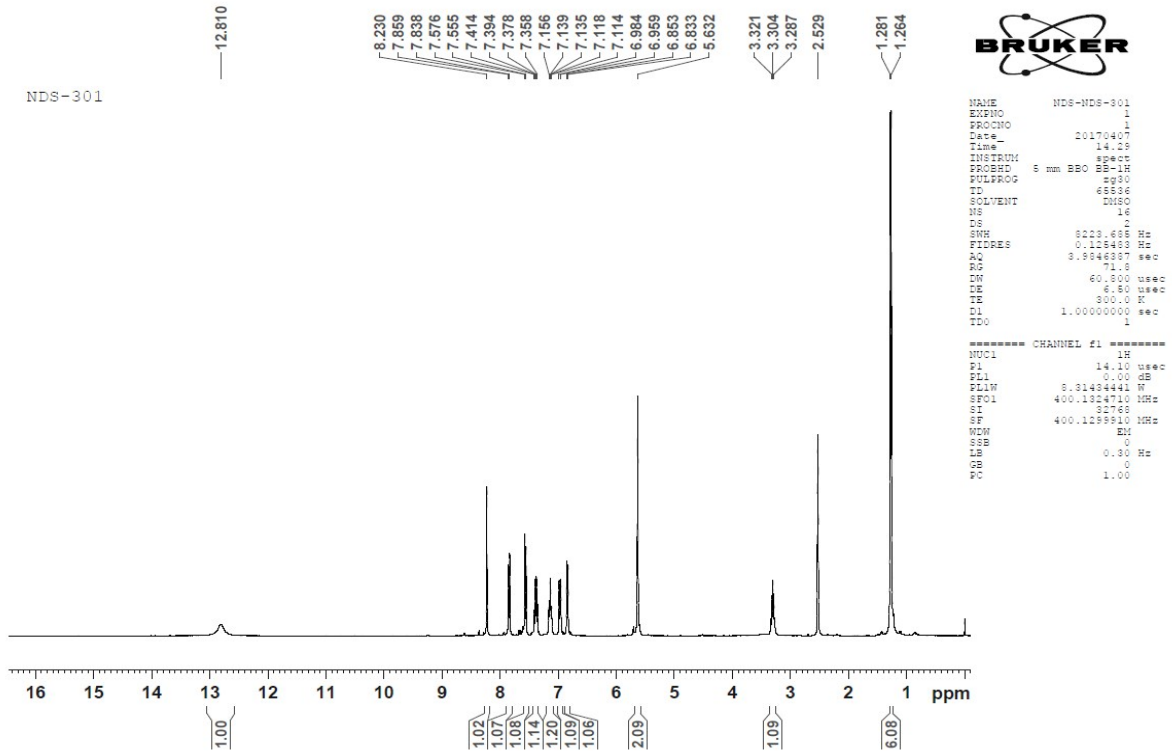
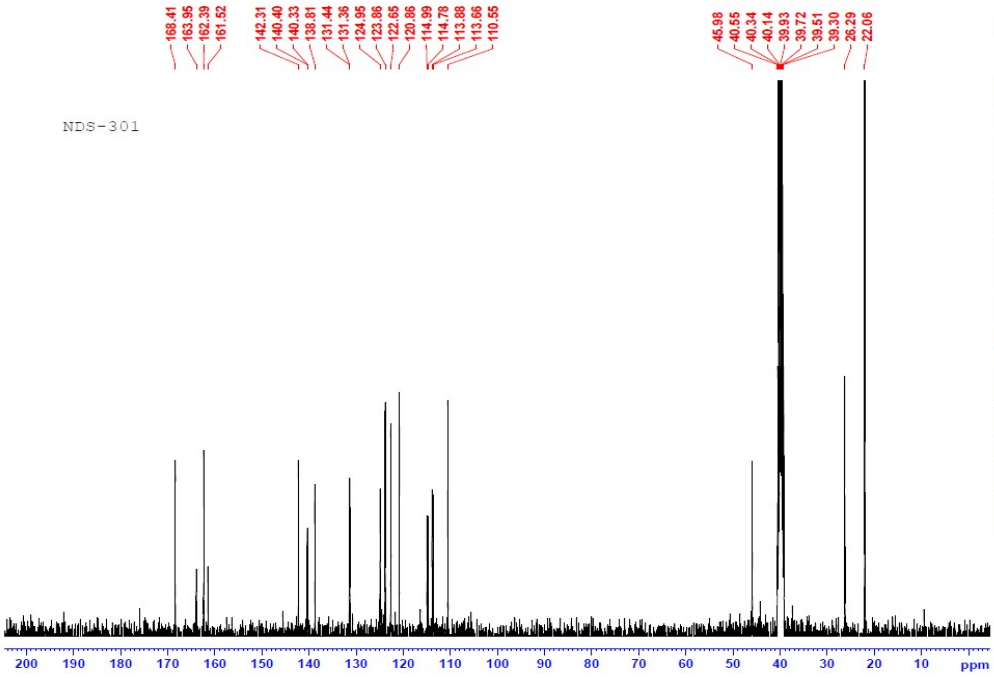
1H-NMR Analysis of synthesized compound: 7a



13C-NMR Analysis of synthesized compound: 7a

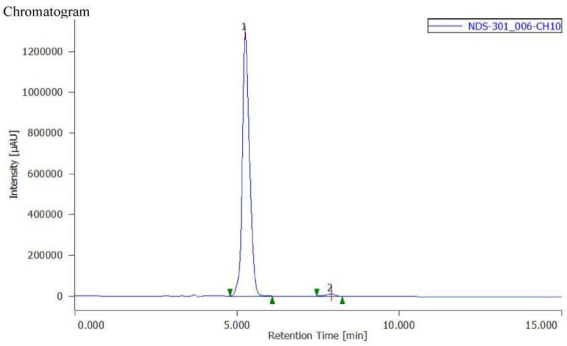


HPLC (percentage purity) of 7a

Benzimidazolederivatives_0914 NDS-301_006 9/16/2017 7:32:49 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



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Peak ID Table	

Peak Information

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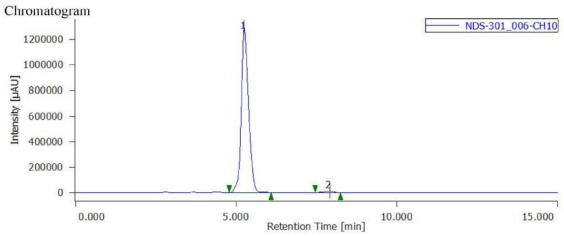
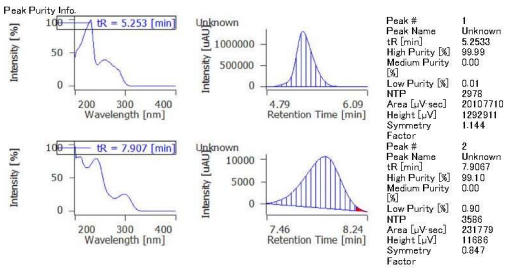
HPLC (peak purity) of 7a

Benzimidazolederivatives_0914 NDS-301_006 9/22/2017 10:53:15 AM

Institute of Pharmacy, Nirma University

Report - HPLC peak purity





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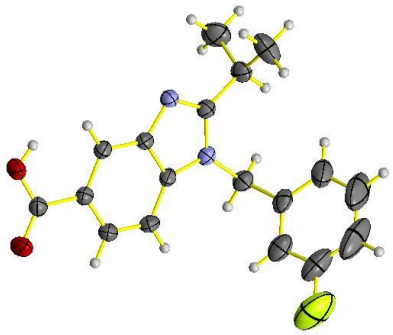
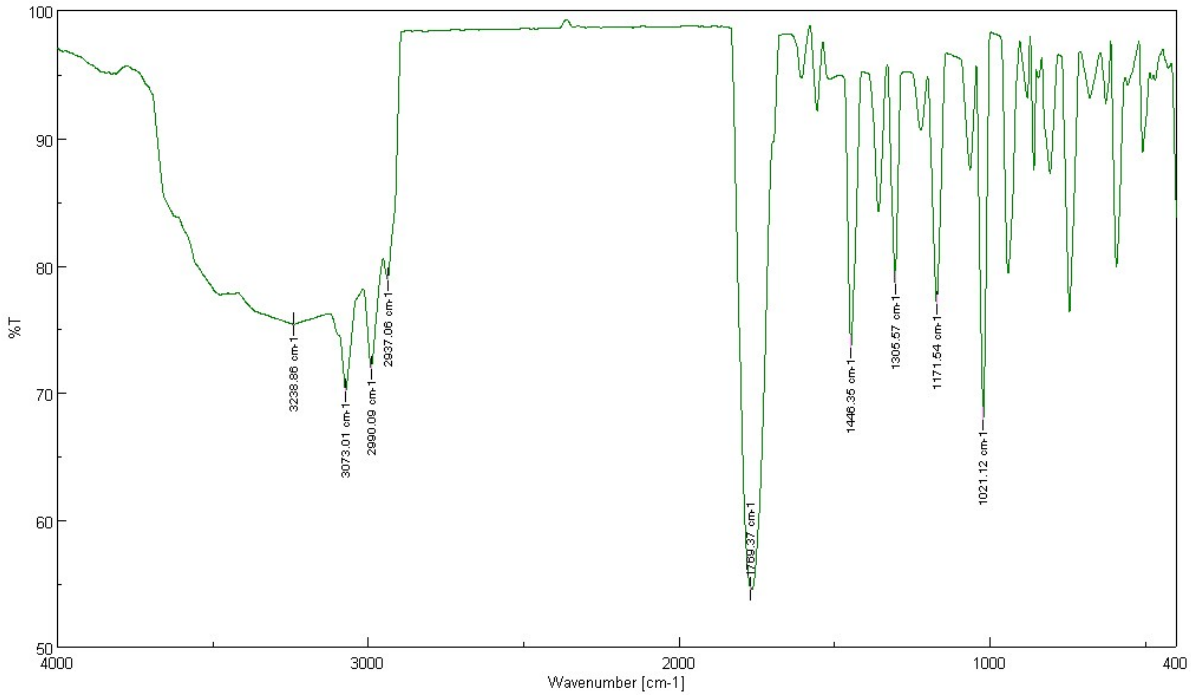
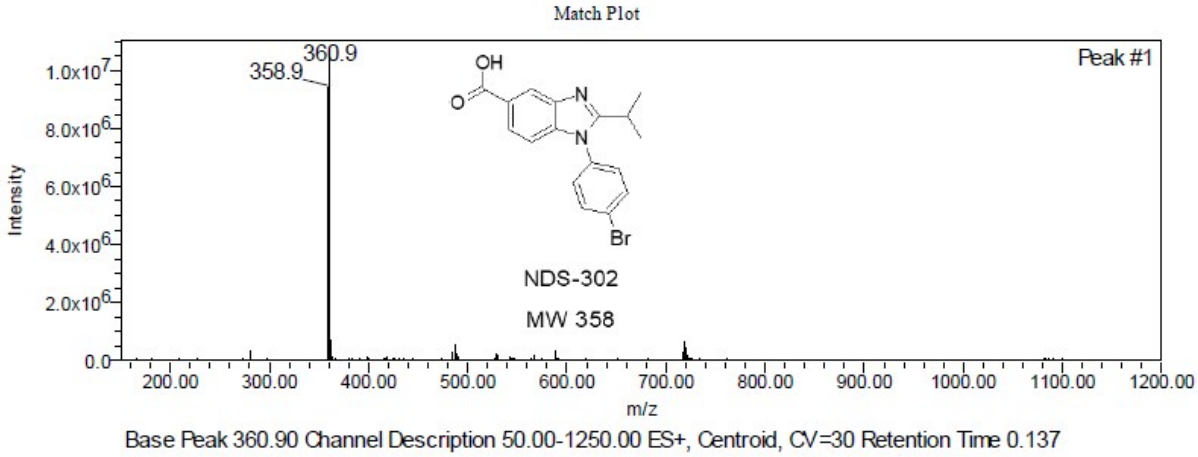


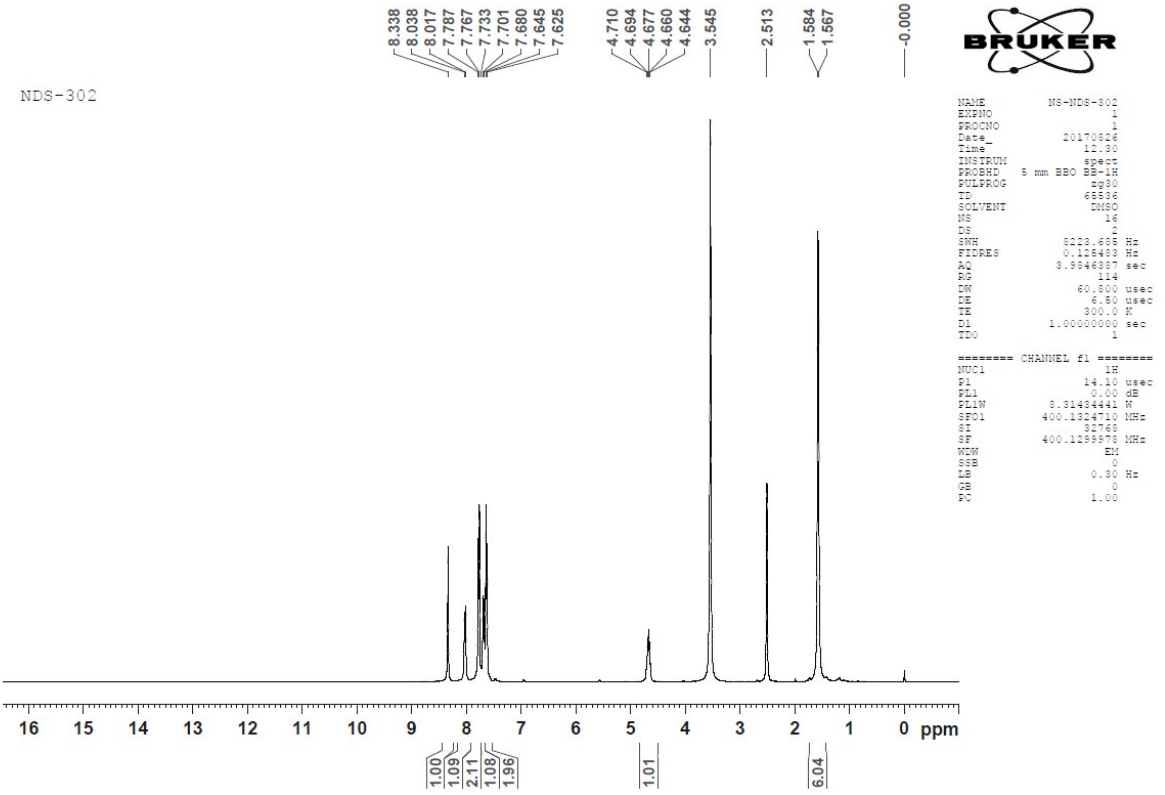
FTIR spectra of 7b



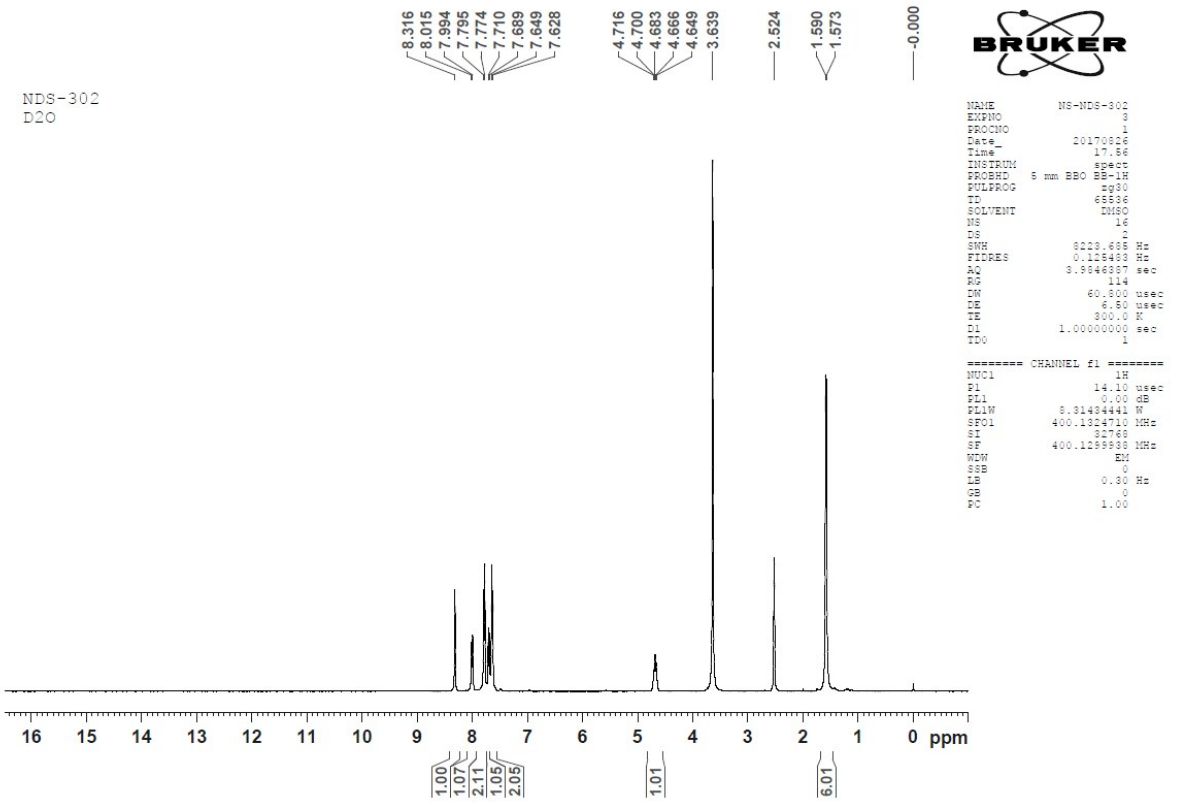
MASS Analysis of synthesized compound: 7b M+1: 359 and M+3: 361



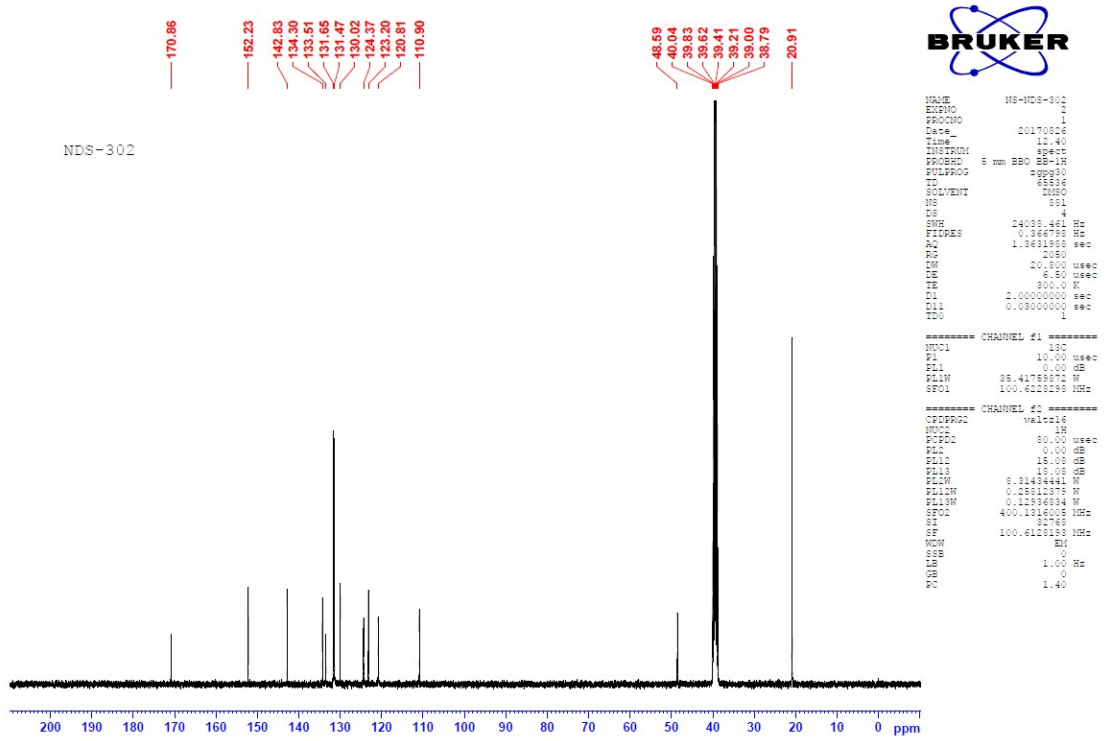
1H-NMR Analysis of synthesized compound: 7b



1H-NMR-D2O exchange analysis of synthesized compound: 7b



13C-NMR Analysis of synthesized compound: 7b

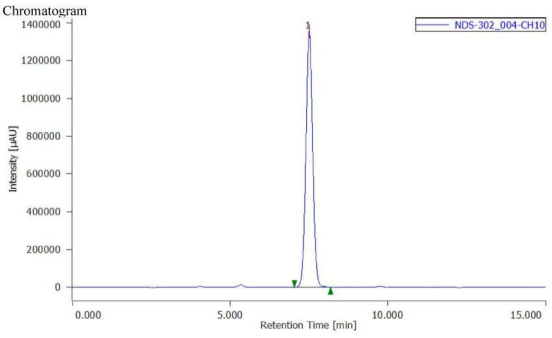


HPLC (percentage purity) of 7b

Benzimidazolederivatives_0914 NDS-302_004 9/16/2017 7:32:12 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



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Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

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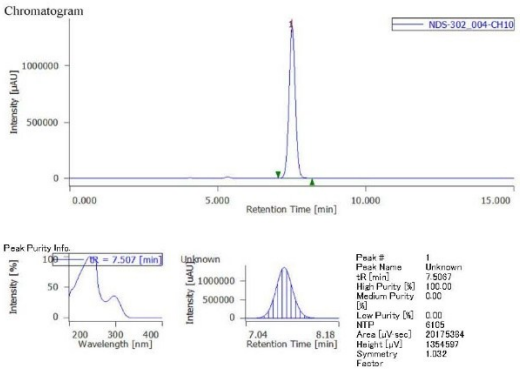
HPLC (peak purity) of 7b

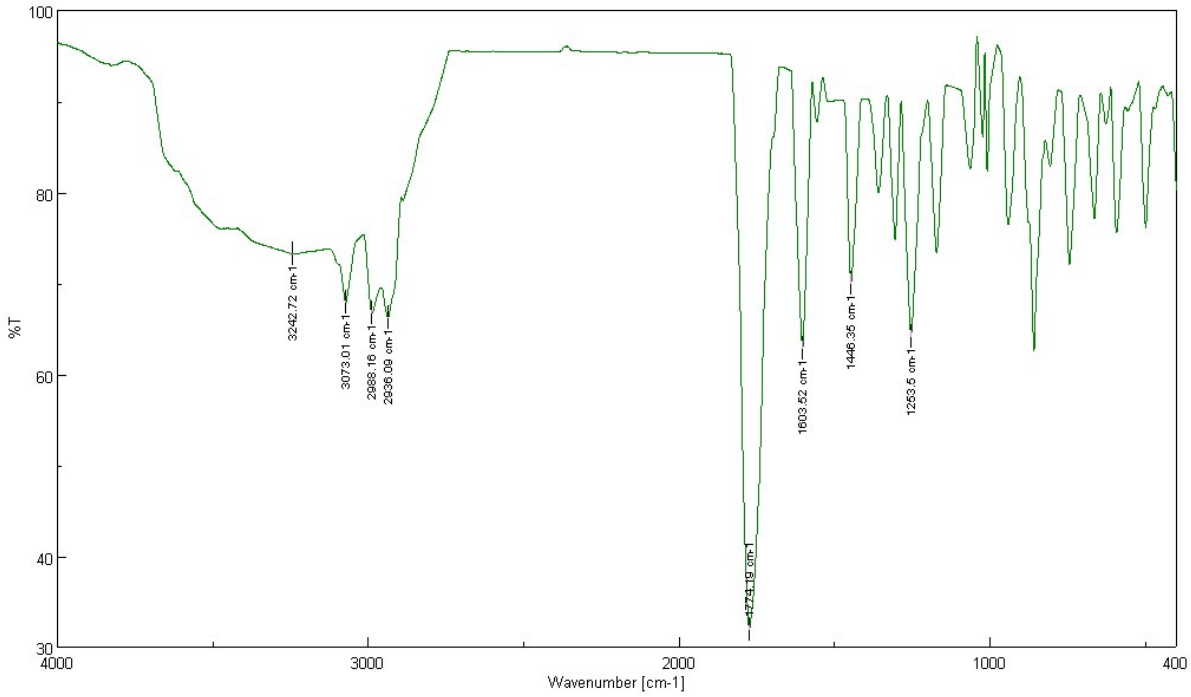
Benzimidazolederivatives_0914 NDS-302_004 9/22/2017 10:52:37 AM

Institute of Pharmacy, Nirma University

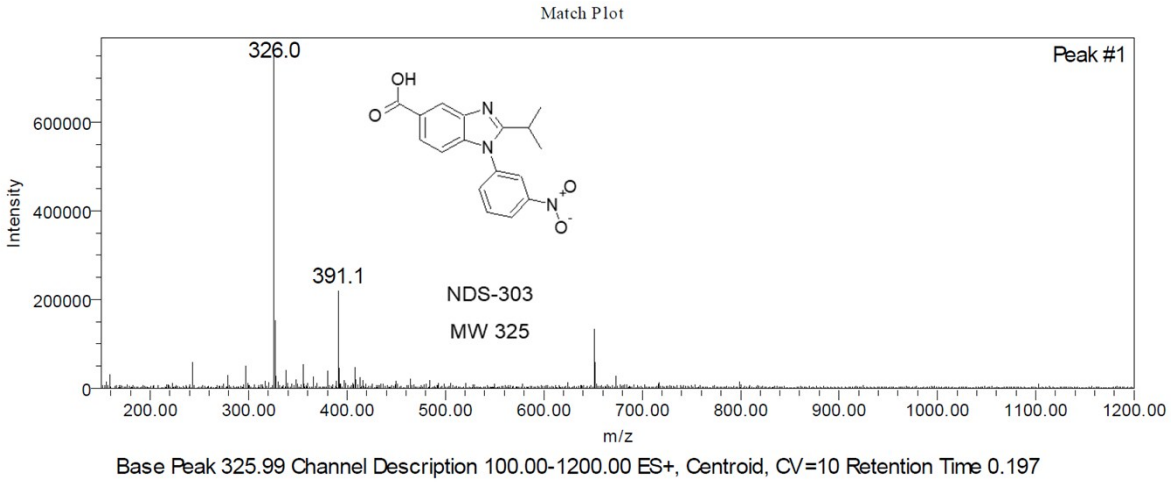
Report - HPLC peak purity



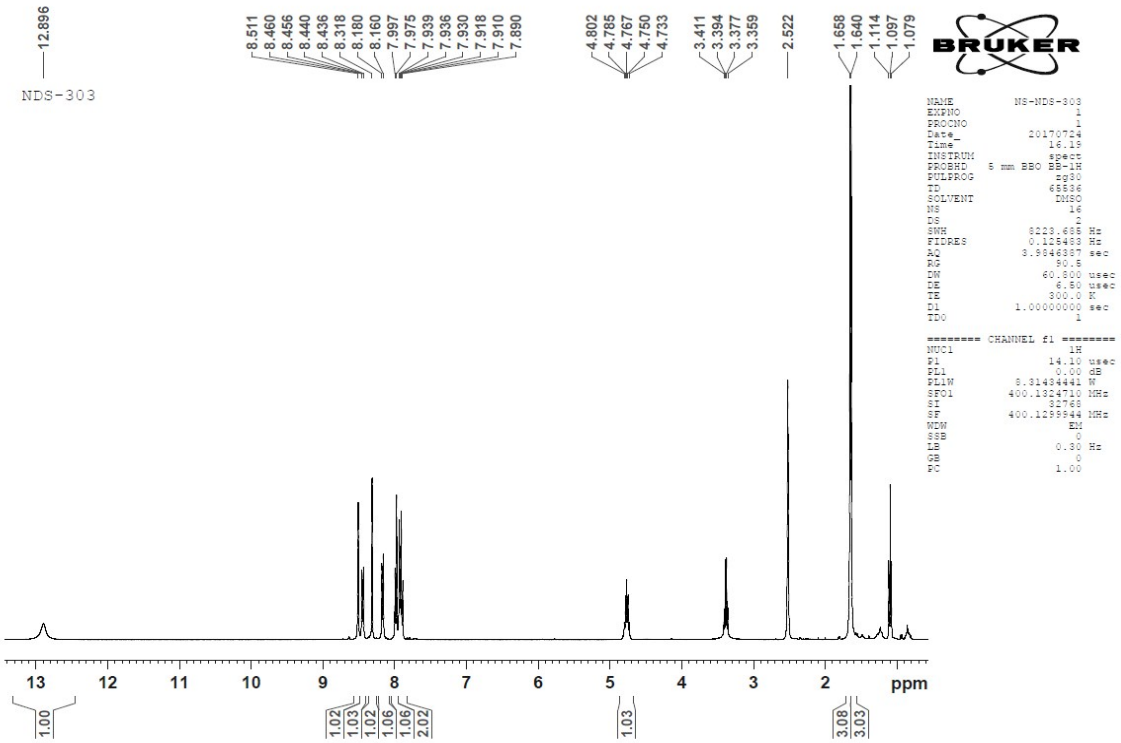
FTIR spectra of 7c



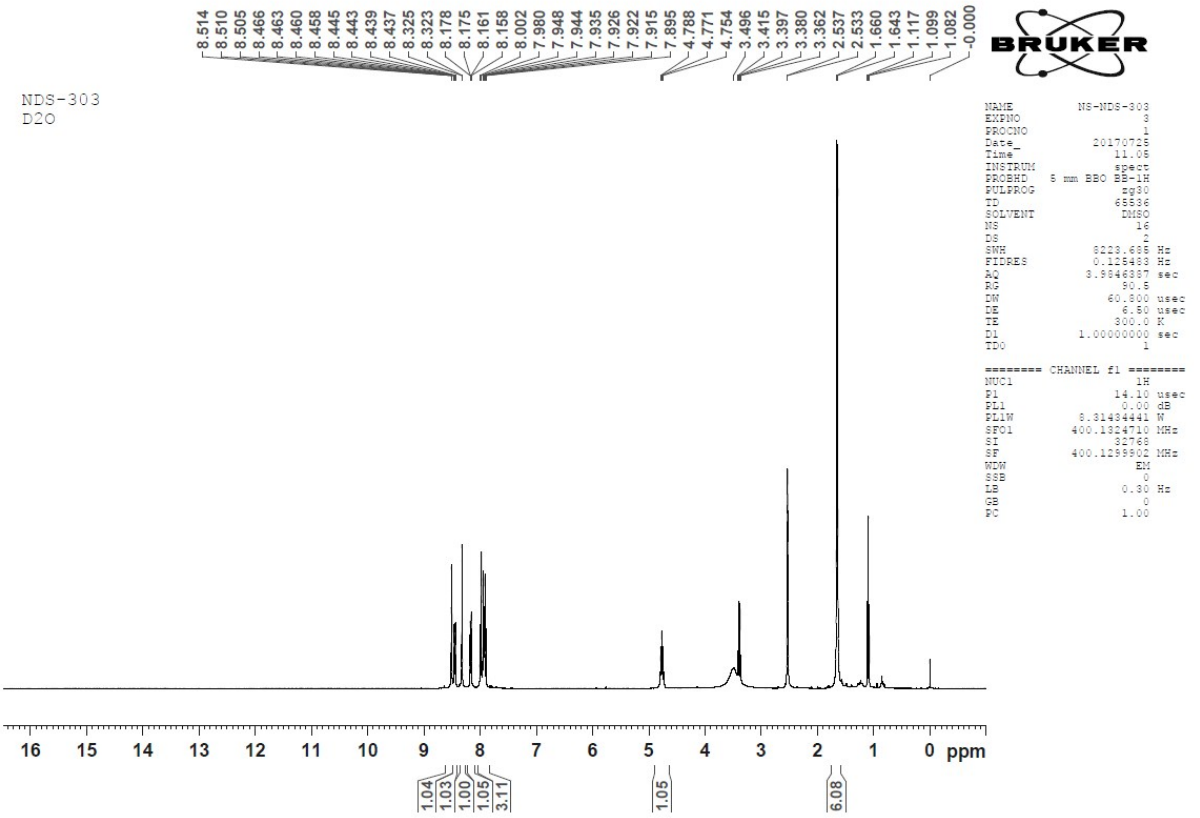
MASS Analysis of synthesized compound: 7c M+1: 326



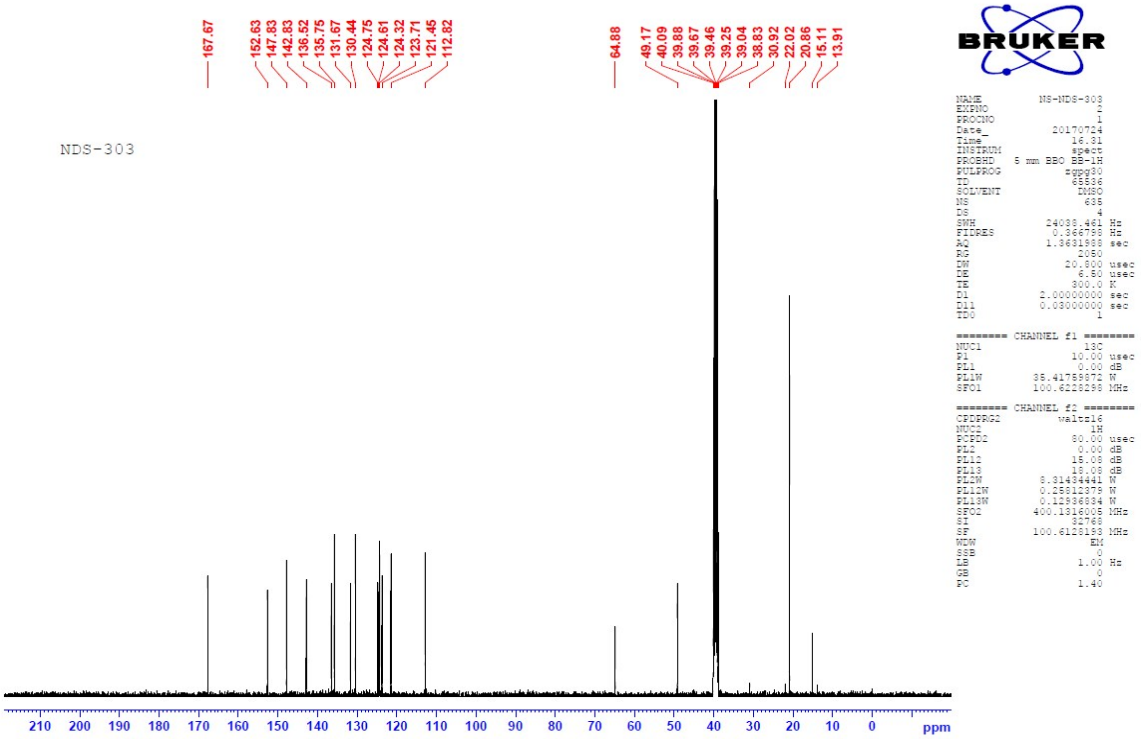
1H-NMR Analysis of synthesized compound: 7c



1H-NMR-D2O exchange analysis of synthesized compound: 7c



13C-NMR Analysis of synthesized compound: 7c

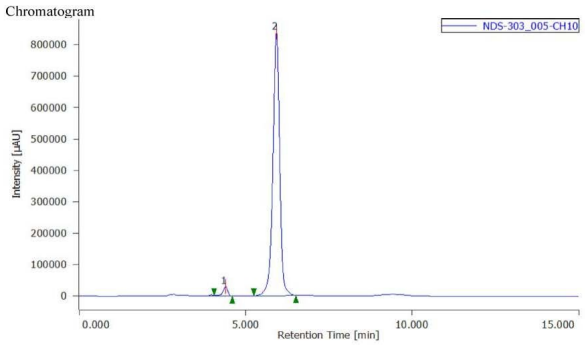


HPLC (percentage purity) of 7c

Benzimidazolederivatives_0914 NDS-303_005 9/16/2017 7:32:33 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



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Peak ID Table	test

Peak Information

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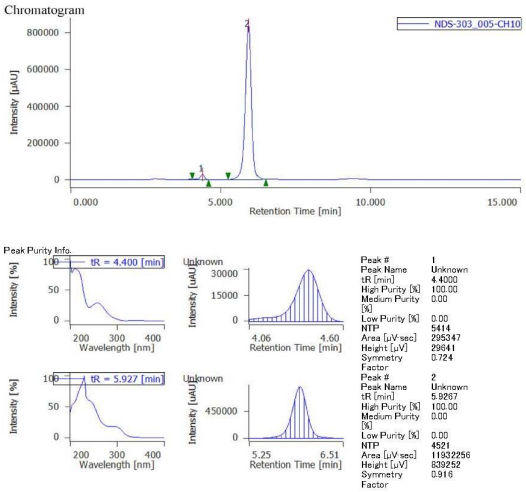
2	Unknown	10	5.927	11932256	839252	97.585	96.589	4521	N/A	0.916

HPLC (peak purity) of 7c

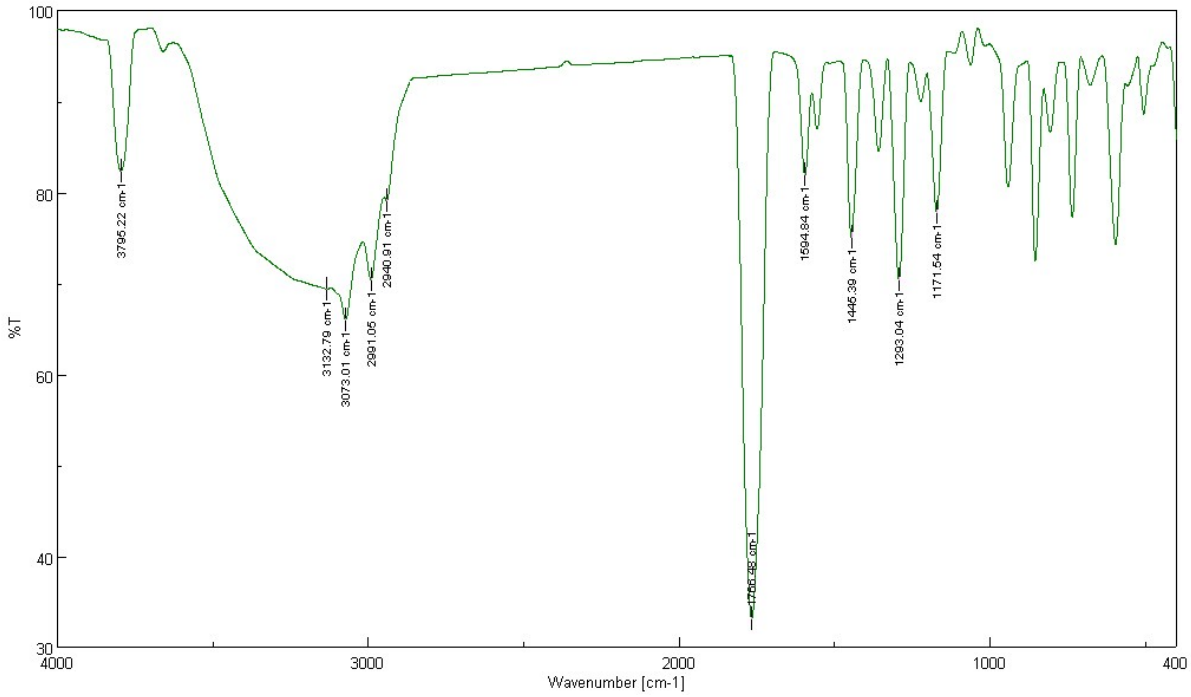
Benzimidazolederivatives_0914 NDS-303_005 9/22/2017 10:52:55 AM

Institute of Pharmacy, Nirma University

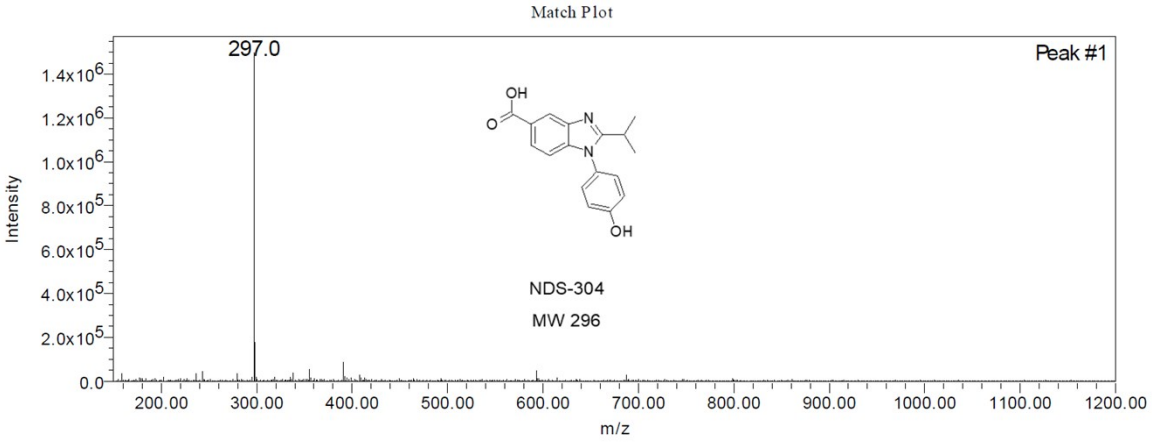
Report - HPLC peak purity



FTIR spectra of 7d



MASS Analysis of synthesized compound: 7d M+1: 297



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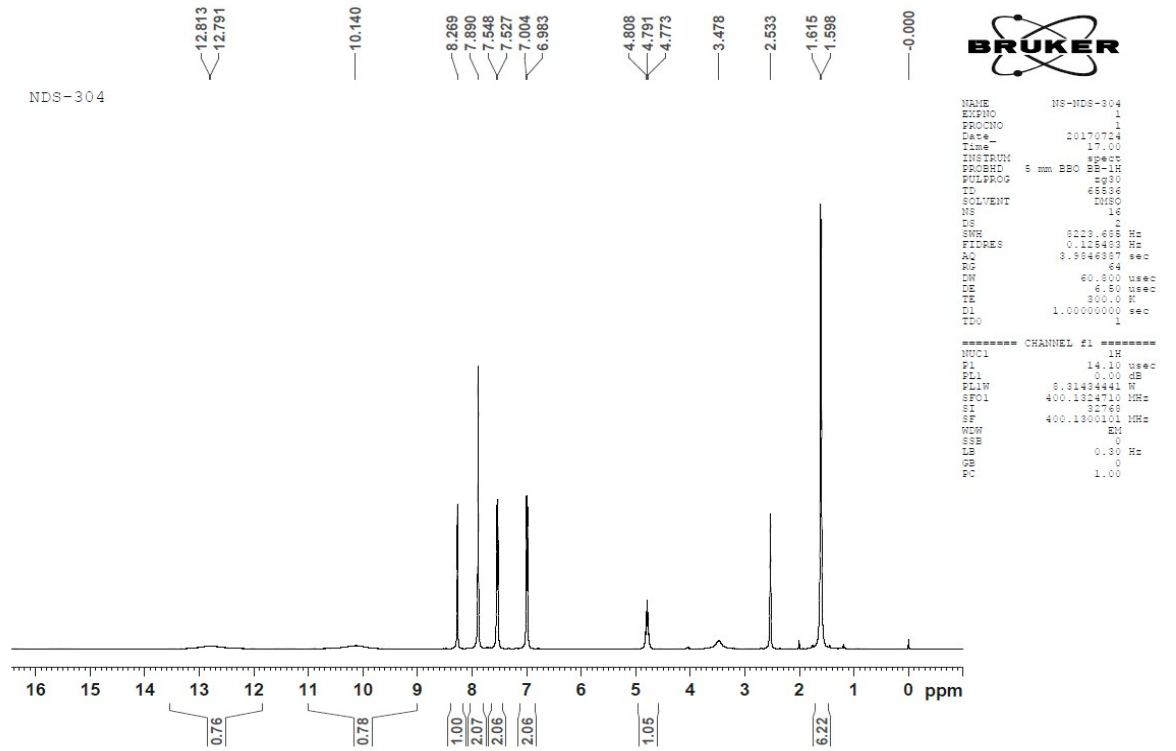
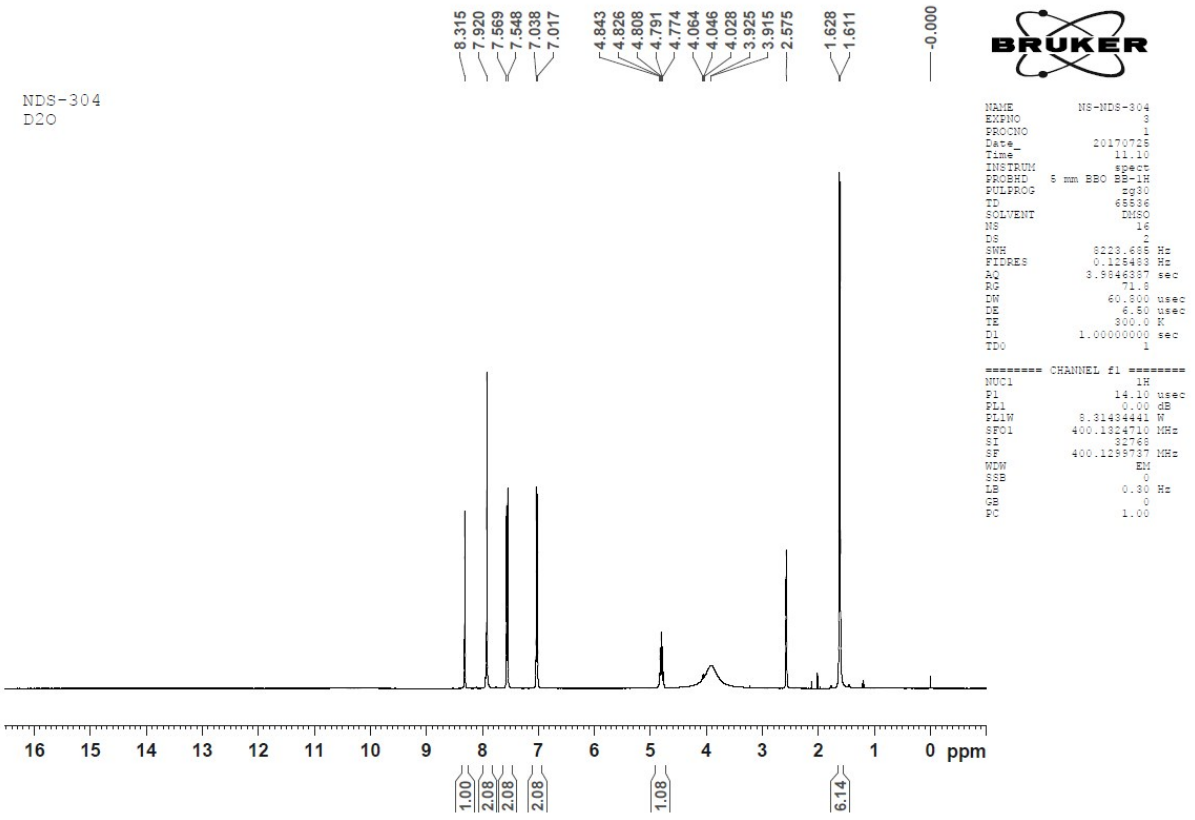
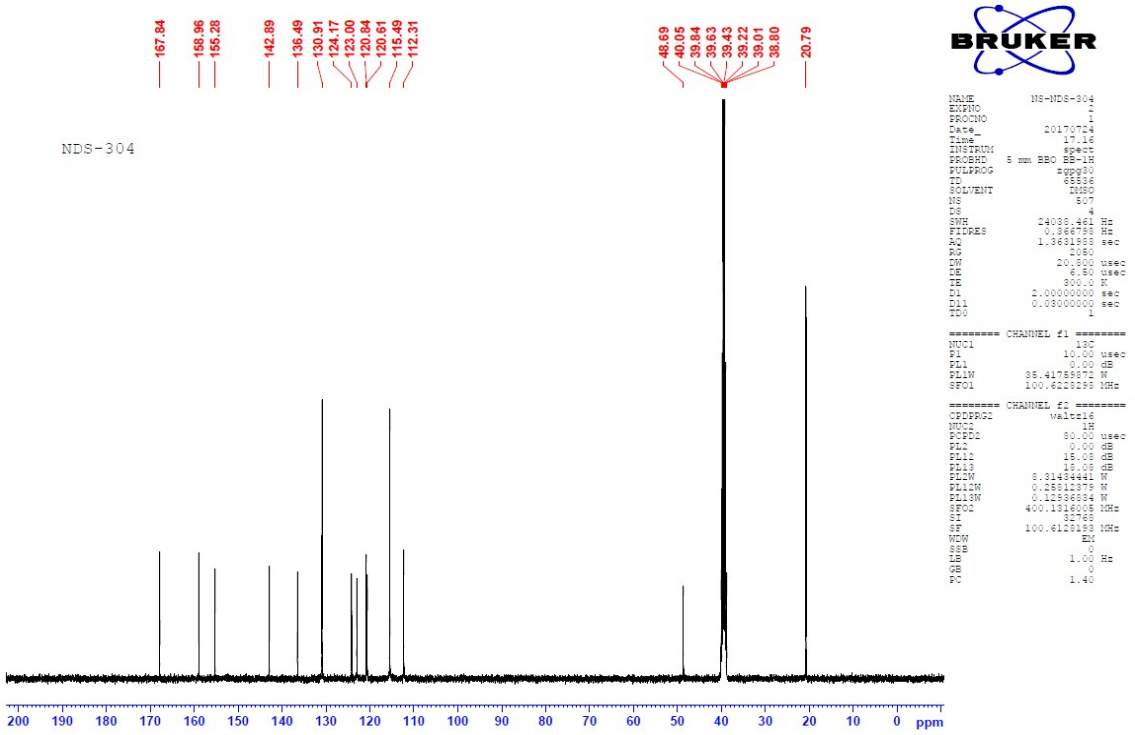
1H-NMR Analysis of synthesized compound: 7d



1H-NMR-D2O exchange analysis of synthesized compound: 7d



13C-NMR Analysis of synthesized compound: 7d



BRUKER

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AQ               1.3631895 sec
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DE                  6.50 usec
TE                 300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                 10.00 usec
PL1                 0.00 dB
PL1W         35.41758972 W
SFO1        100.6228296 MHz

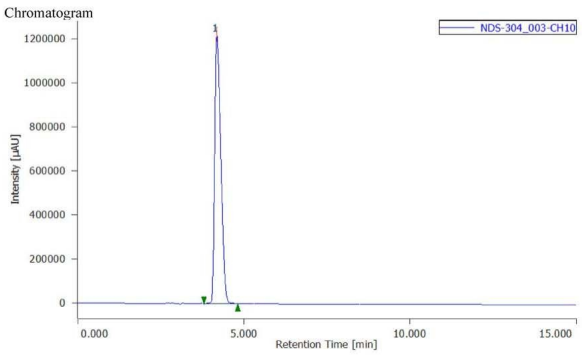
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               16.06 dB
PL13               18.09 dB
PL2W          8.31434441 W
PL12W         0.25912379 W
PL13W         0.12936884 W
SFO2        400.1316005 MHz
SI                   32768
SF          100.6128193 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

HPLC (percentage purity) of 7d

Benzimidazolederivatives_0914 NDS-304_003 9/18/2017 7:31:37 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information	
User Name	Administrator
Date Modified	9/14/2017 5:23:48 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 11:28:04 AM
Volume	20.00 [µL]
Sample #	2
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

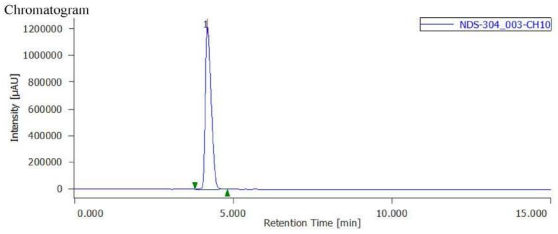
#	Peak Name	CH	tR [min]	Area [µV*sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.190	15686190	1223283	100.000	100.000	2414	N/A	1.486

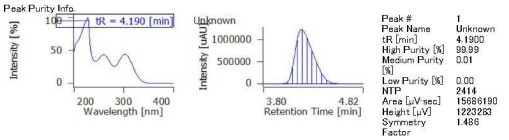
HPLC (peak purity) of 7d

Benzimidazolederivatives_0914 NDS-304_003 9/22/2017 10:52:13 AM

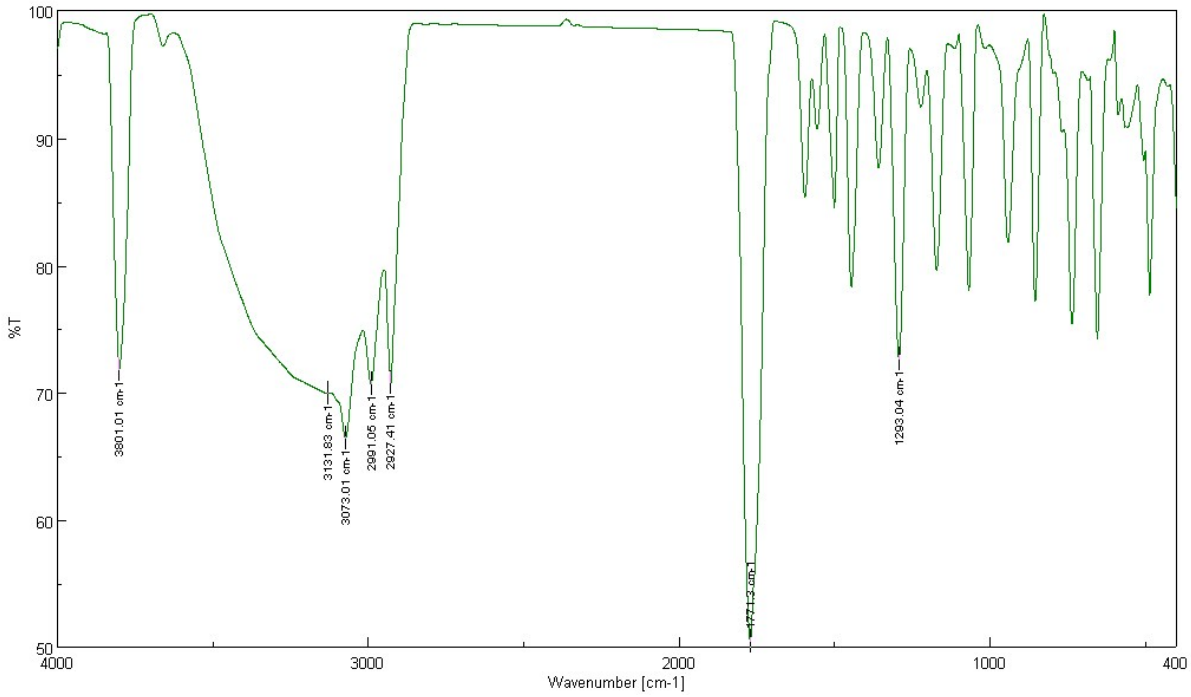
Institute of Pharmacy, Nirma University

Report - HPLC peak purity

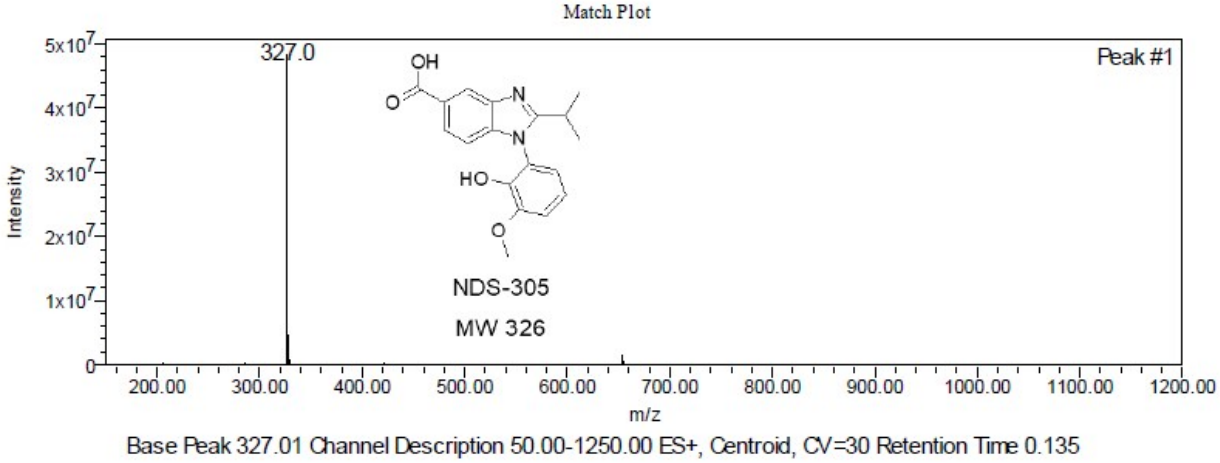




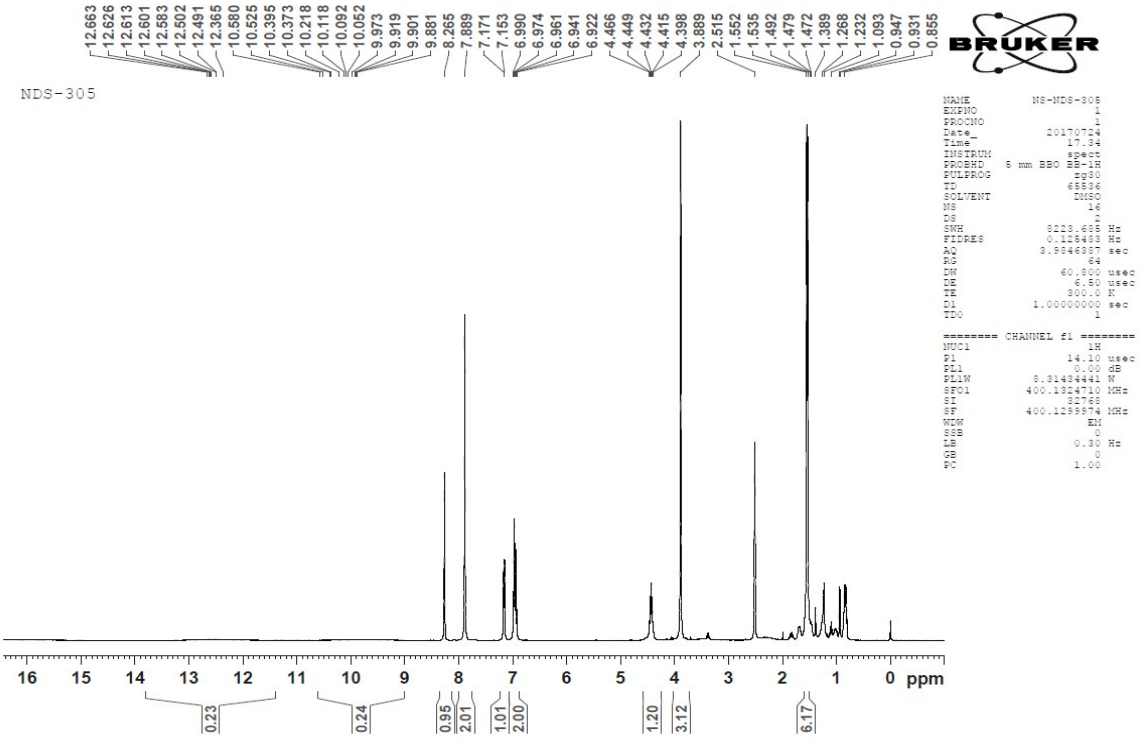
FTIR spectra of 7e



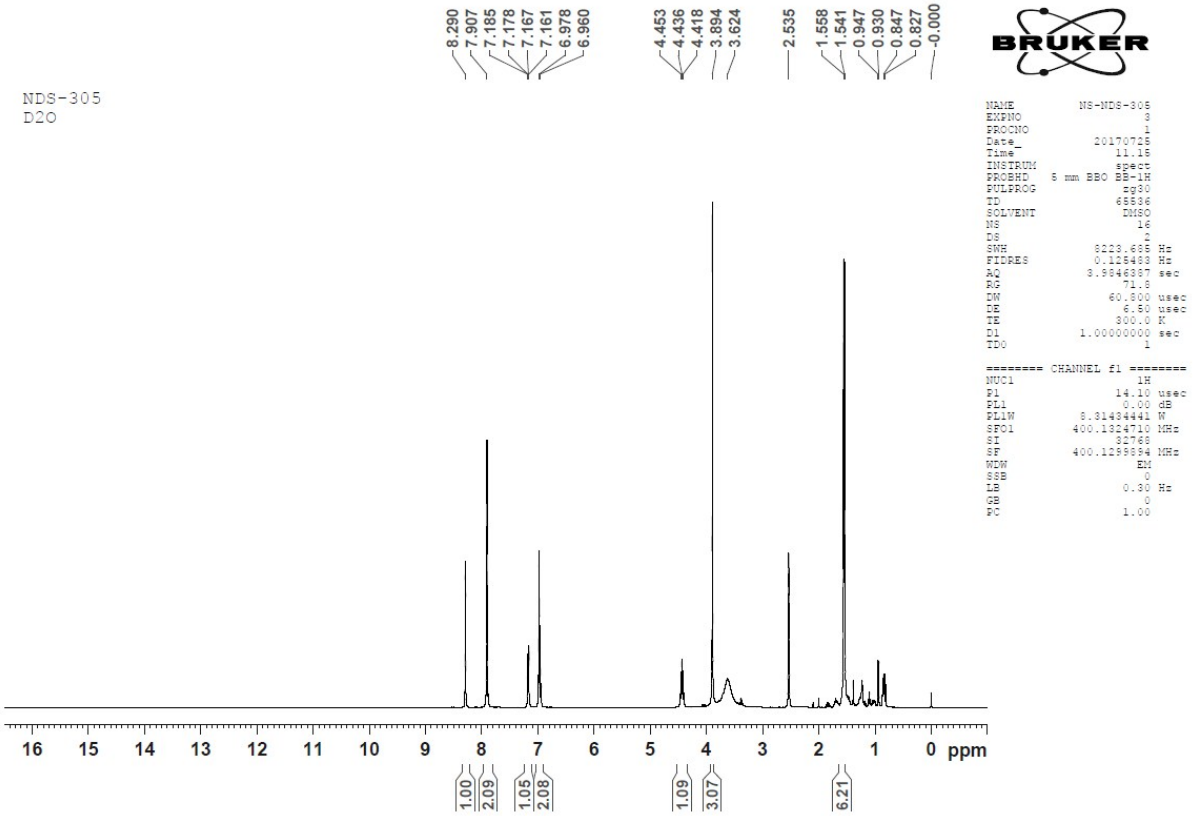
MASS Analysis of synthesized compound: 7e M+1: 327



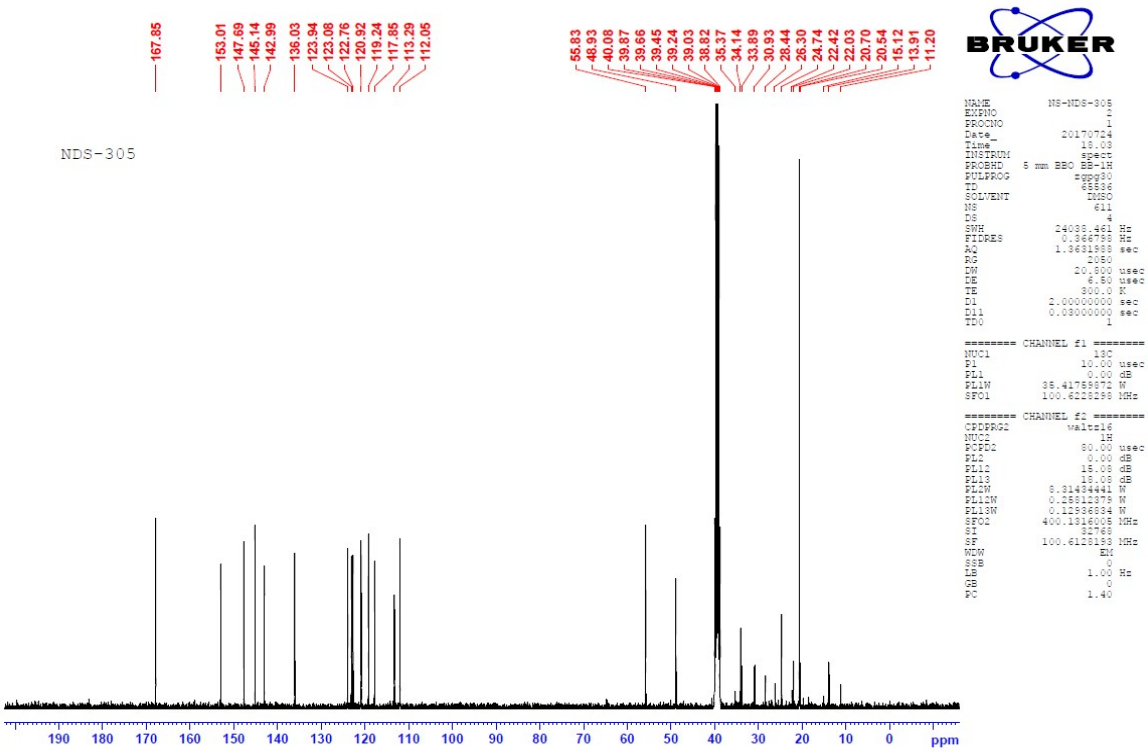
1H-NMR Analysis of synthesized compound: 7e



1H-NMR-D2O exchange analysis of synthesized compound: 7e



13C-NMR Analysis of synthesized compound: 7e

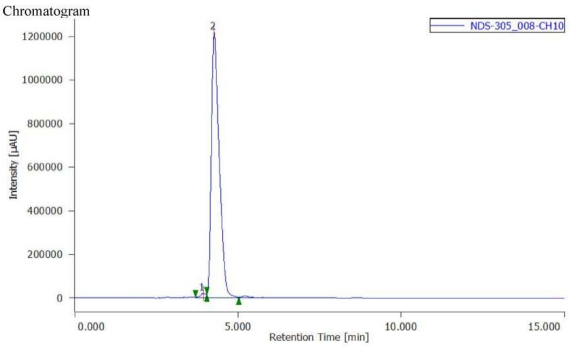


HPLC (percentage purity) of 7e

Benzimidazolederivatives_0914 NDS-305_008 9/16/2017 7:33:25 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information	
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Date Modified	9/14/2017 5:23:59 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 12:56:26 PM
Volume	20.00 [µL]
Sample #	7
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

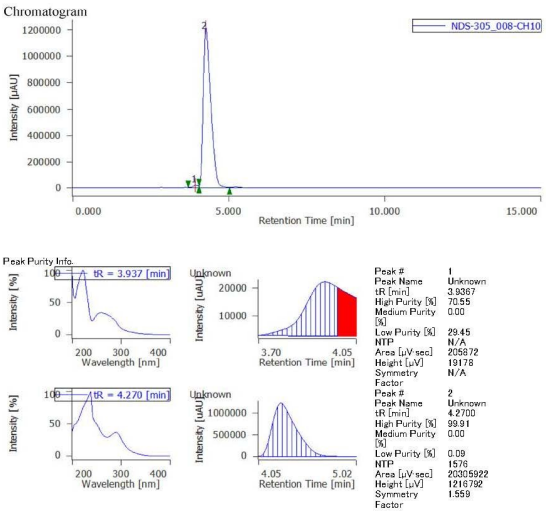
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.937	205872	19178	1.004	1.552	N/A	N/A	N/A
2	Unknown	10	4.270	20305922	1216792	98.996	98.448	1576	N/A	1.559

HPLC (peak purity) of 7e

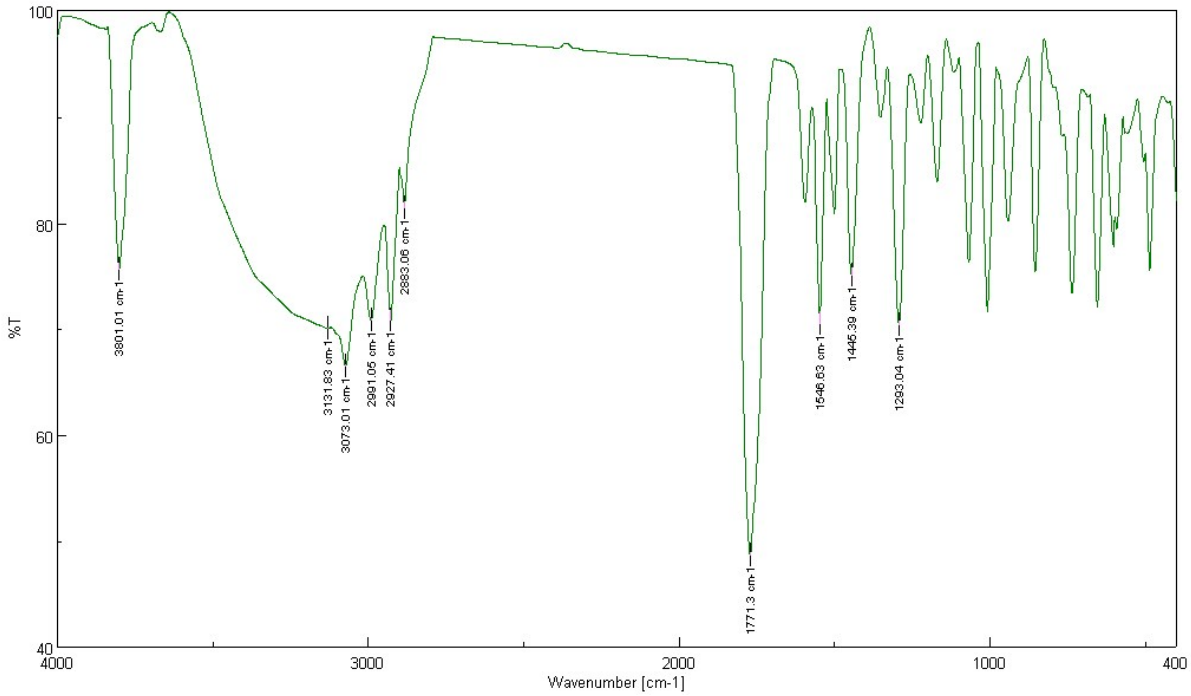
Benzimidazolederivatives_0914 NDS-305_008 9/22/2017 10:53:33 AM

Institute of Pharmacy, Nirma University

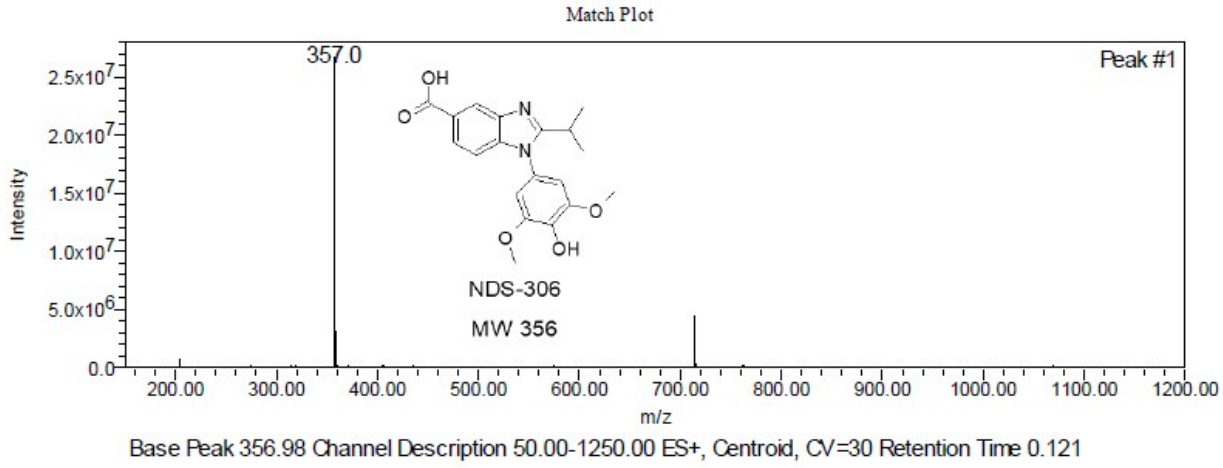
Report - HPLC peak purity



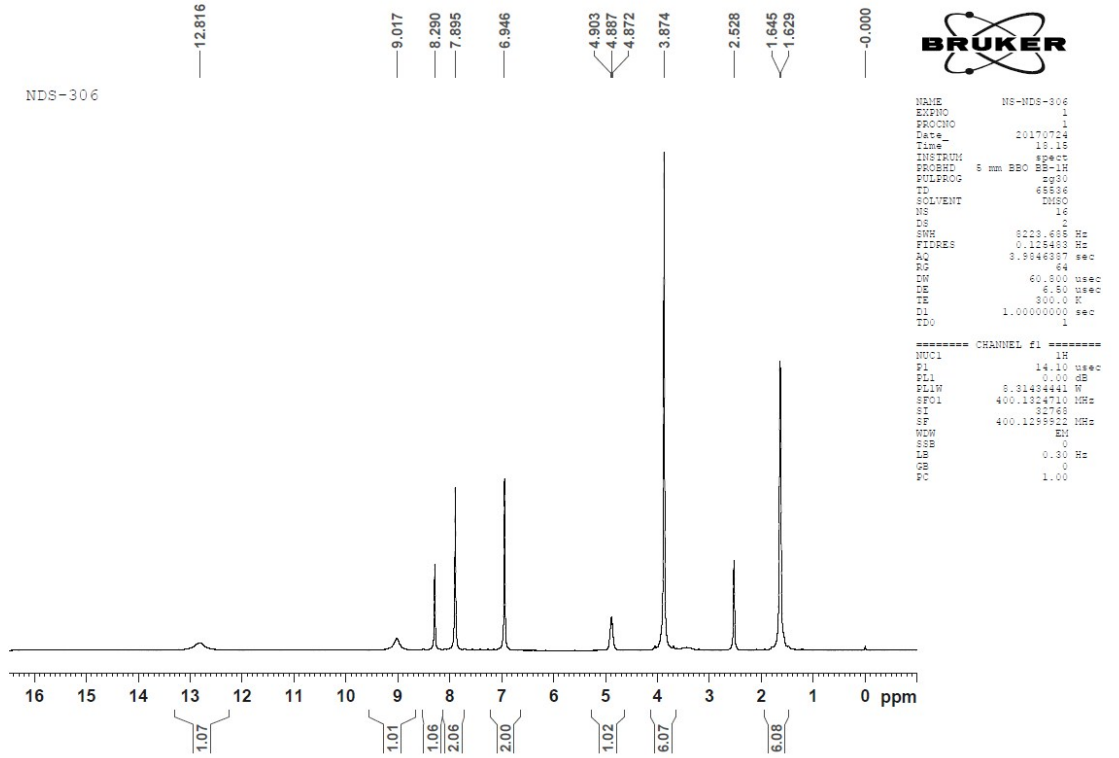
FTIR spectra of 7f



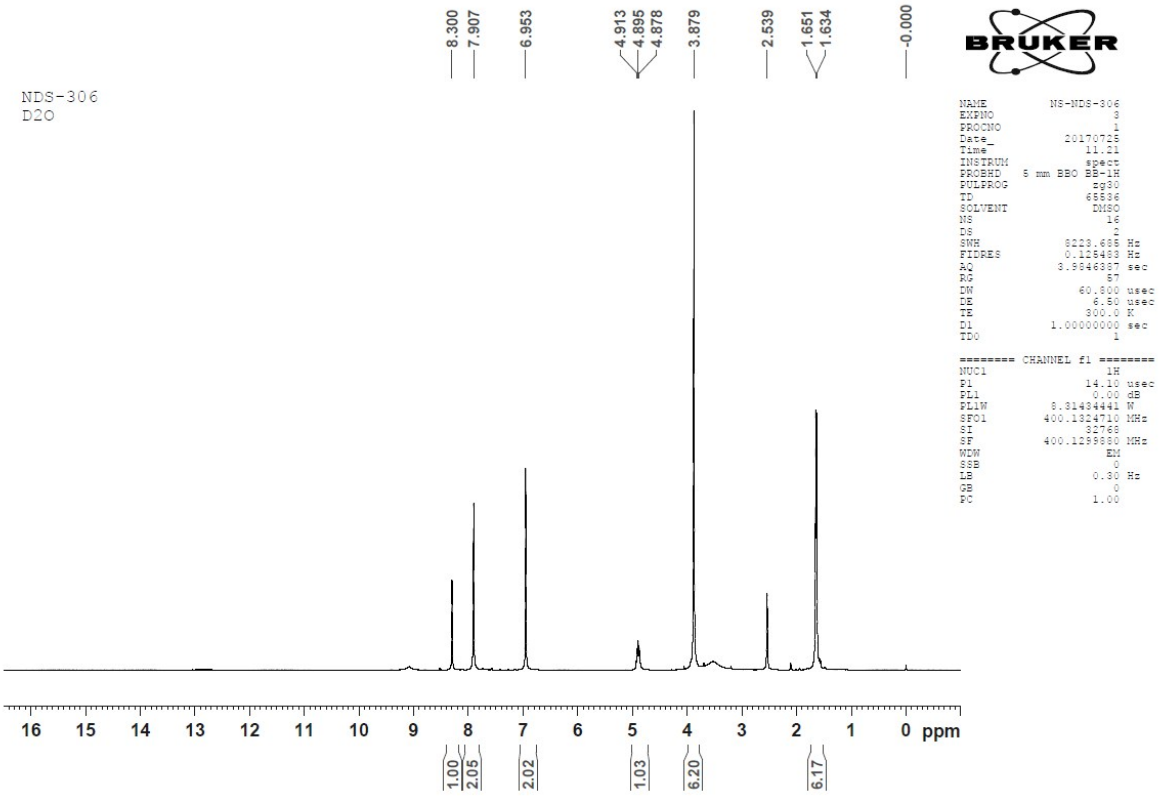
MASS Analysis of synthesized compound: 7f M+1: 357



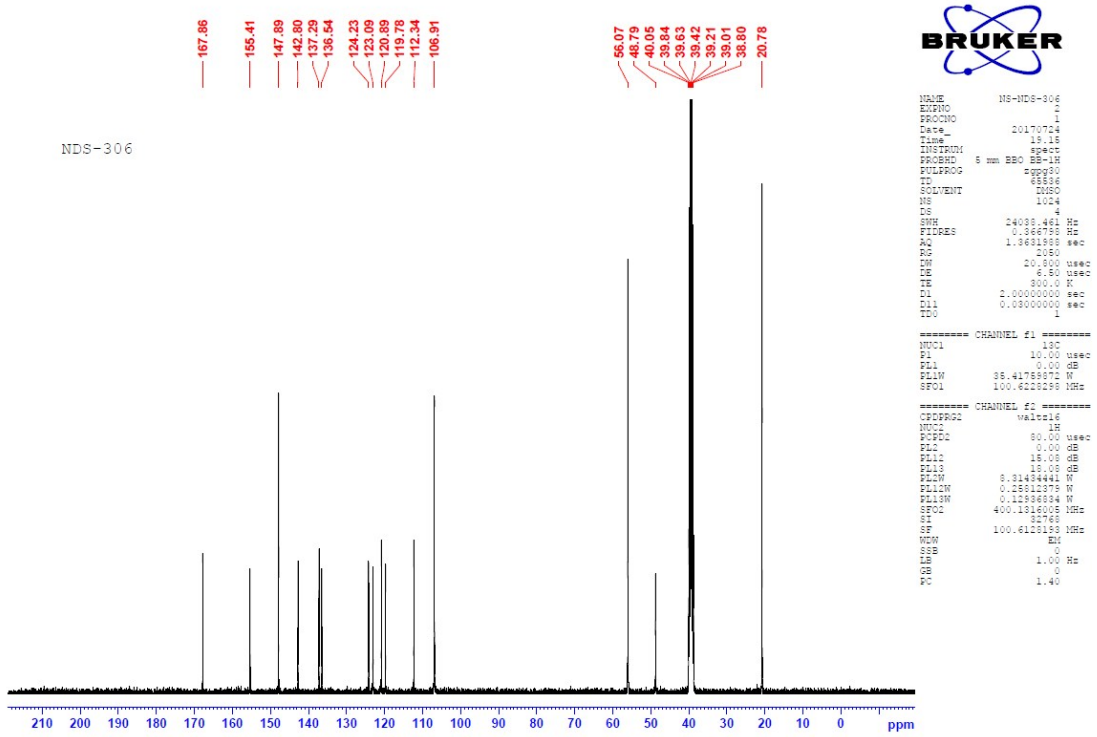
1H-NMR Analysis of synthesized compound: 7f



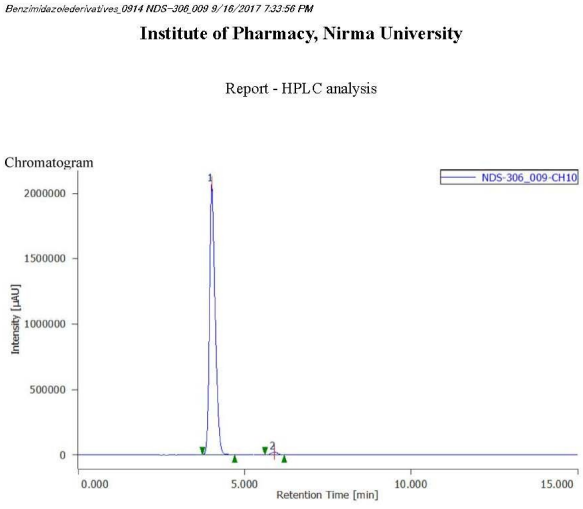
1H-NMR-D2O exchange analysis of synthesized compound: 7f



13C-NMR Analysis of synthesized compound: 7f



HPLC (percentage purity) of 7f



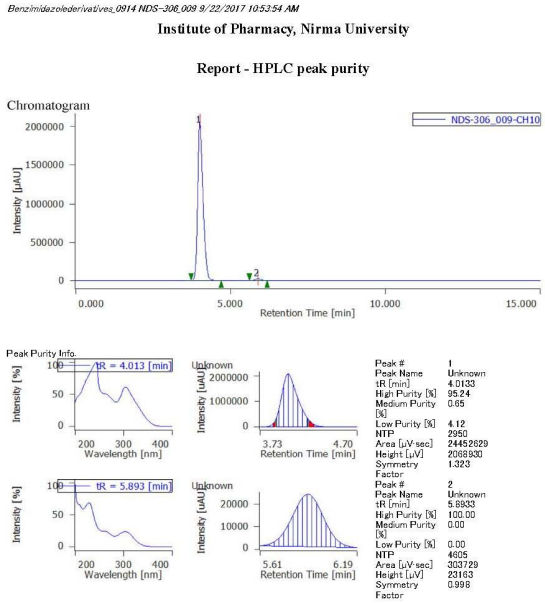
Chromatogram Information

User Name	Administrator
Date Modified	9/14/2017 5:24:01 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 1:13:26 PM
Volume	20.00 [µL]
Sample #	8
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

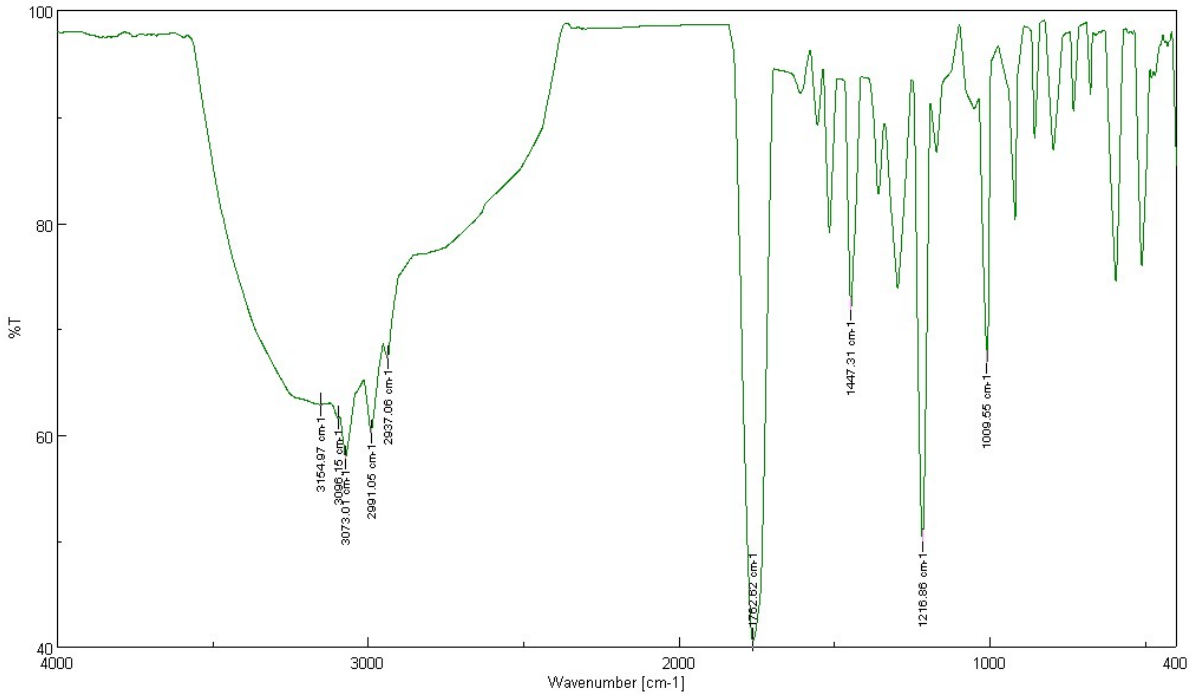
Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.013	24452629	2068930	98.773	98.893	2950	5.782	1.323
2	Unknown	10	5.893	303729	23163	1.227	1.107	4605	N/A	0.998

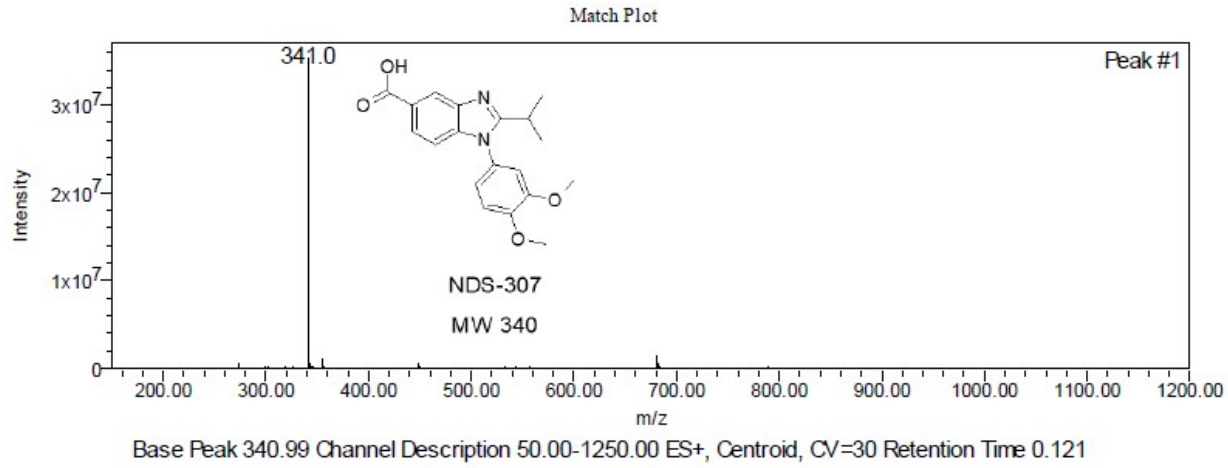
HPLC (peak purity) of 7f



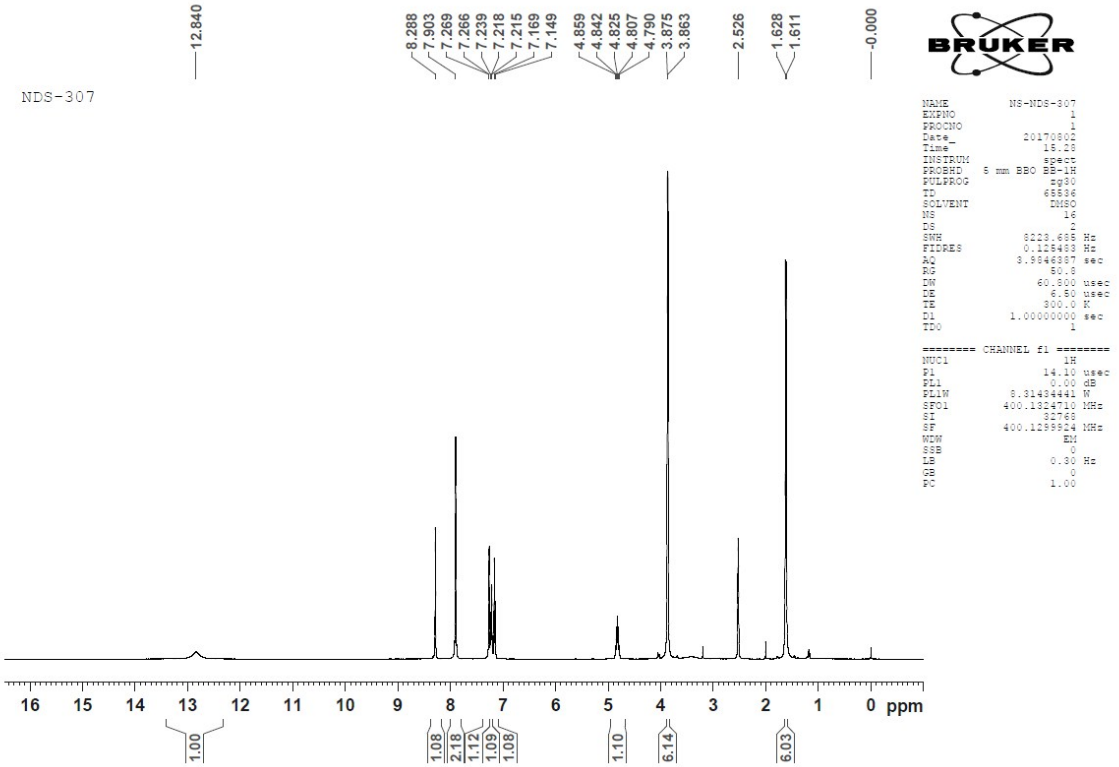
FTIR spectra of 7g



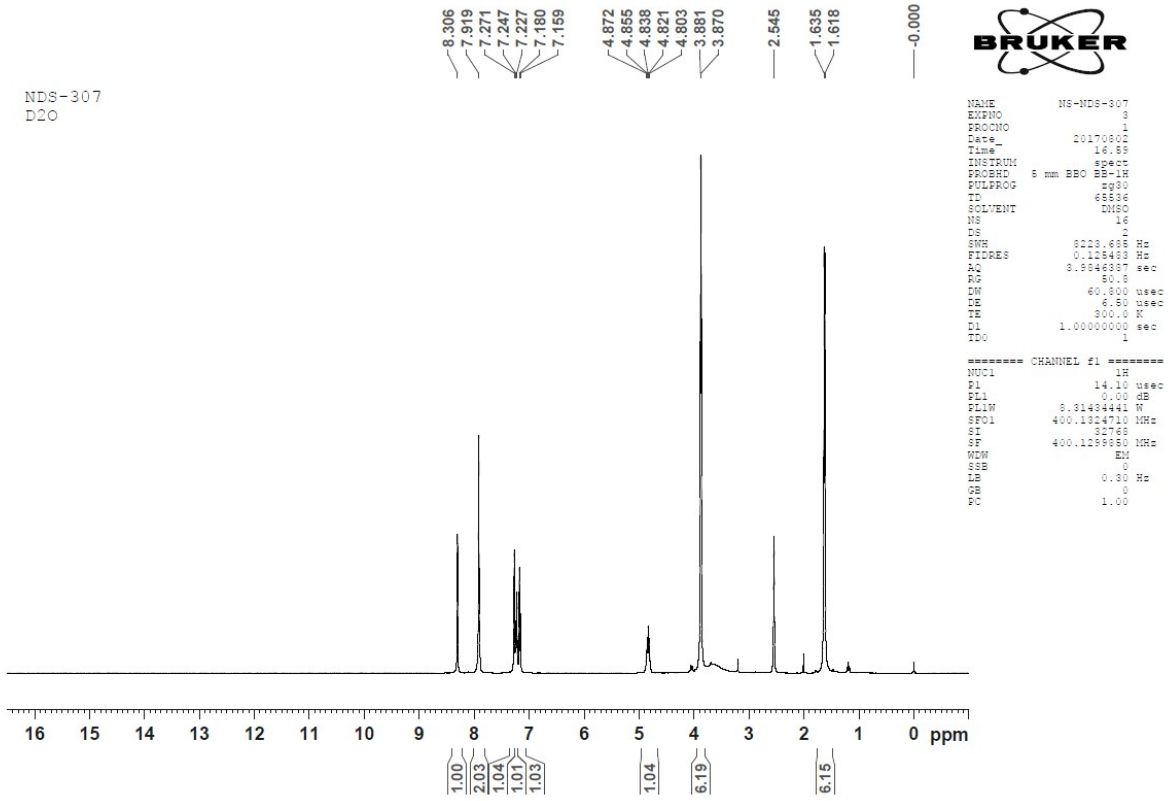
MASS Analysis of synthesized compound: 7g M+1: 341



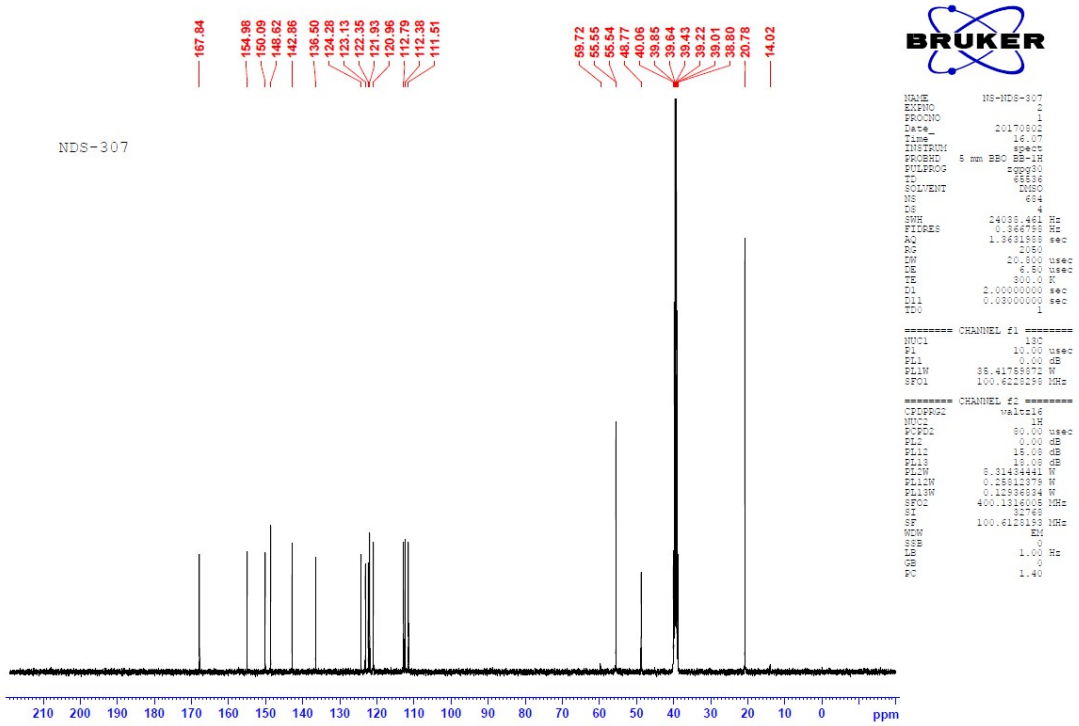
1H-NMR Analysis of synthesized compound: 7g



1H-NMR-D2O exchange analysis of synthesized compound: 7g



13C-NMR Analysis of synthesized compound: 7g

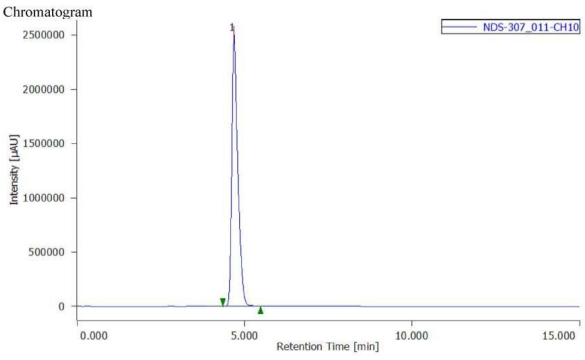


HPLC (percentage purity) of 7g

Benzimidazolederivatives_0914 NDS-307_011 9/16/2017 7:34:22 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information	
User Name	Administrator
Date Modified	9/14/2017 5:24:04 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 1:41:52 PM
Volume	20.00 [µL]
Sample #	10
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

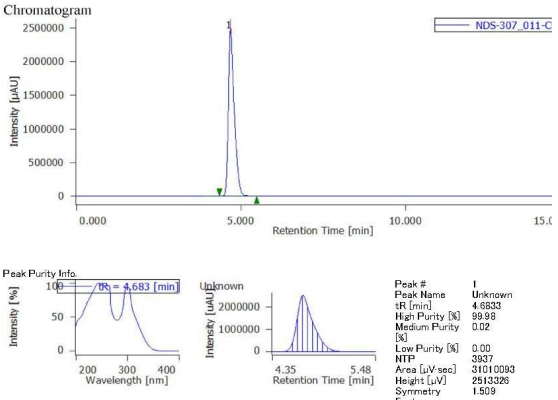
#	Peak Name	CH	tR [min]	Area [µV*sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.683	31010093	2513326	100.000	100.000	3937	N/A	1.509

HPLC (peak purity) of 7g

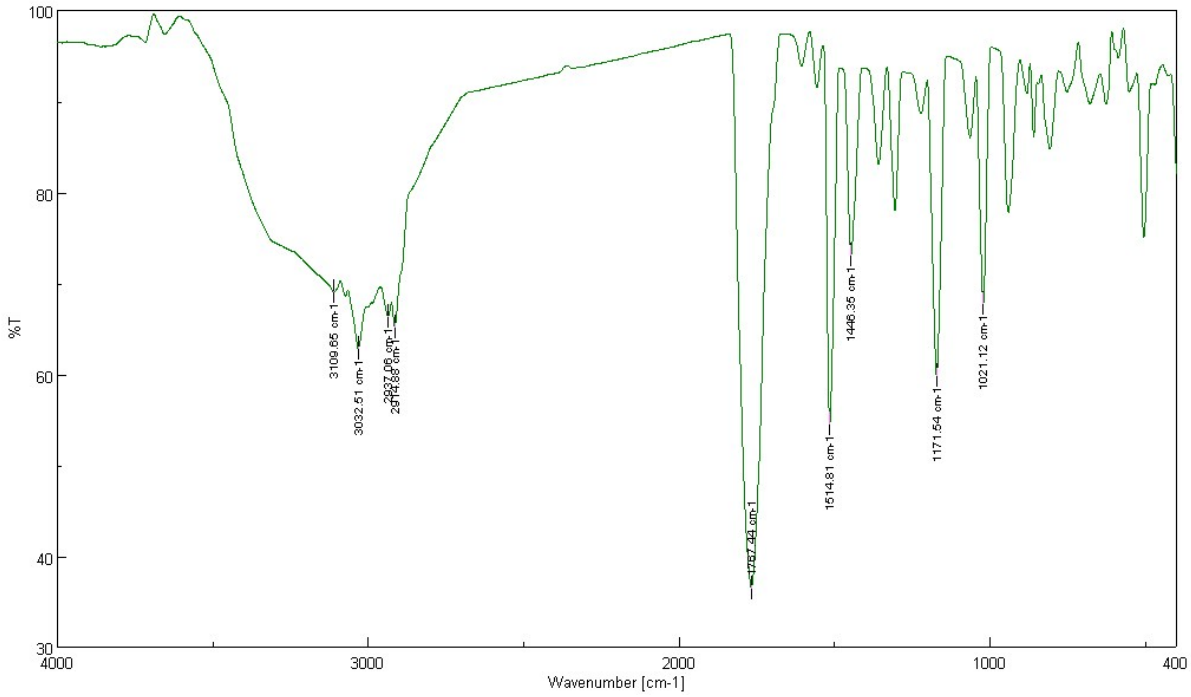
Benzimidazolederivatives_0914 NDS-307_011 9/22/2017 10:54:11 AM

Institute of Pharmacy, Nirma University

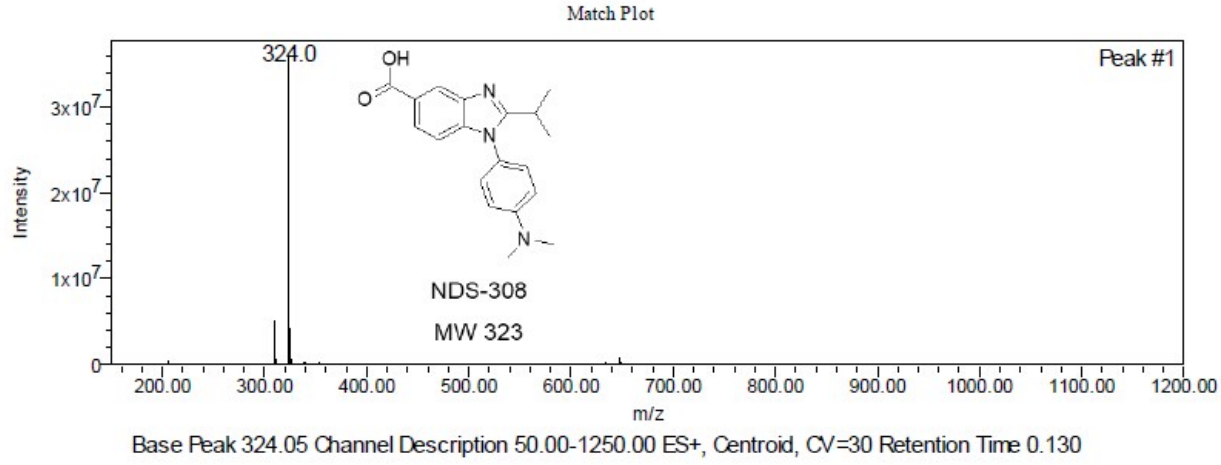
Report - HPLC peak purity



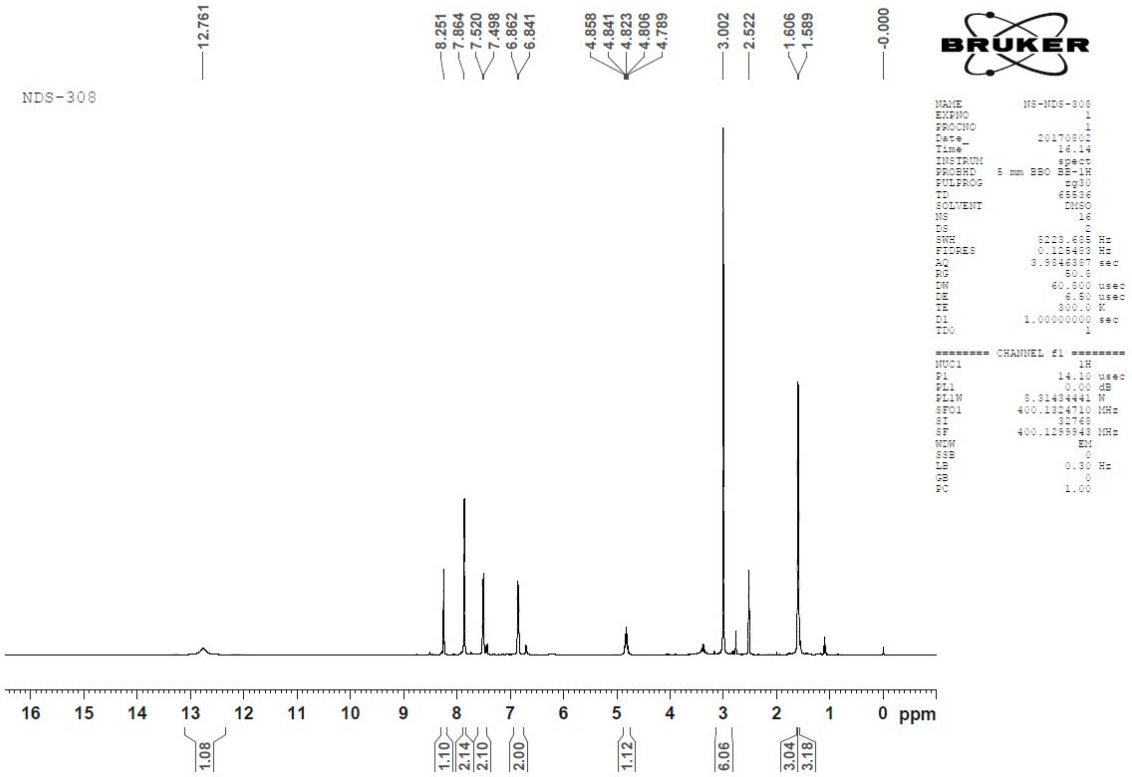
FTIR spectra of 7h



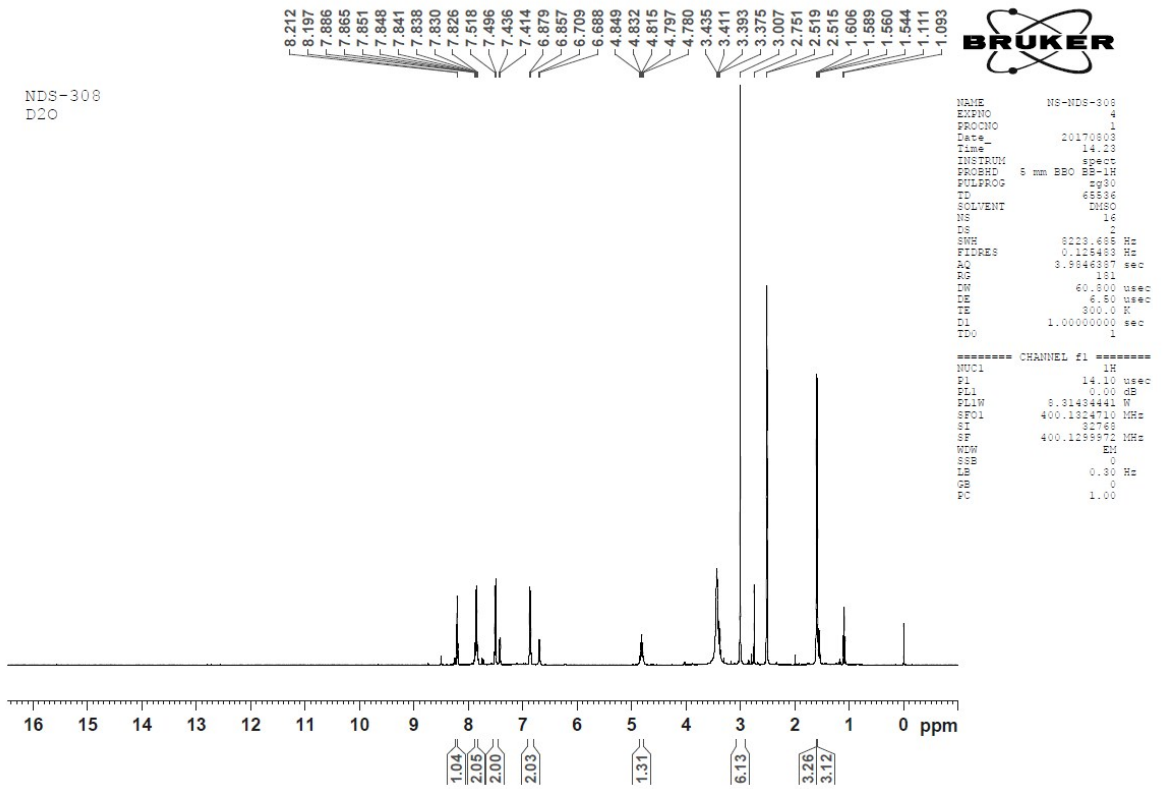
MASS Analysis of synthesized compound: 7h M+1: 324



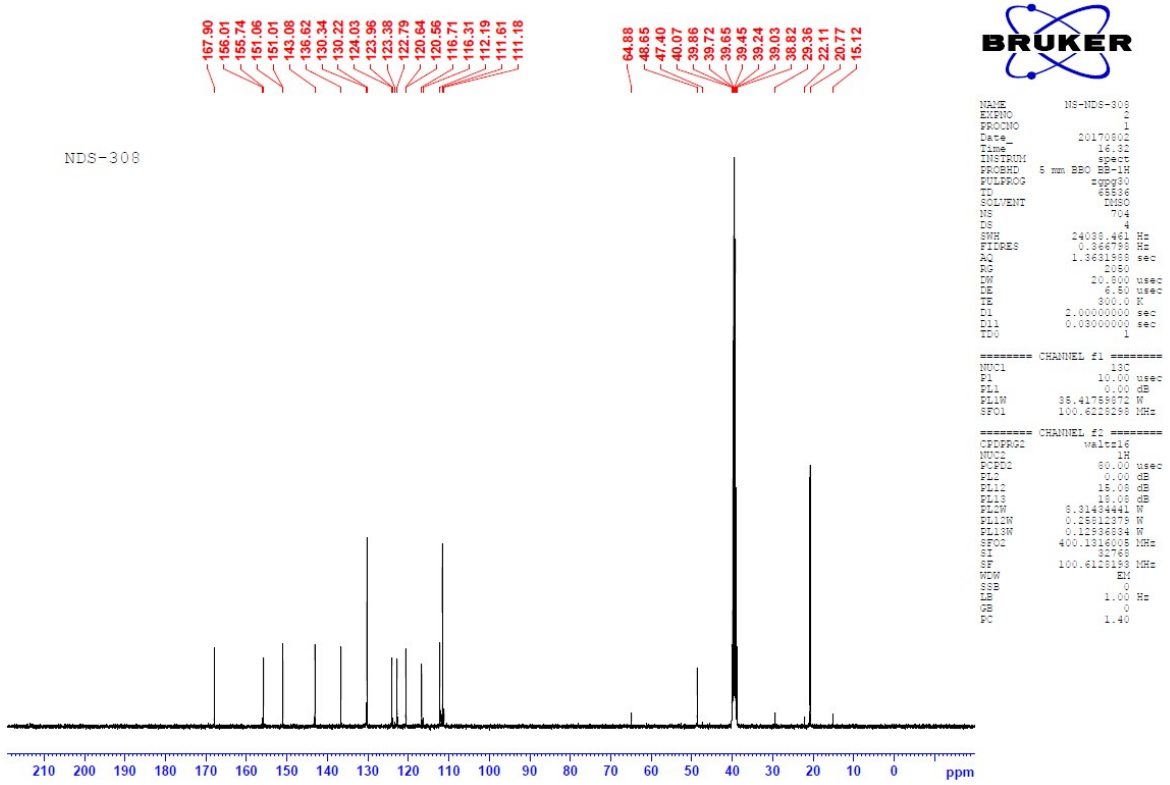
1H-NMR Analysis of synthesized compound: 7h



1H-NMR-D2O exchange analysis of synthesized compound: 7h



13C-NMR Analysis of synthesized compound: 7h

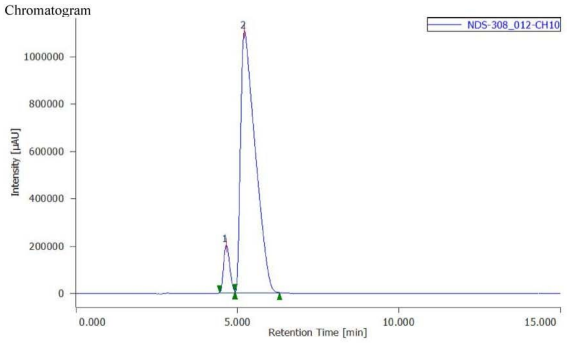


HPLC (percentage purity) of 7h

Benzimidazolederivatives_0914 NDS-308_012 9/16/2017 7:34:39 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

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Date Modified	9/14/2017 5:24:07 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 1:59:49 PM
Volume	20.00 [µL]
Sample #	11
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

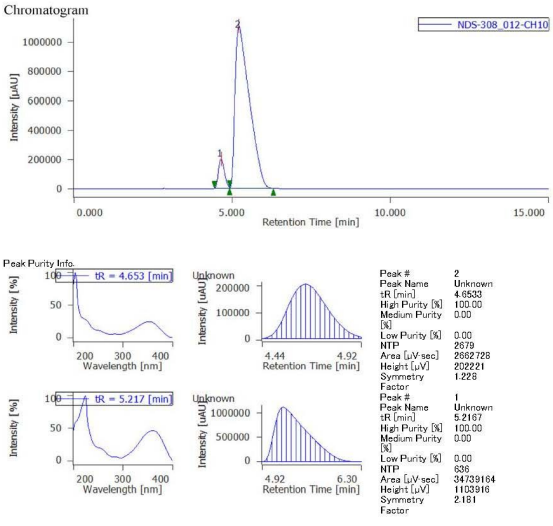
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.653	2662728	202221	7.119	15.482	2679	0.930	1.228
2	Unknown	10	5.217	34739164	1103916	92.881	84.518	636	N/A	2.181

HPLC (peak purity) of 7h

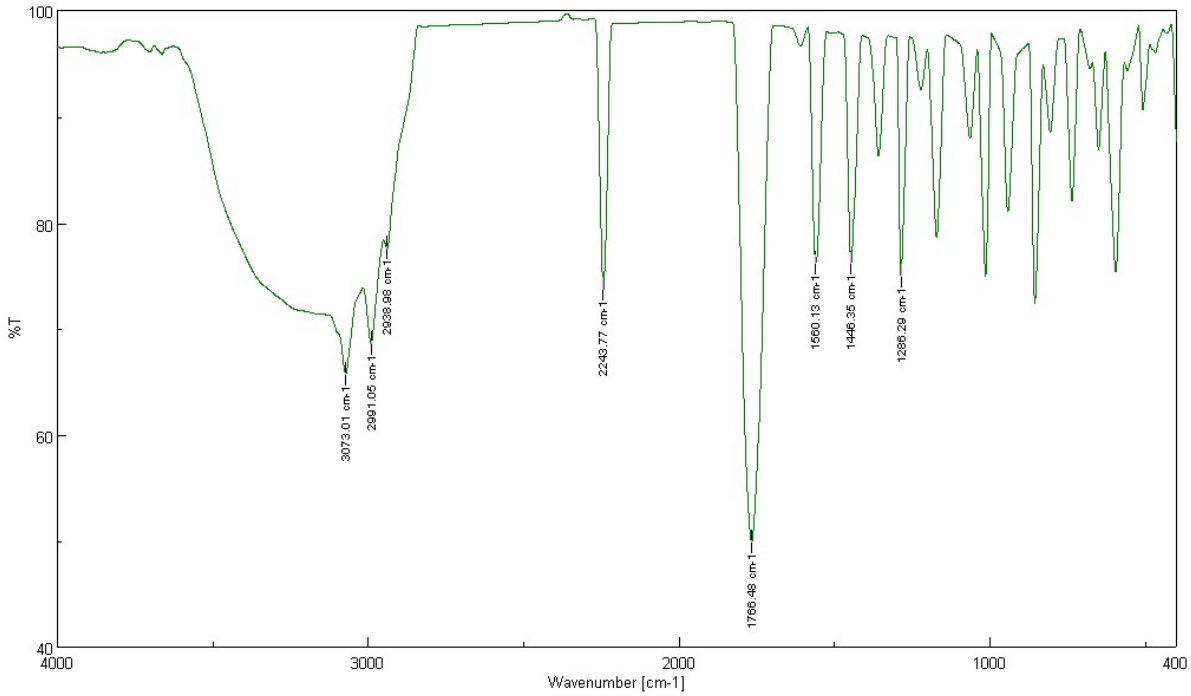
Benzimidazolederivatives_0914 NDS-308_012 9/22/2017 10:54:27 AM

Institute of Pharmacy, Nirma University

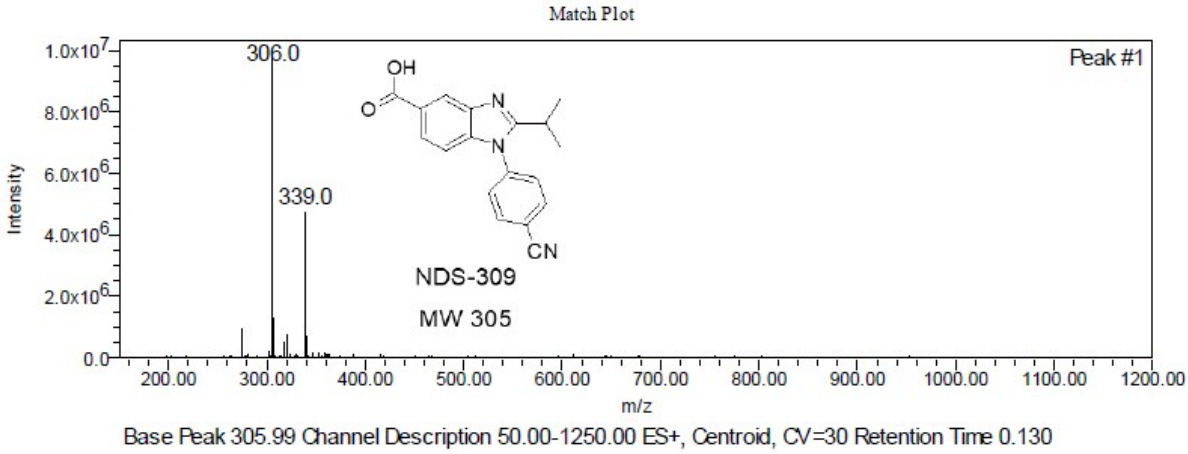
Report - HPLC peak purity



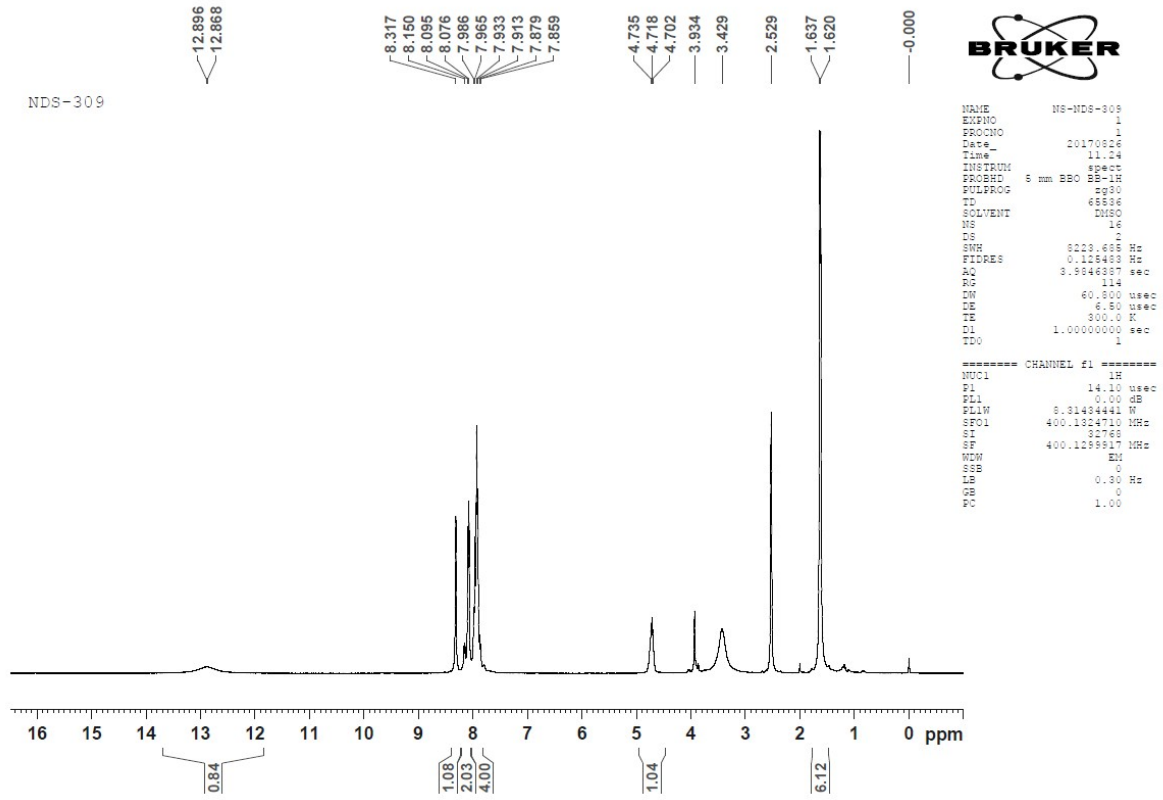
FTIR spectra of 7i



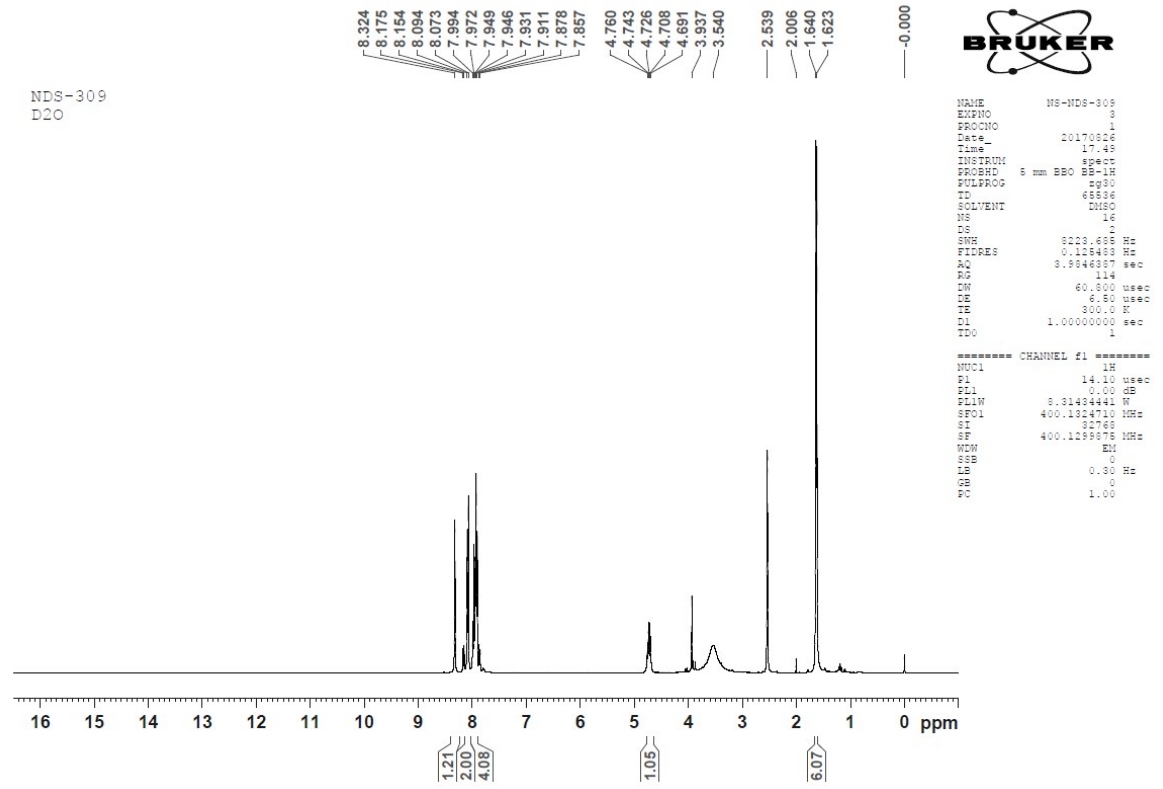
MASS Analysis of synthesized compound: 7i M+1: 306



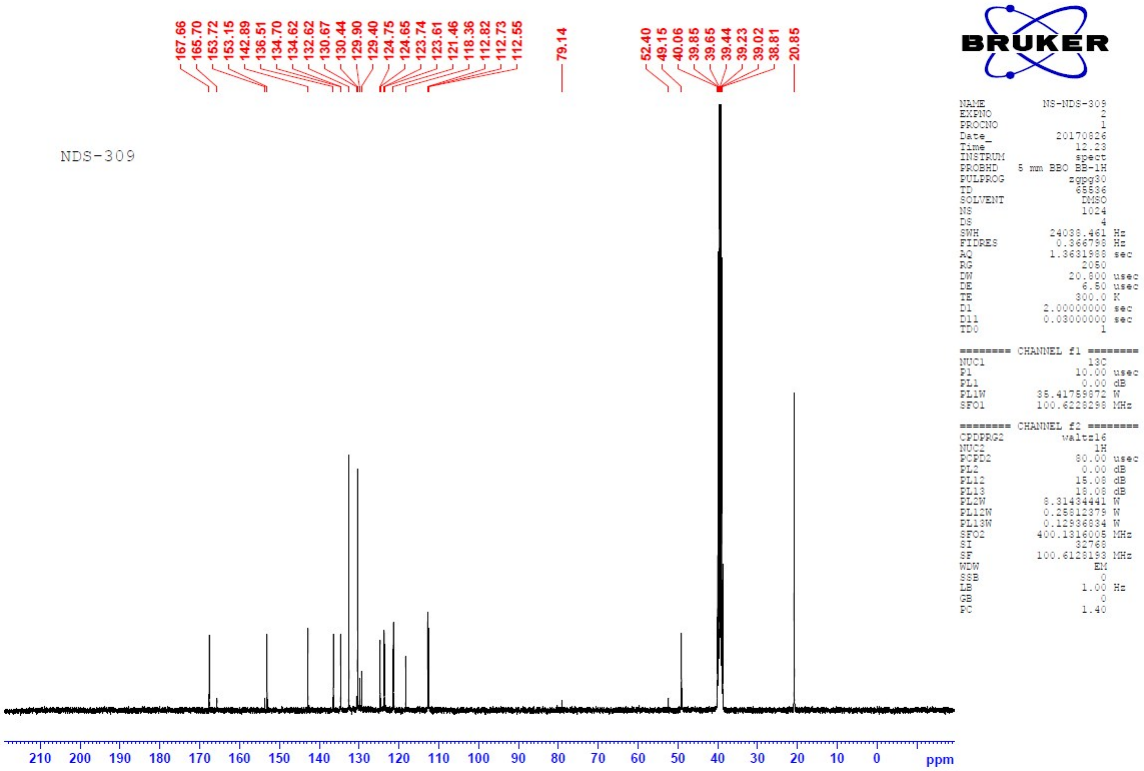
1H-NMR Analysis of synthesized compound: 7i



1H-NMR-D2O exchange analysis of synthesized compound: 7i



13C-NMR Analysis of synthesized compound: 7i

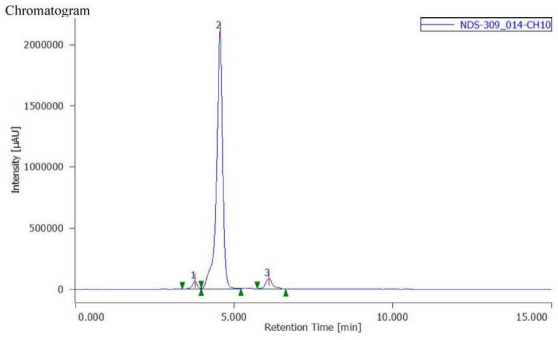


HPLC (percentage purity) of 7i

Benzimidazolederivatives_0914 NDS-309_014 9/16/2017 7:35:21 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information	
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Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 2:43:41 PM
Volume	20.00 [µL]
Sample #	13
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

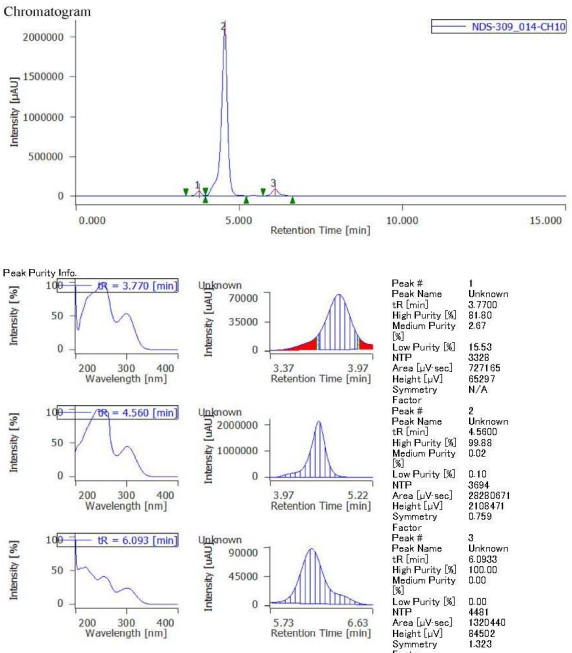
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.770	727165	65297	2.398	2.891	3328	2.755	N/A
2	Unknown	10	4.560	28280671	2108471	93.249	93.367	3694	4.545	0.759
3	Unknown	10	6.093	1320440	84502	4.354	3.742	4481	N/A	1.323

HPLC (peak purity) of 7i

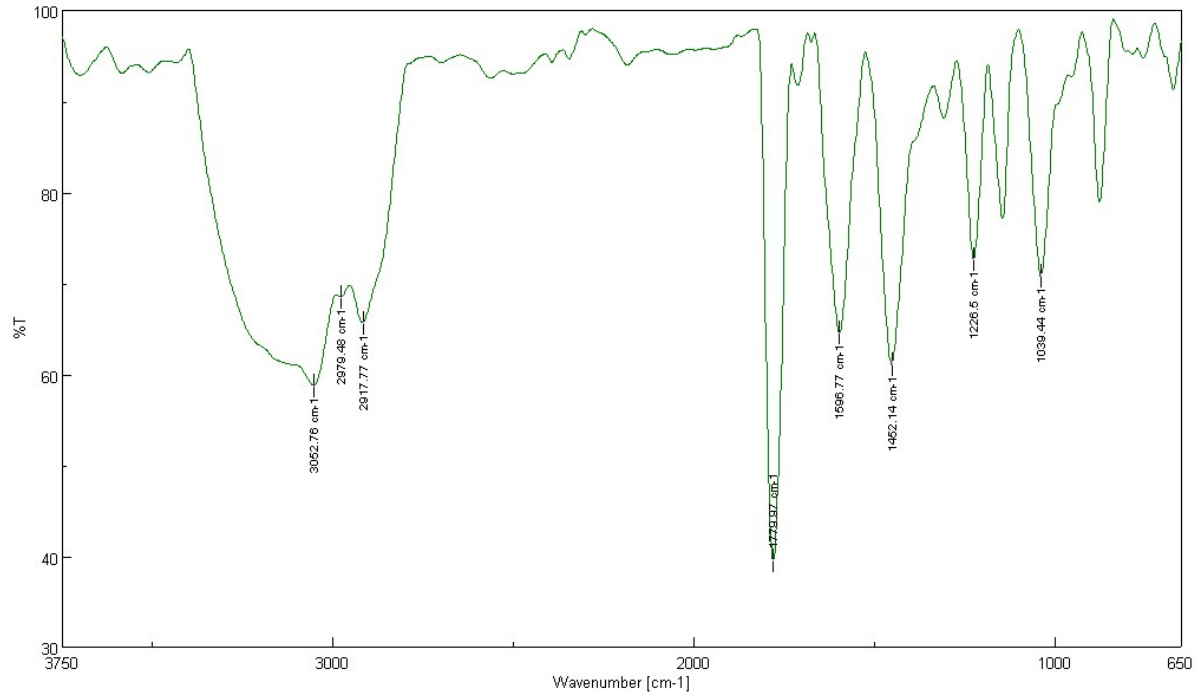
Benzimidazolederivatives_0914 NDS-309_014 9/22/2017 10:54:44 AM

Institute of Pharmacy, Nirma University

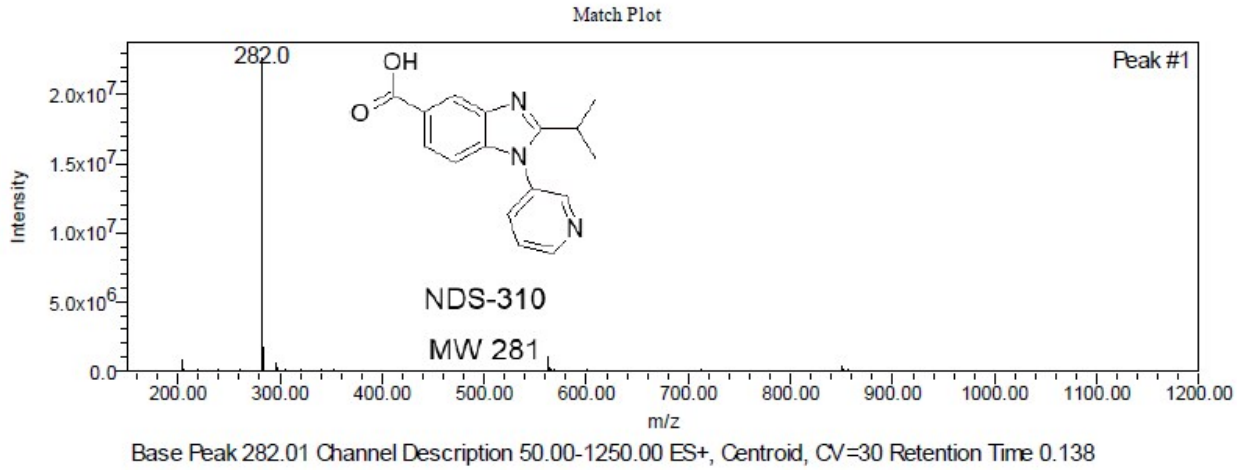
Report - HPLC peak purity



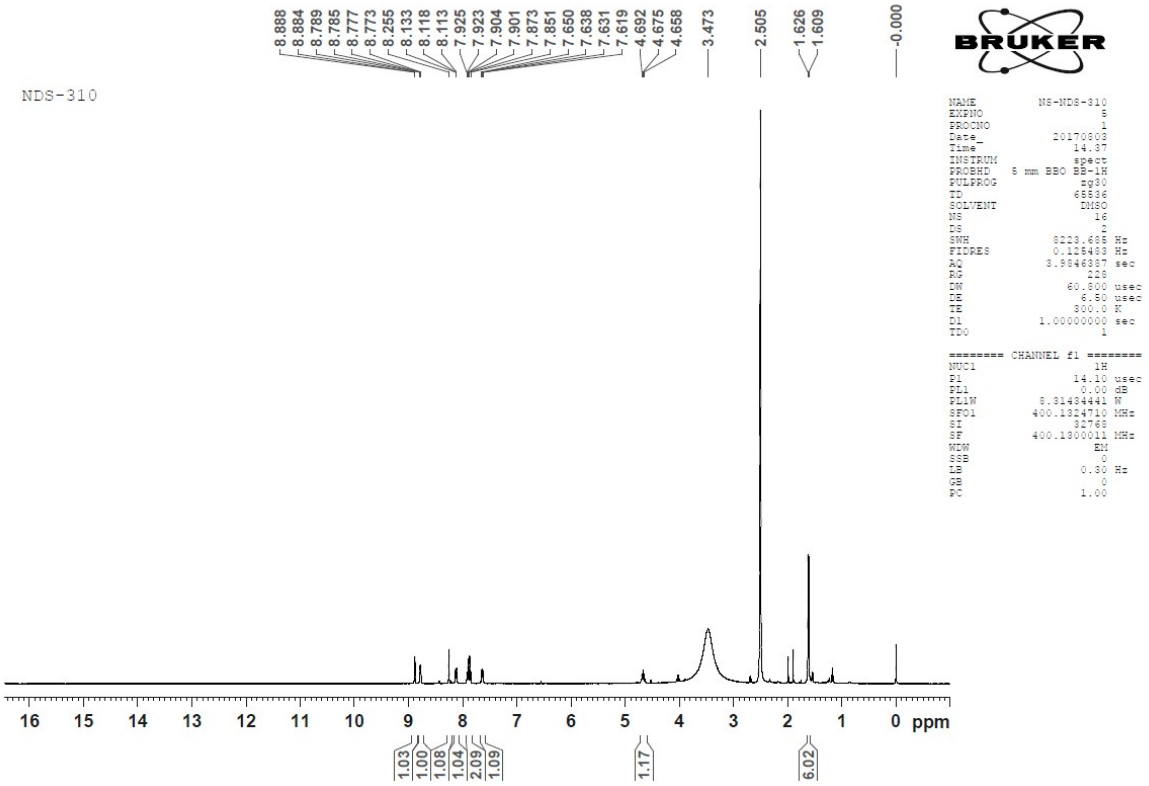
FTIR spectra of 7j



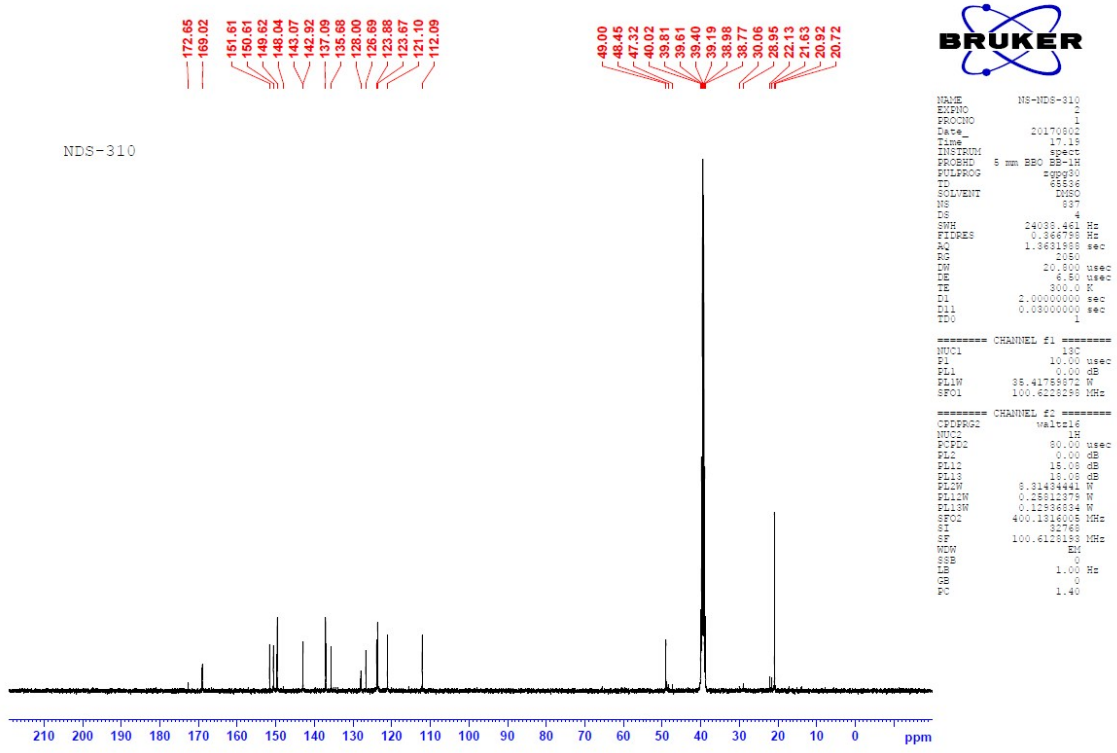
MASS Analysis of synthesized compound: 7j M+1: 282



1H-NMR Analysis of synthesized compound: 7j



13C-NMR Analysis of synthesized compound: 7j

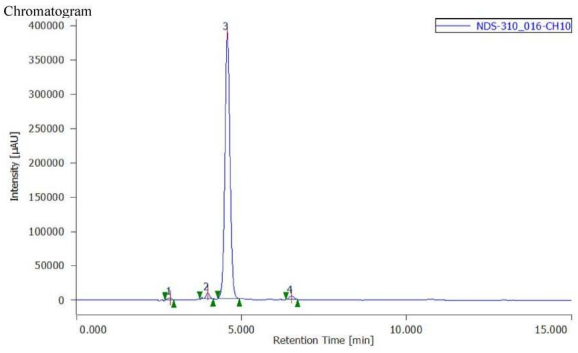


HPLC (percentage purity) of 7j

Benzimidazolederivatives_0914 NDS-310_016 9/16/2017 7:35:29 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

User Name	Administrator
Date Modified	9/14/2017 5:24:12 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 3:43:19 PM
Volume	20.00 [µL]
Sample #	15
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

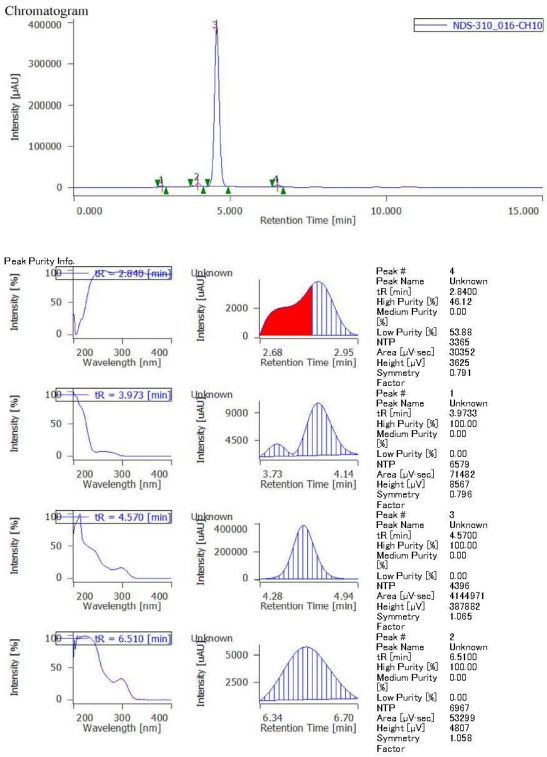
#	Peak Name	CH	tR [min]	Area [µV*sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	2.840	30352	3625	0.706	0.895	3365	4.943	0.791
2	Unknown	10	3.973	71482	8567	1.662	2.116	6579	2.532	0.796
3	Unknown	10	4.570	4144971	387882	96.392	95.801	4396	6.627	1.065
4	Unknown	10	6.510	53299	4807	1.239	1.187	6967	N/A	1.058

HPLC (peak purity) of 7j

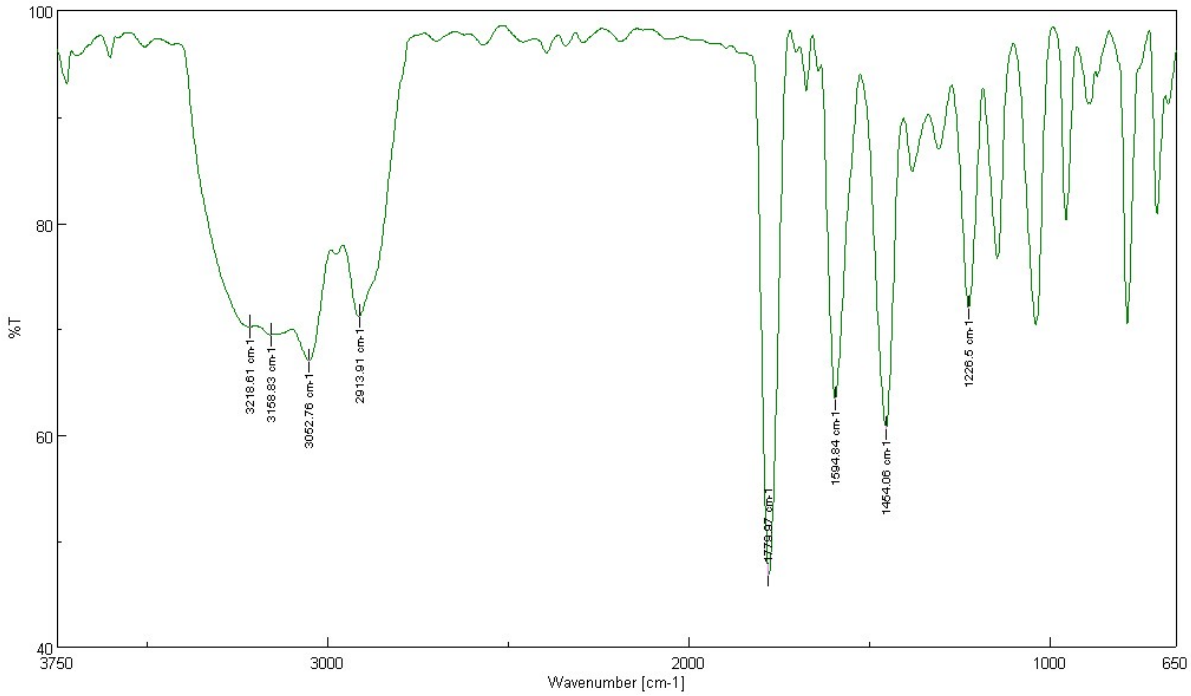
Benzimidazolederivatives_0914 NDS-310_016 9/22/2017 10:55:00 AM

Institute of Pharmacy, Nirma University

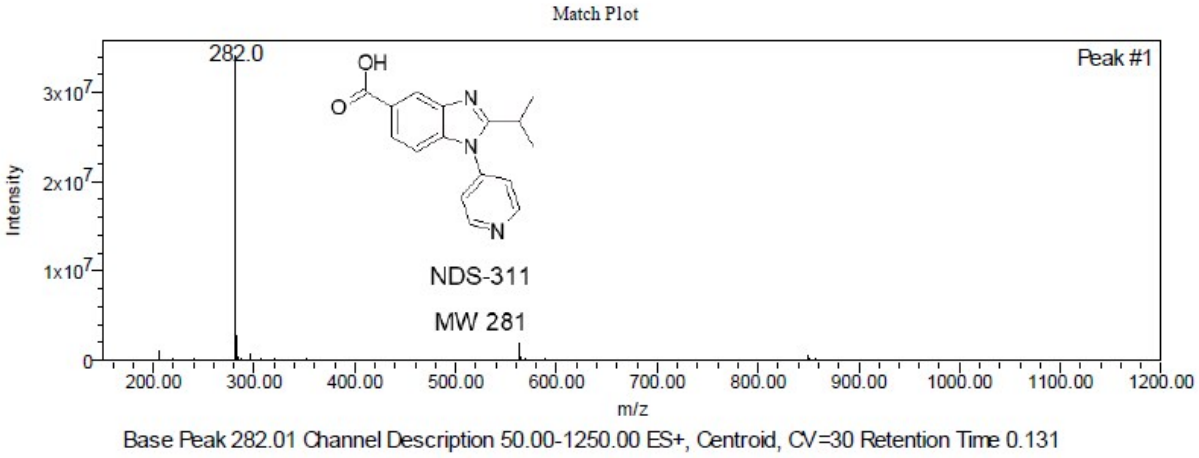
Report - HPLC peak purity



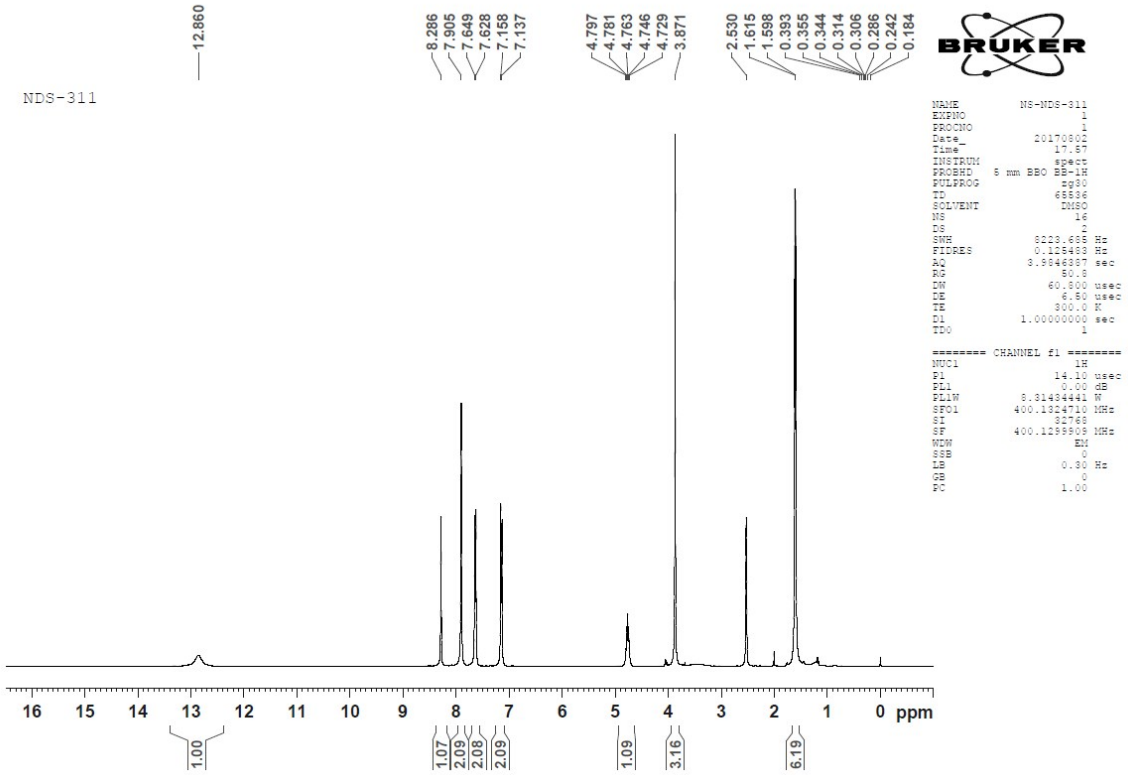
FTIR spectra of 7k



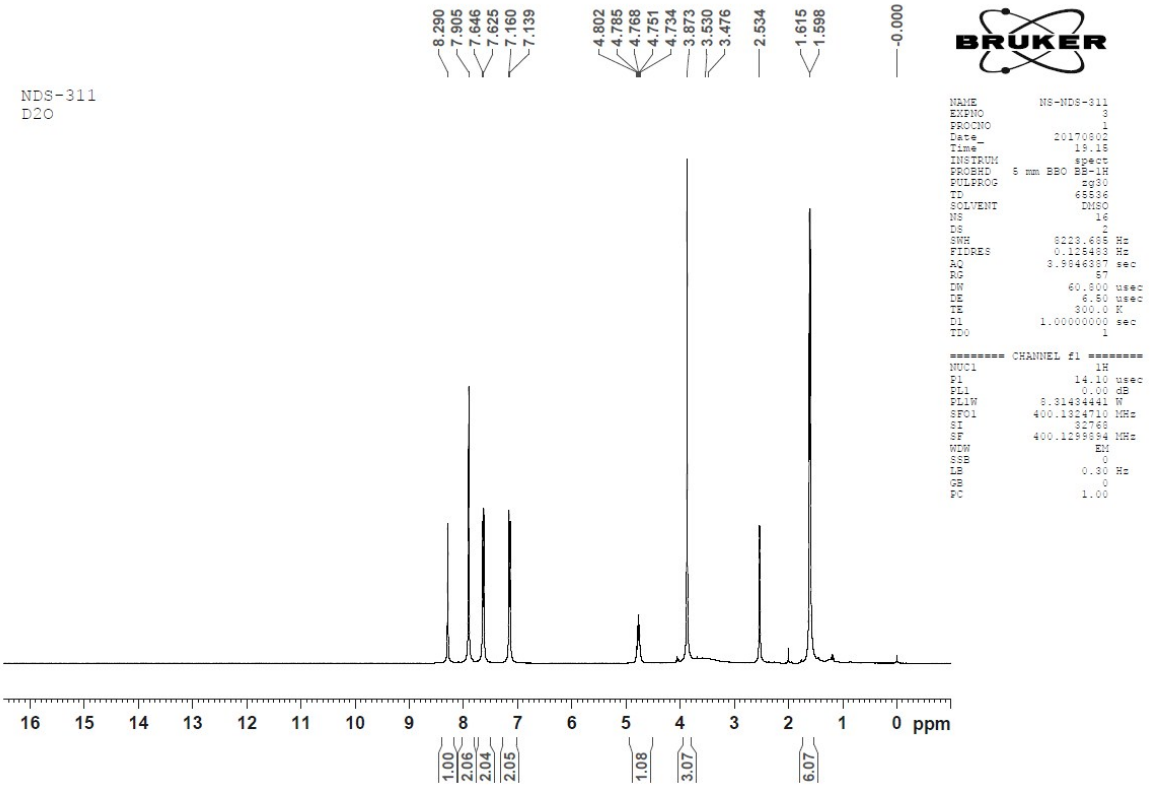
MASS Analysis of synthesized compound: 7k M+1: 282



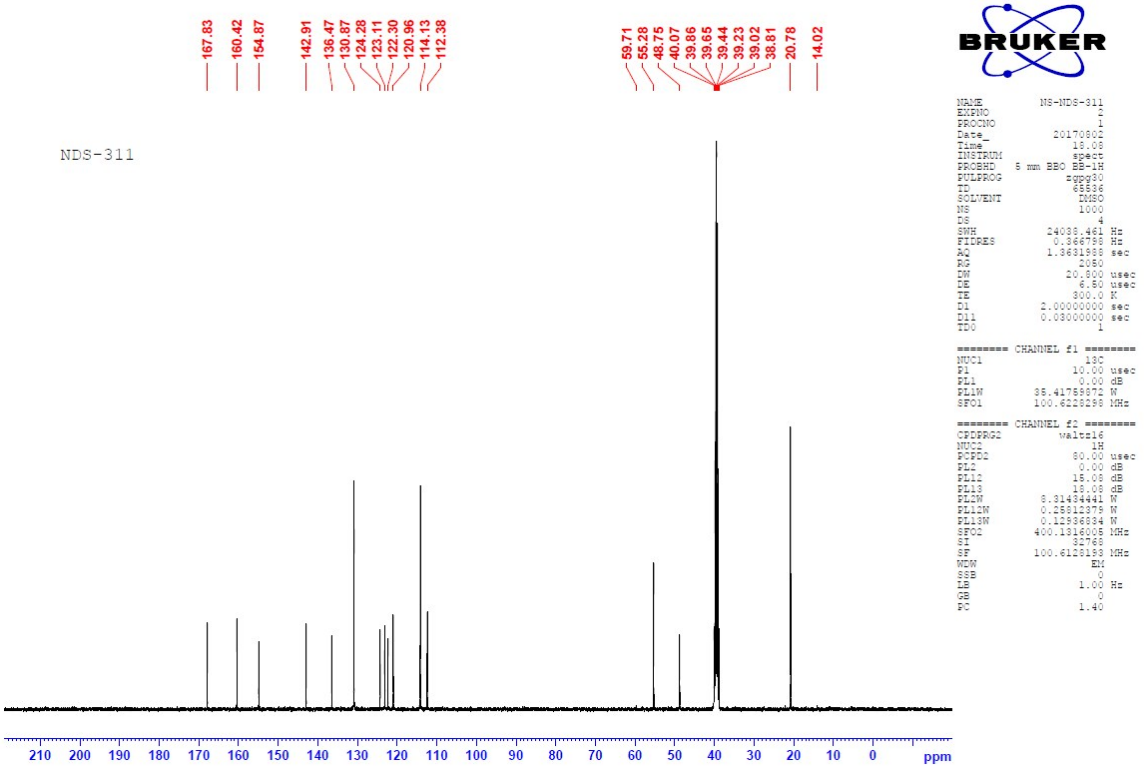
1H-NMR Analysis of synthesized compound: 7k



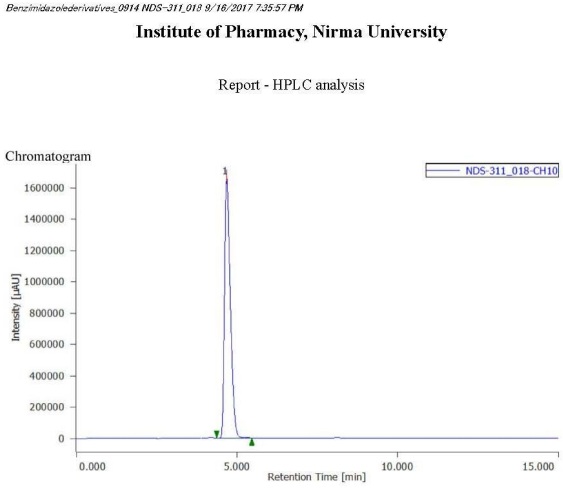
1H-NMR-D2O exchange analysis of synthesized compound: 7k



13C-NMR Analysis of synthesized compound: 7k



HPLC (percentage purity) of 7k



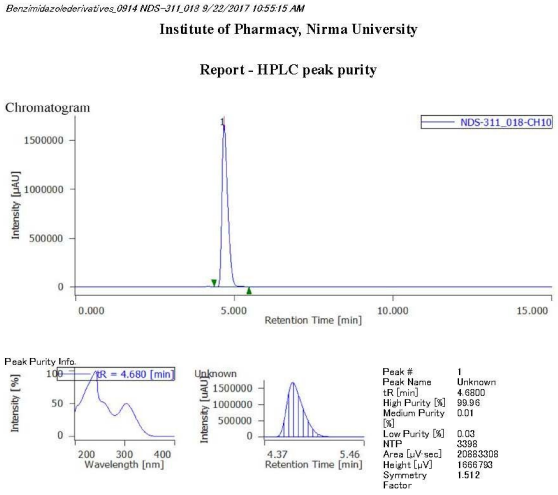
Chromatogram Information

User Name	Administrator
Date Modified	9/14/2017 5:24:15 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 4:23:55 PM
Volume	20.00 [µL]
Sample #	17
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

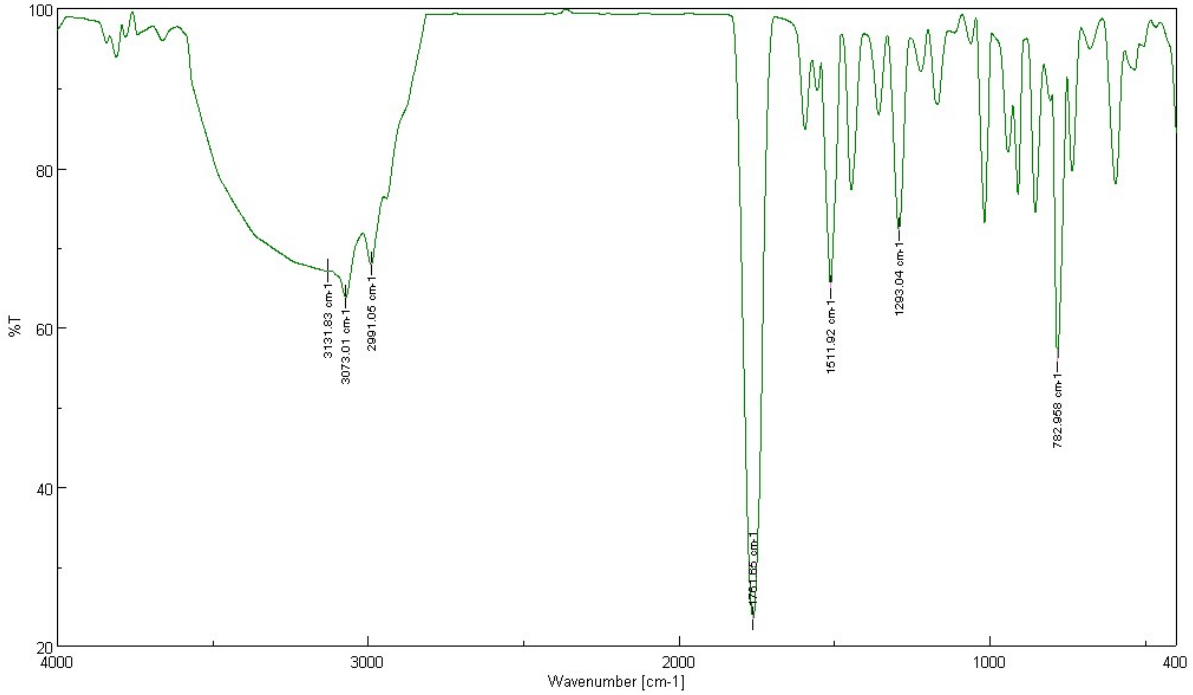
Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.680	20883308	1666793	100.000	100.000	3398	N/A	1.512

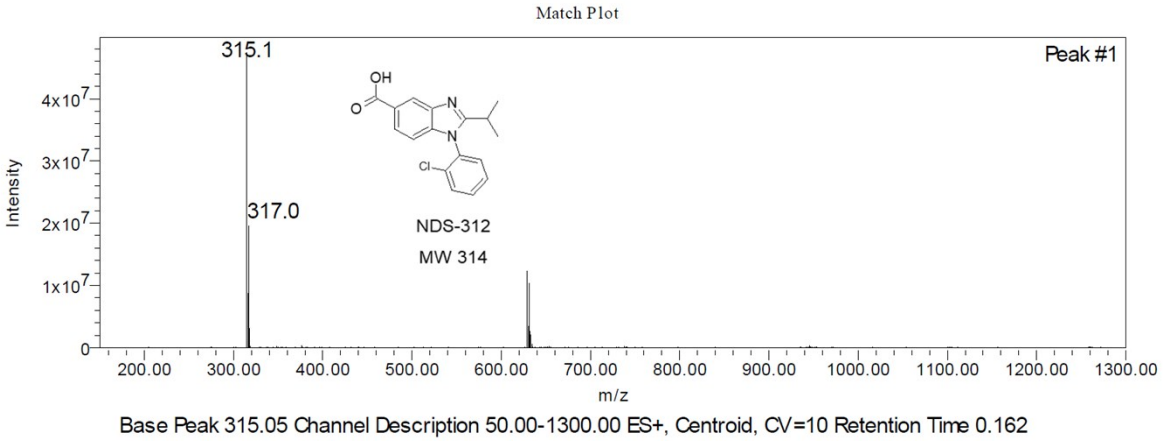
HPLC (peak purity) of 7k



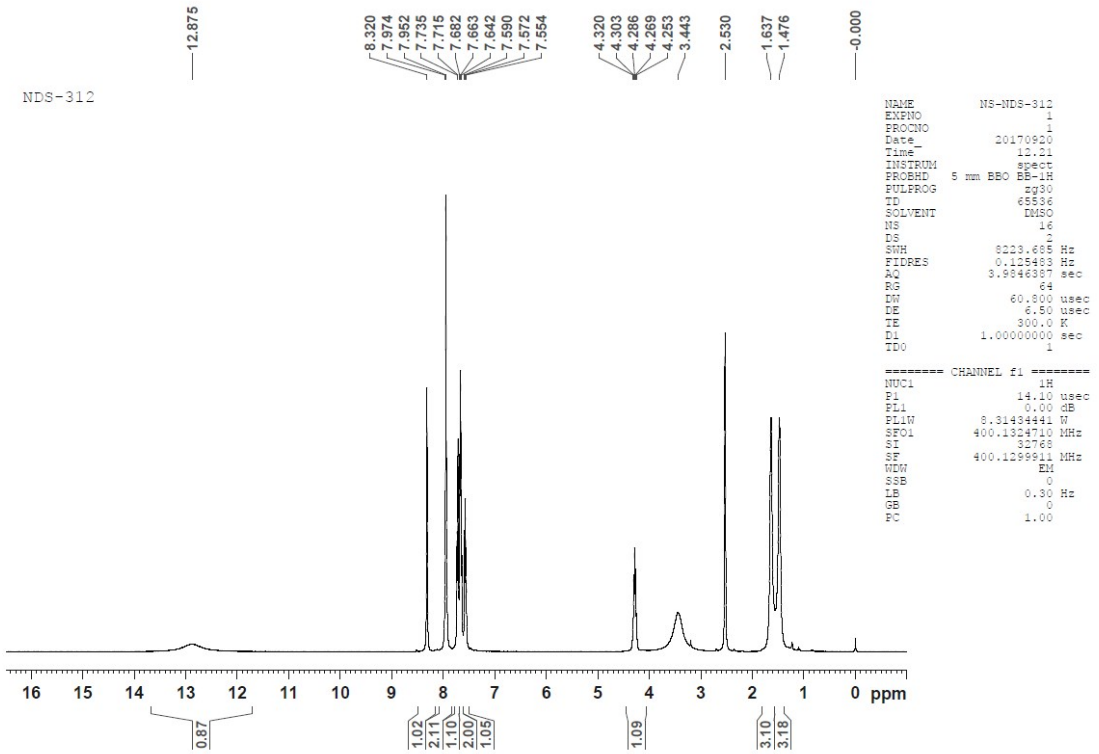
FTIR spectra of 7l



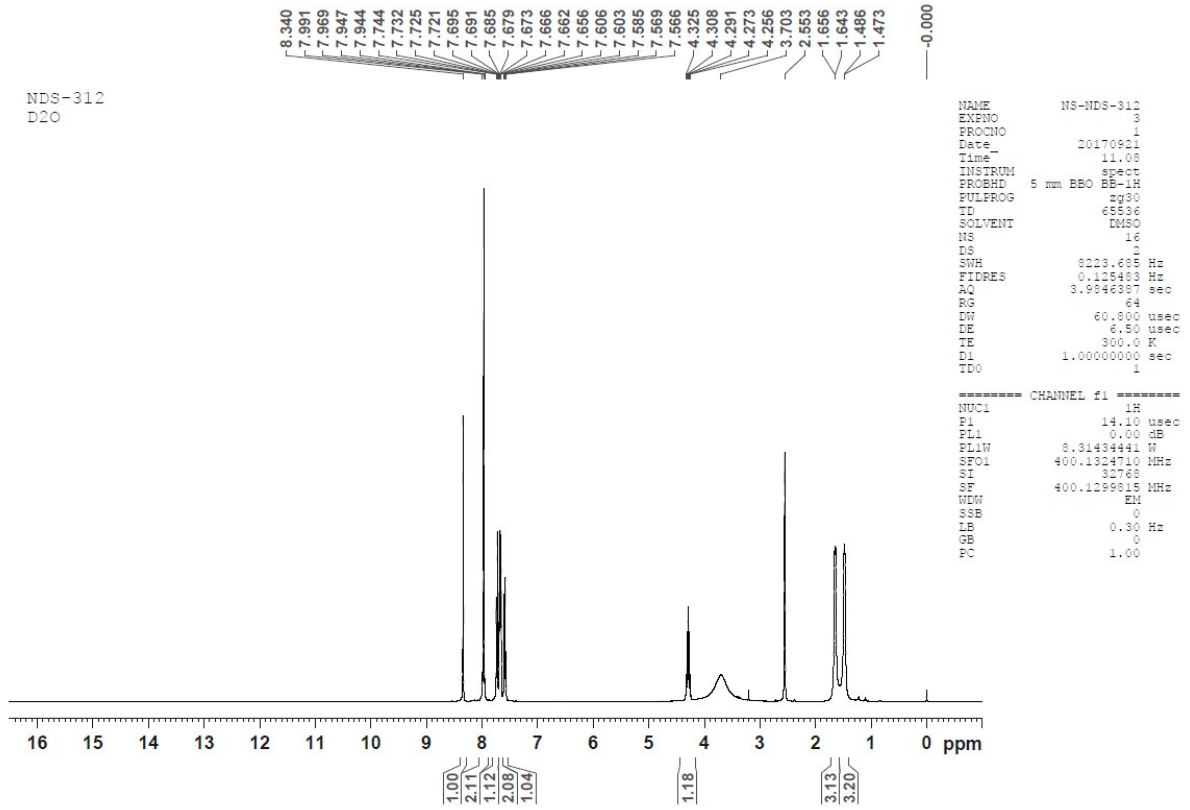
MASS Analysis of synthesized compound: 7l M+1: 315, M+3: 317



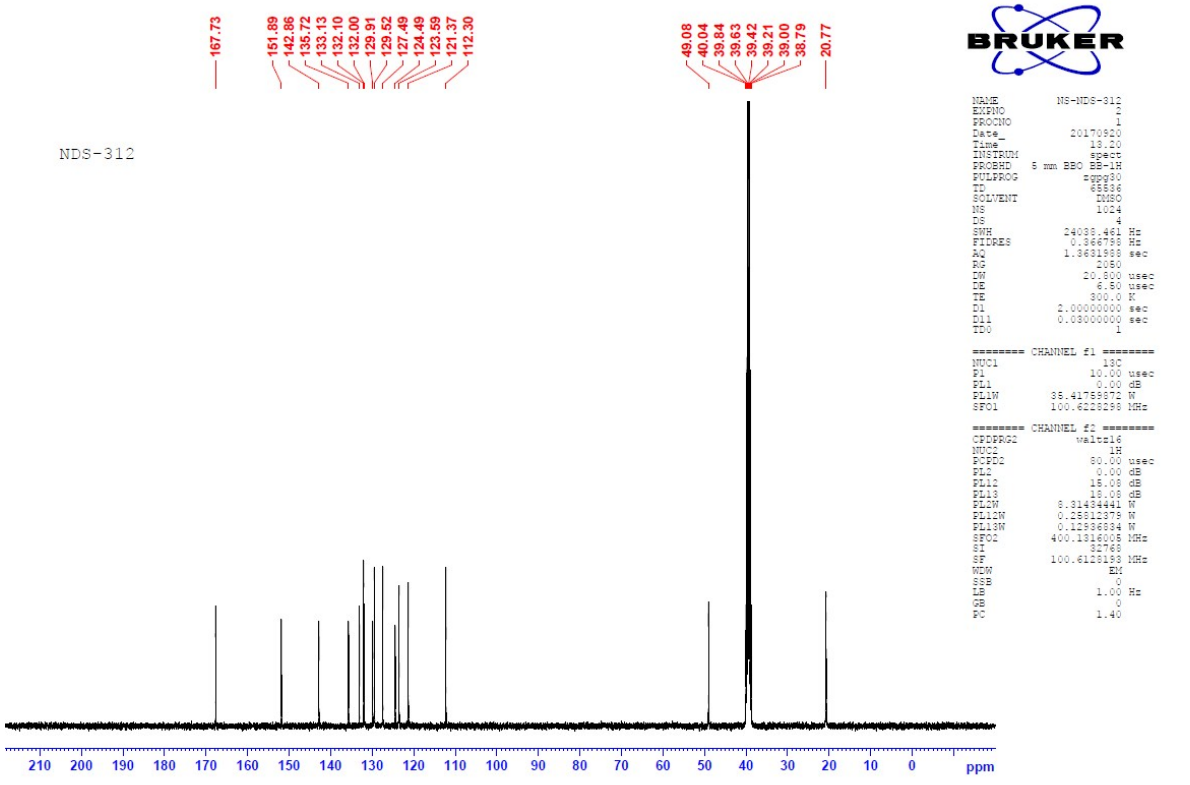
1H-NMR Analysis of synthesized compound: 7l



1H-NMR-D2O exchange analysis of synthesized compound: 7l



13C-NMR Analysis of synthesized compound: 7l

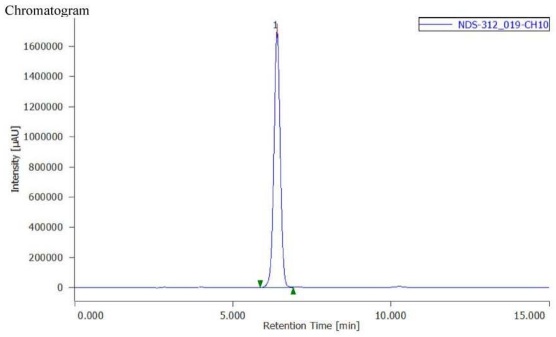


HPLC (percentage purity) of 7l

Benzimidazolederivatives_0914 NDS-312_019 9/16/2017 7:36:14 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information	
User Name	Administrator
Date Modified	9/14/2017 5:24:17 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 4:41:05 PM
Volume	20.00 [µL]
Sample #	18
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

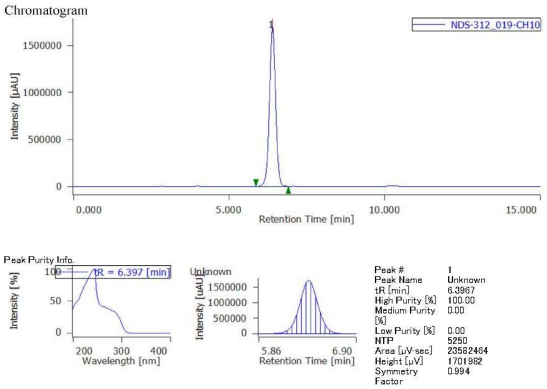
P	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	6.397	23582464	1701982	100.000	100.000	5250	N/A	0.994

HPLC (peak purity) of 7l

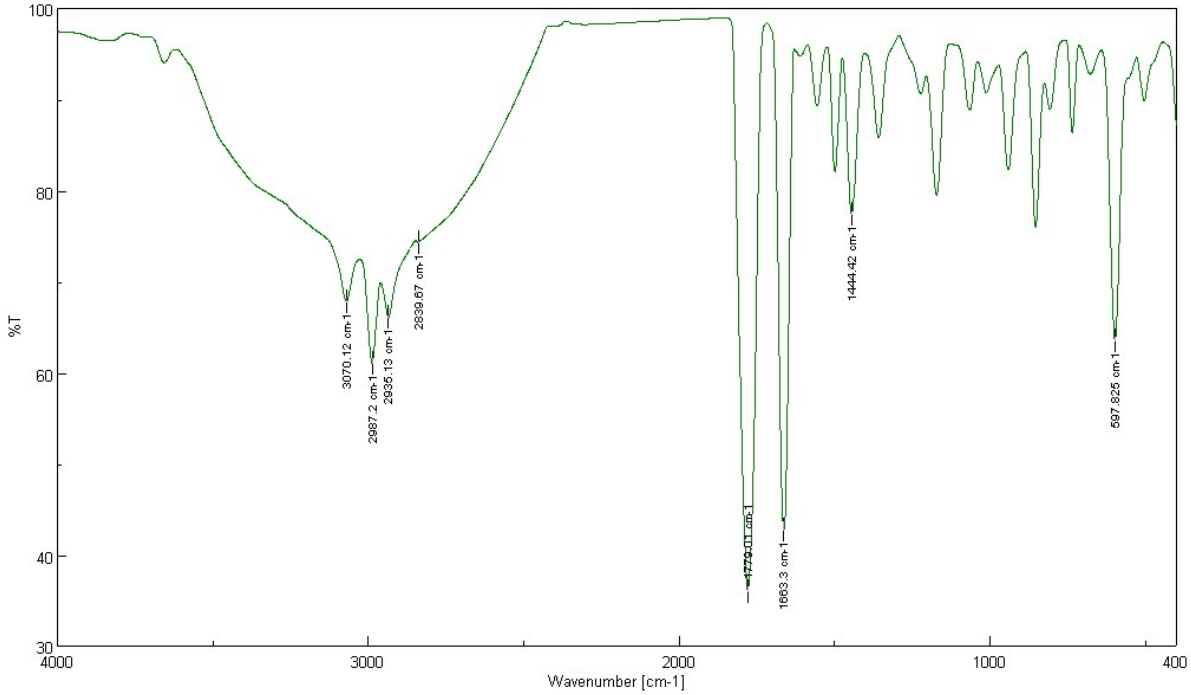
Benzimidazolederivatives_0914 NDS-312_019 9/22/2017 10:55:51 AM

Institute of Pharmacy, Nirma University

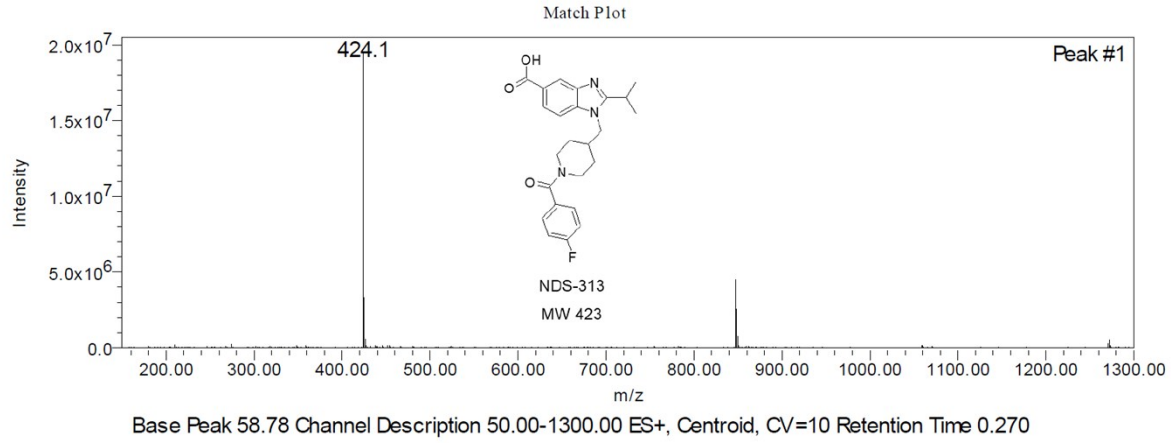
Report - HPLC peak purity



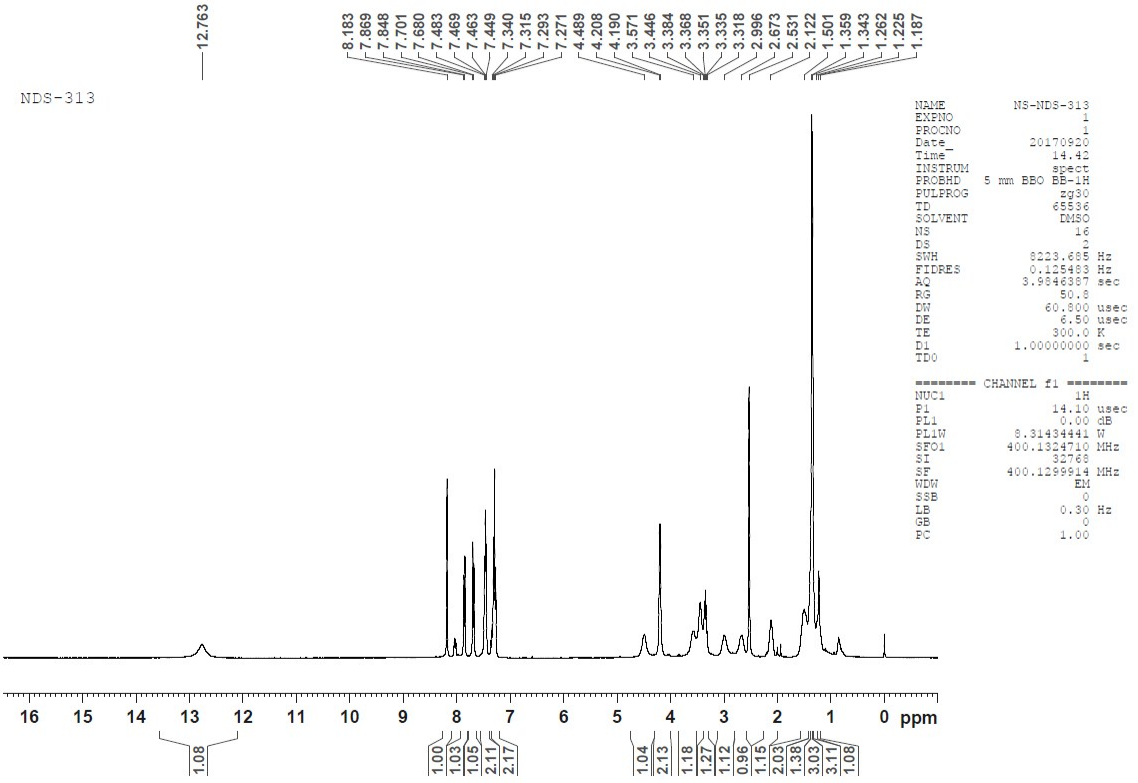
FTIR spectra of 7m



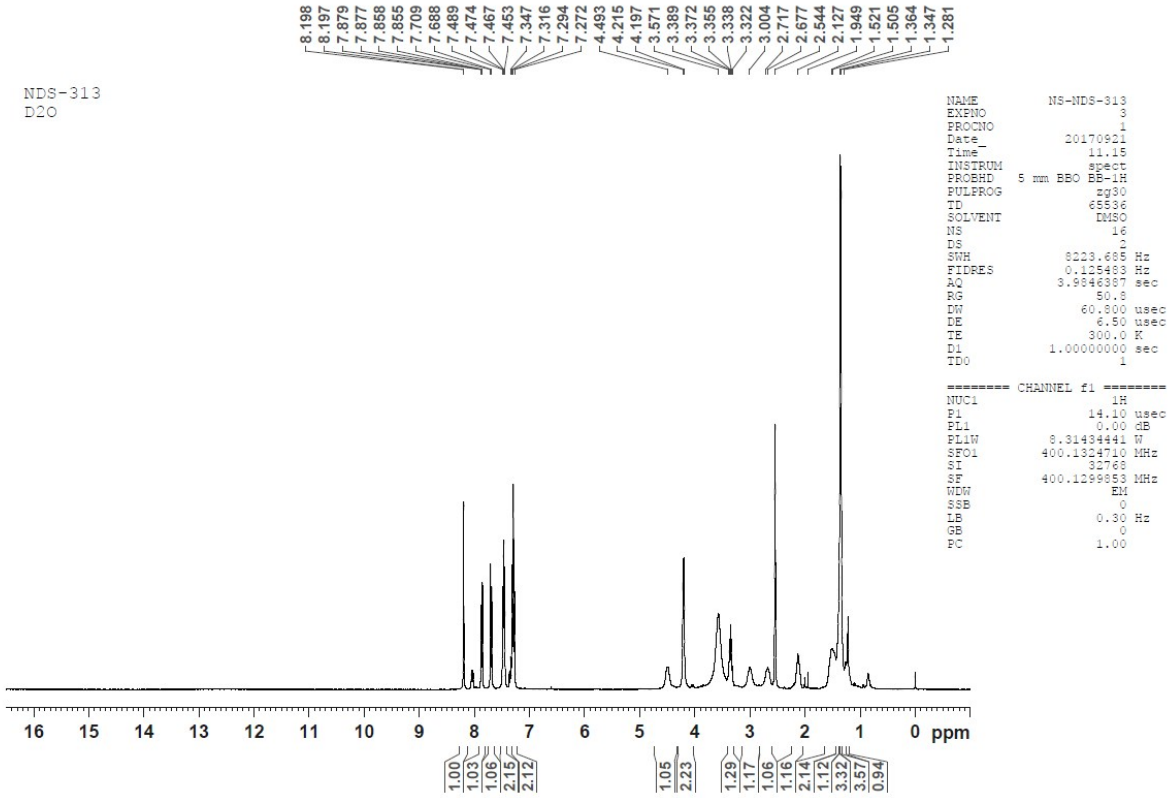
MASS Analysis of synthesized compound: 7m M+1: 424



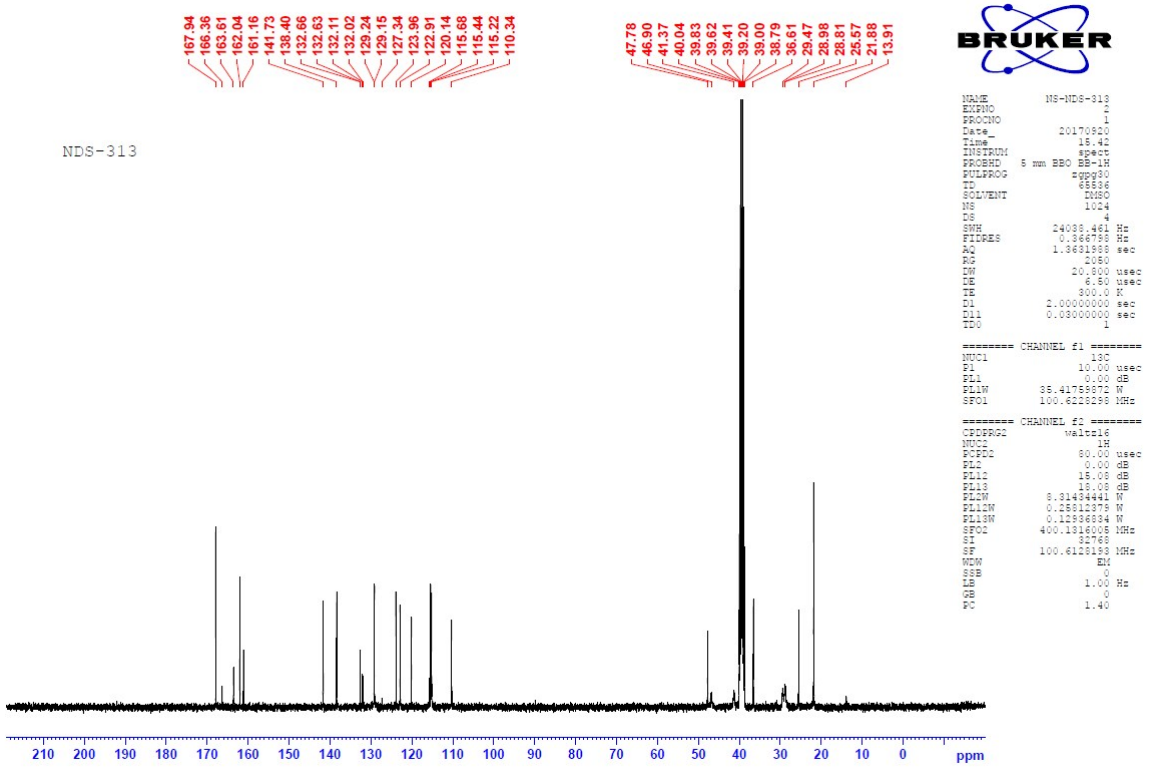
1H-NMR Analysis of synthesized compound: 7m



1H-NMR-D2O exchange analysis of synthesized compound: 7m



13C-NMR Analysis of synthesized compound: 7m



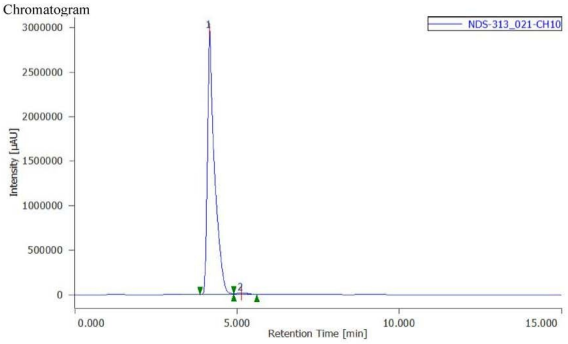
HPLC (percentage purity) of 7m

Benzimidazolederivatives_0914 NDS-313_021 9/16/2017 7:36:37 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis

Chromatogram



Chromatogram Information

User Name	Administrator
Date Modified	9/14/2017 5:32:08 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 5:10:28 PM
Volume	20.00 [µL]
Sample #	20
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.160	44711344	2966155	99.139	99.486	2754	N/A	1.893
2	Unknown	10	5.143	388208	15324	0.861	0.514	599	N/A	N/A

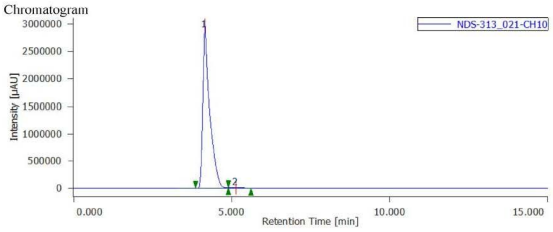
HPLC (peak purity) of 7m

Benzimidazolederivatives_0914 NDS-313_021 9/22/2017 10:56:12 AM

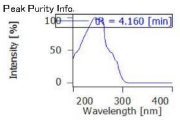
Institute of Pharmacy, Nirma University

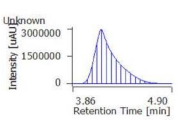
Report - HPLC peak purity

Chromatogram

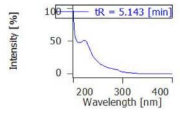


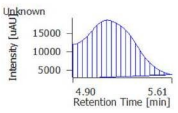
Peak Purity Info





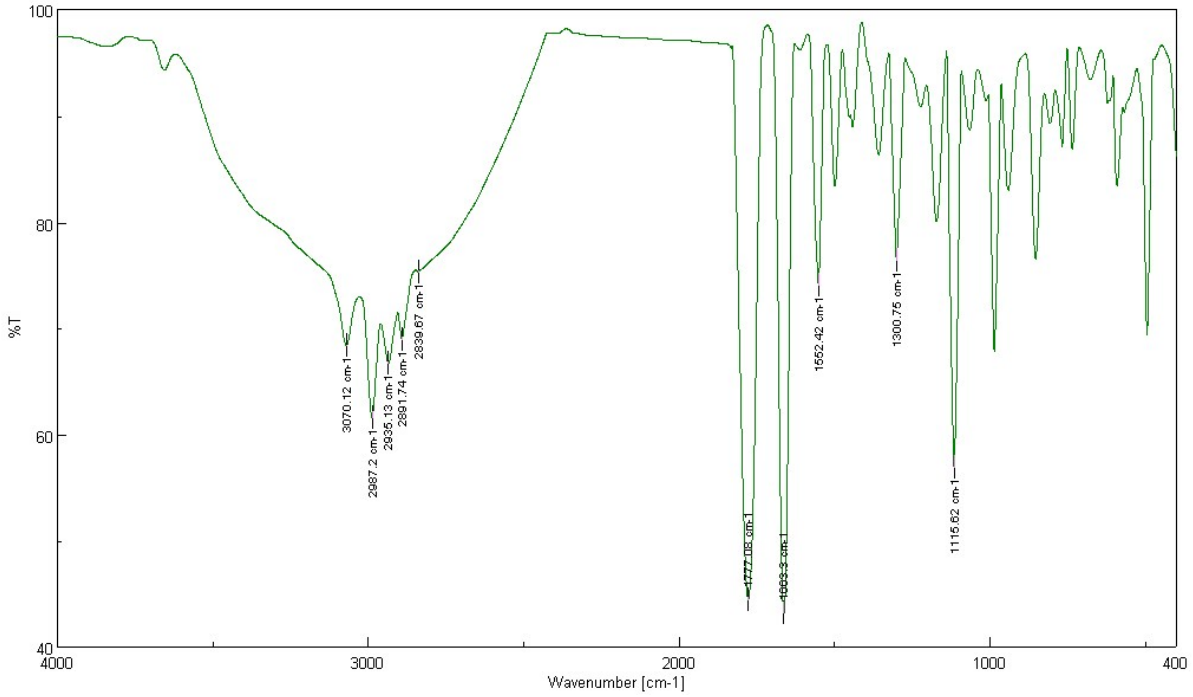
Peak #	1
Peak Name	Unknown
tR [min]	4.1600
High Purity [%]	99.86
Medium Purity [%]	0.00
Low Purity [%]	0.04
NTP	2754
Area [µV·sec]	44711344
Height [µV]	2966155
Symmetry Factor	1.893



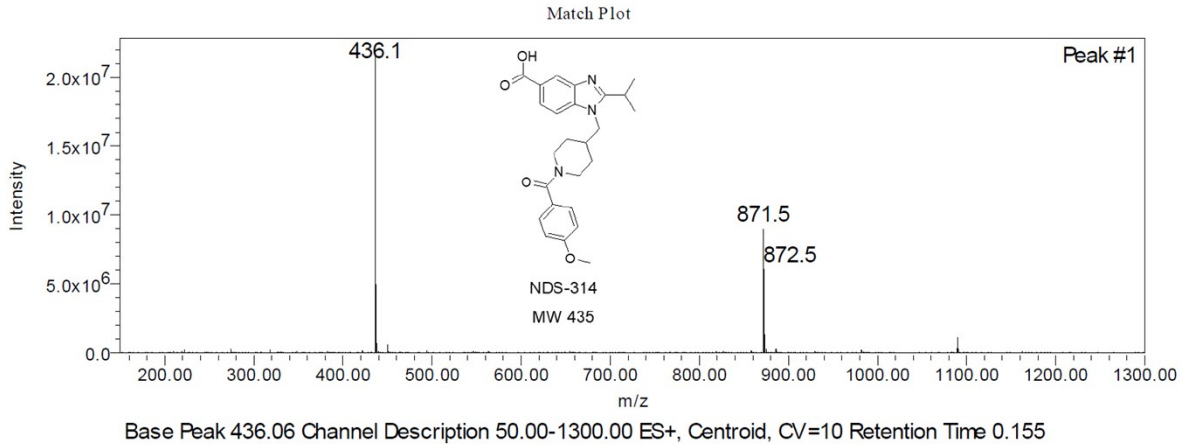


Peak #	2
Peak Name	Unknown
tR [min]	5.1433
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	599
Area [µV·sec]	388208
Height [µV]	15324
Symmetry Factor	N/A

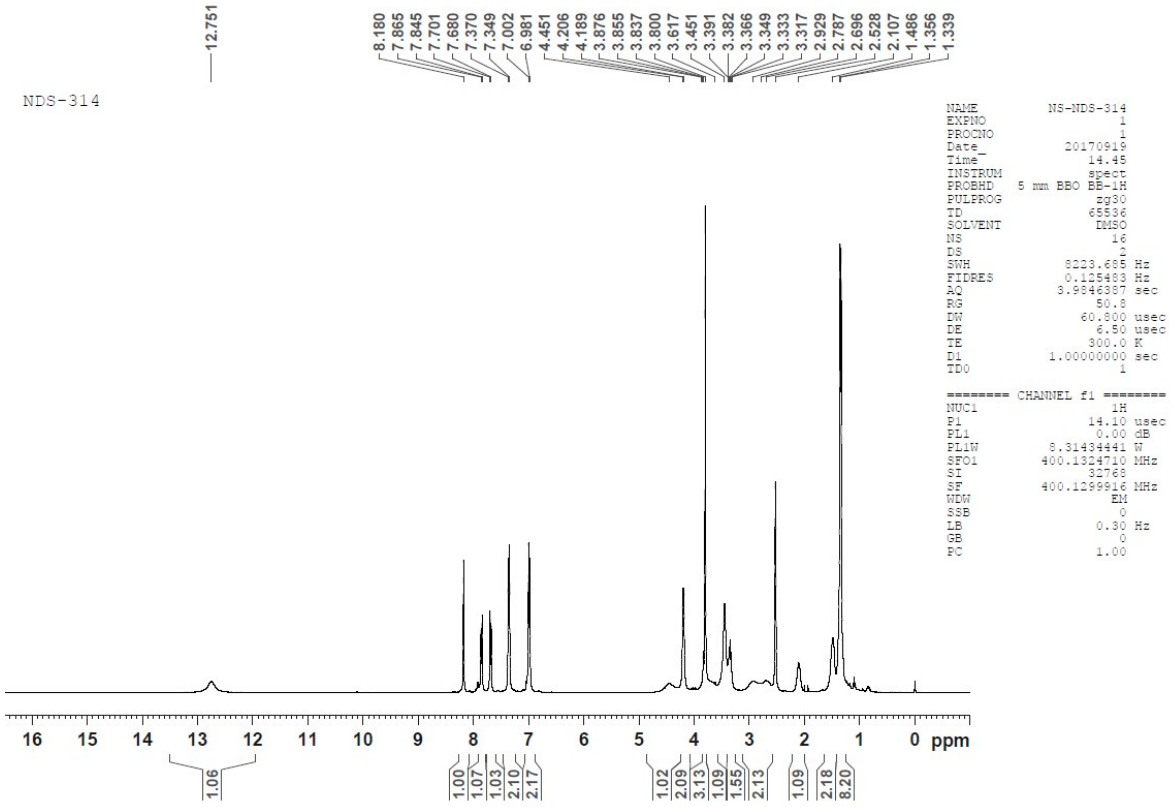
FTIR spectra of 7n



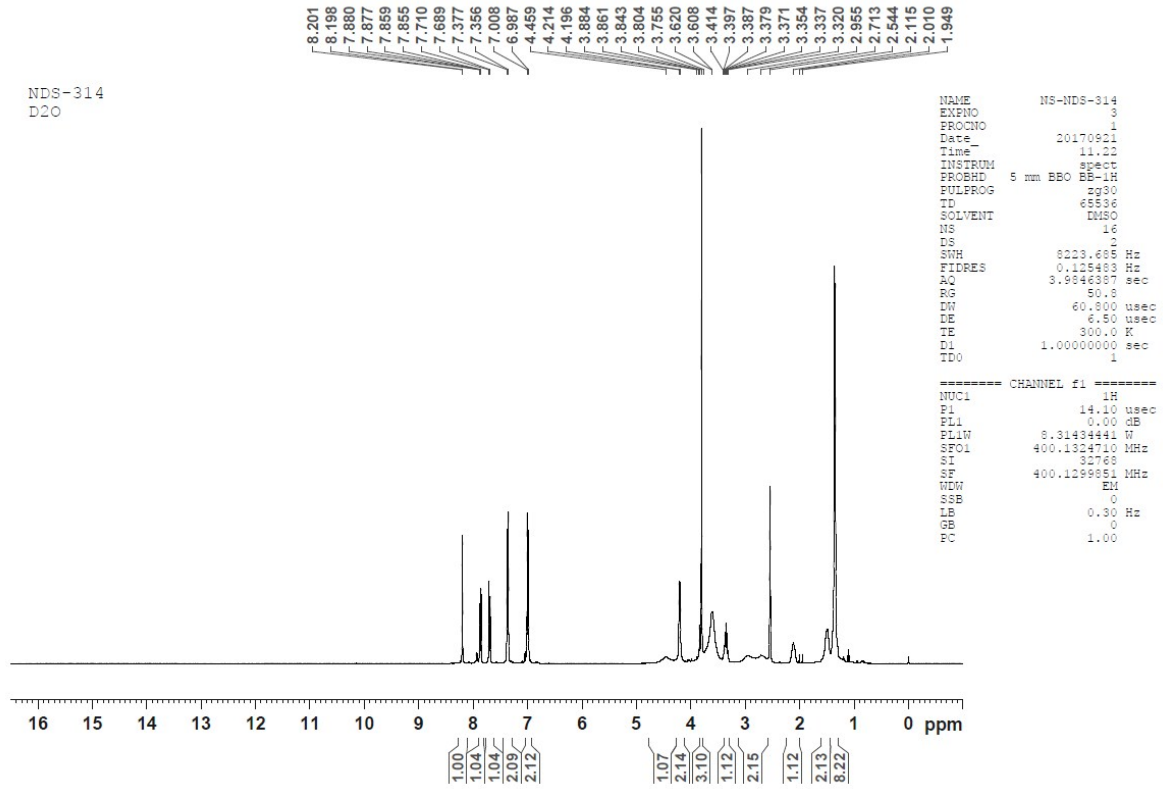
MASS Analysis of synthesized compound: 7n M+1: 436



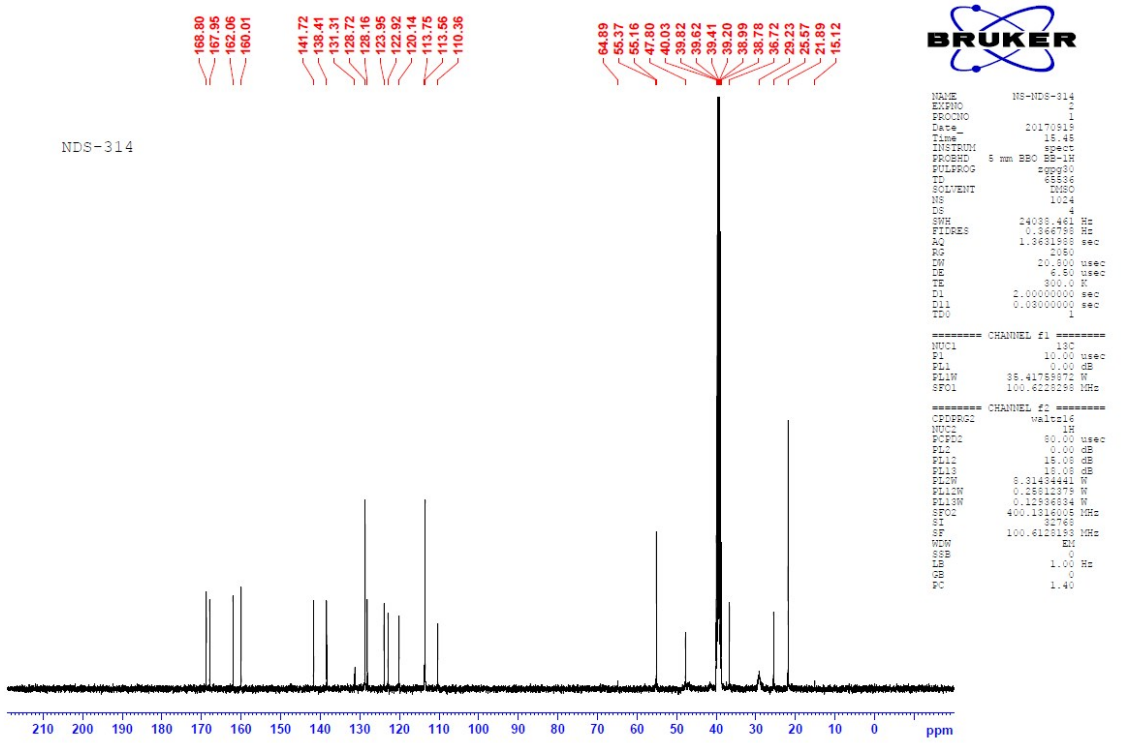
1H-NMR Analysis of synthesized compound: 7n



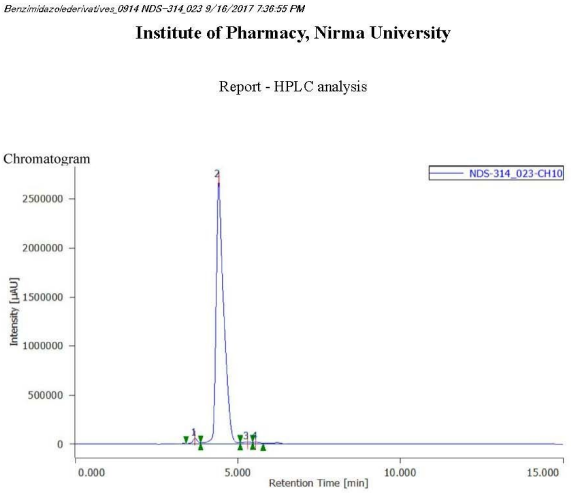
1H-NMR-D2O exchange analysis of synthesized compound: 7n



13C-NMR Analysis of synthesized compound: 7n



HPLC (percentage purity) of 7n



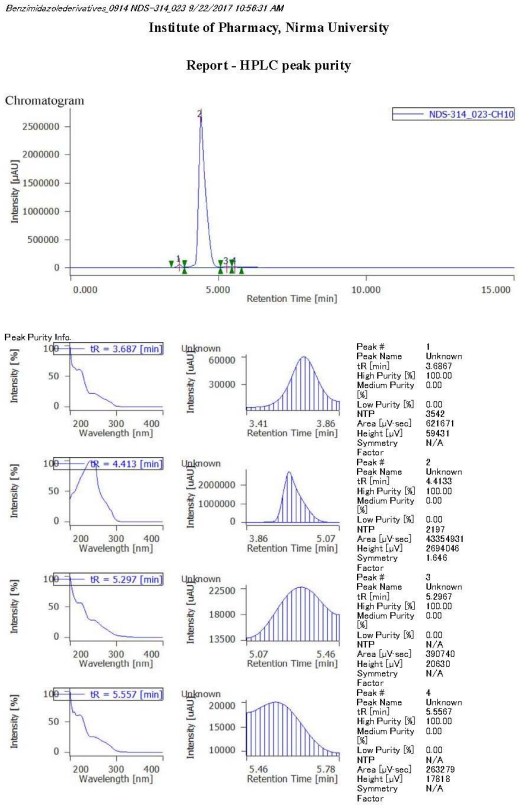
Chromatogram Information

User Name	Administrator
Date Modified	9/14/2017 6:43:51 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 5:37:11 PM
Volume	20.00 [µL]
Sample #	22
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

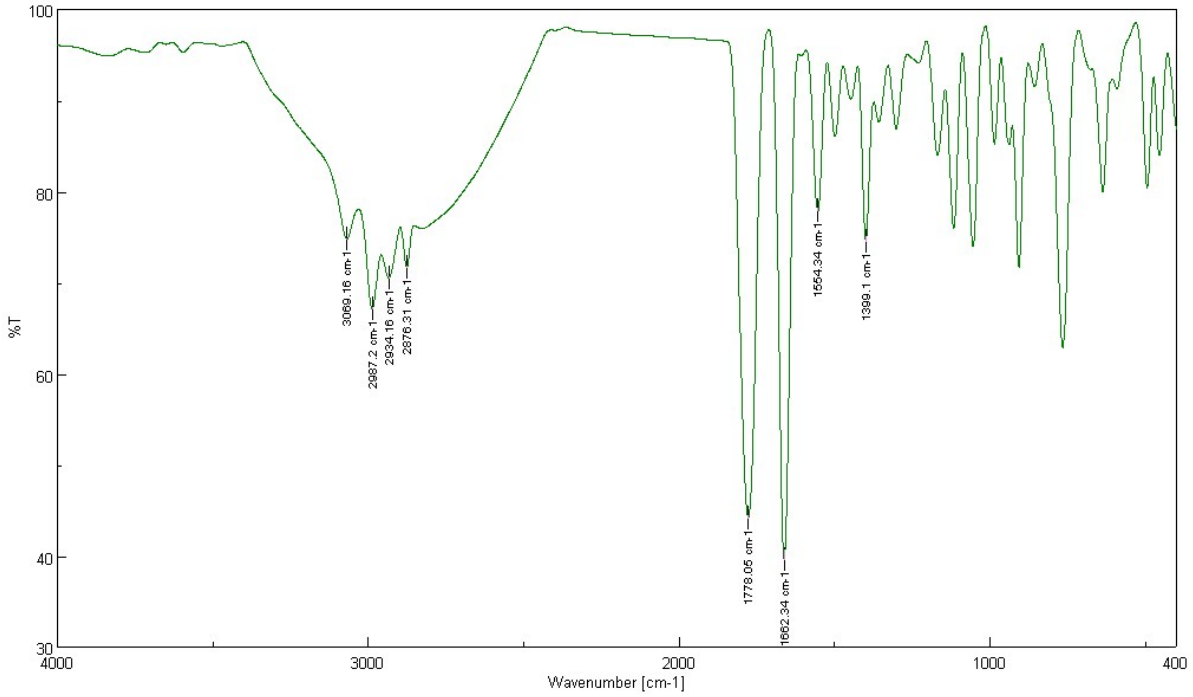
Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.687	621671	59431	1.393	2.129	3542	2.211	N/A
2	Unknown	10	4.413	43354931	2694046	97.142	96.494	2197	N/A	1.646
3	Unknown	10	5.297	390740	20630	0.875	0.739	N/A	N/A	N/A
4	Unknown	10	5.557	263279	17818	0.590	0.638	N/A	N/A	N/A

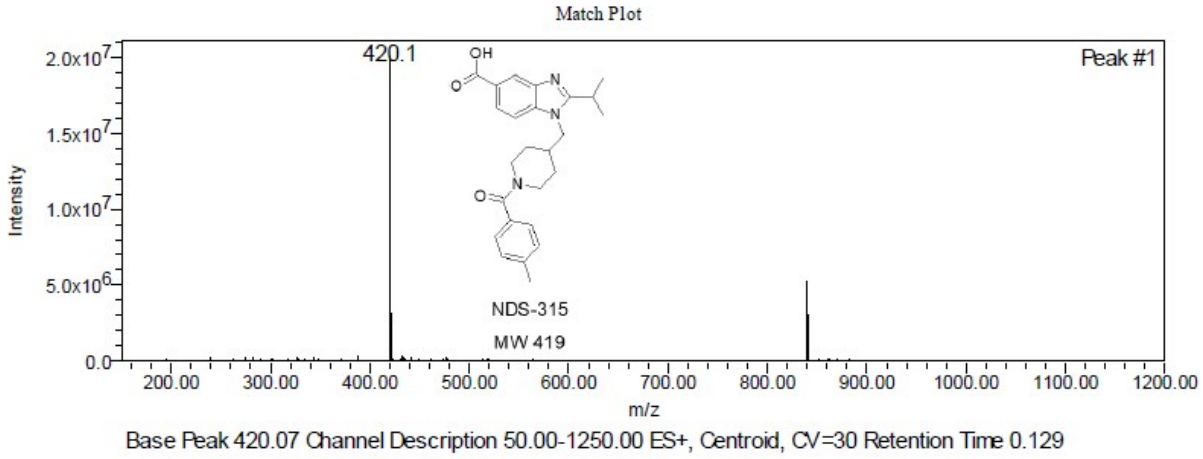
HPLC (peak purity) of 7n



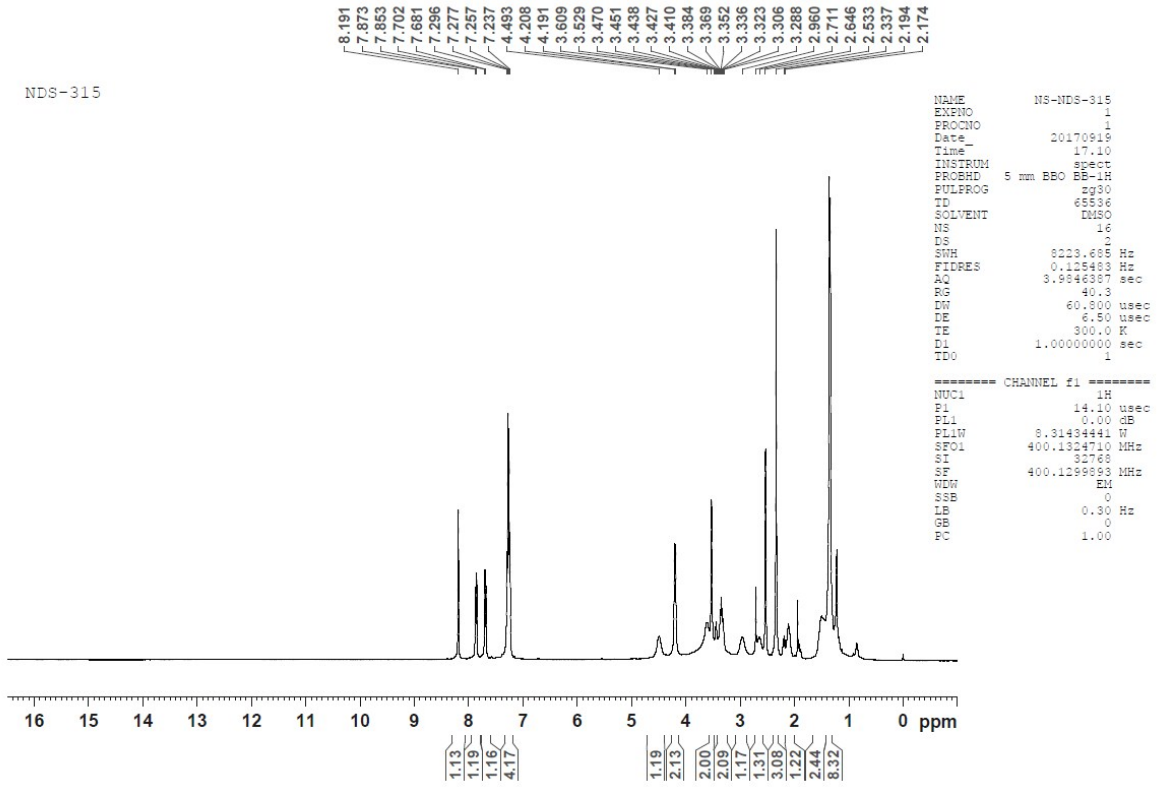
FTIR spectra of 7o



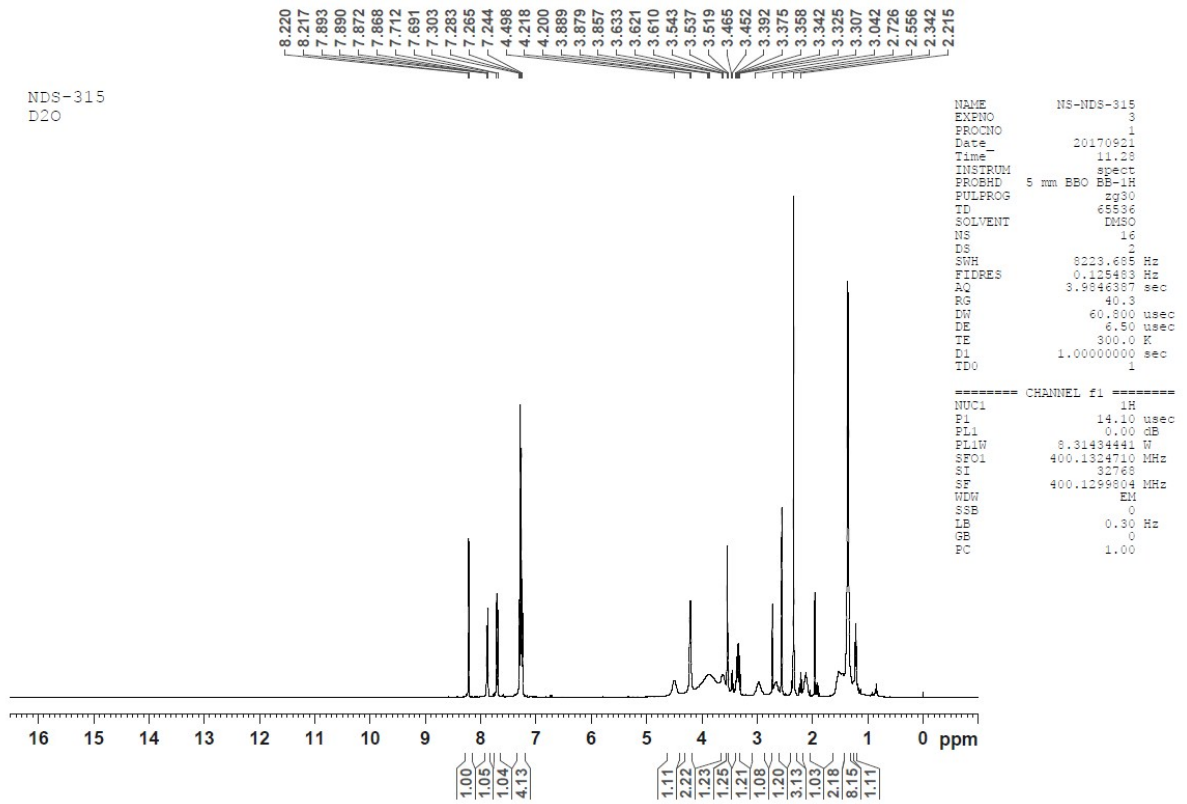
MASS Analysis of synthesized compound: 7o M+1: 420



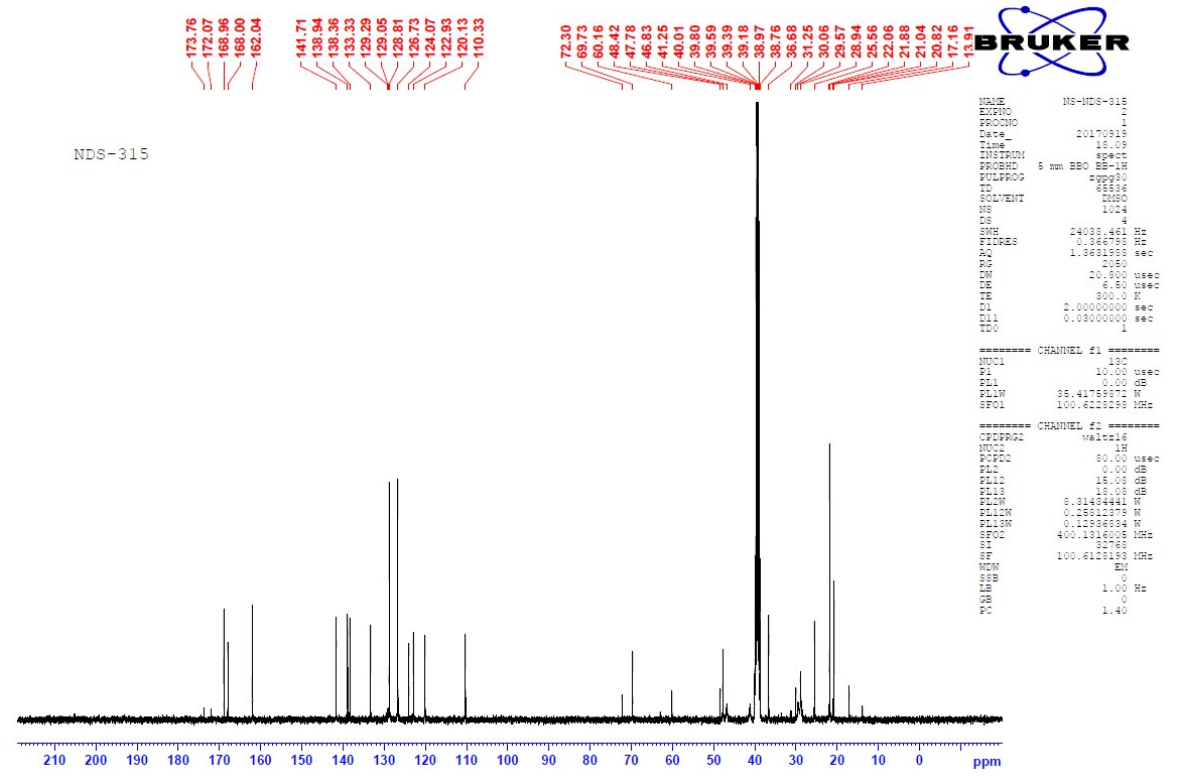
1H-NMR Analysis of synthesized compound: 7o



1H-NMR-D2O exchange analysis of synthesized compound: 7o



13C-NMR Analysis of synthesized compound: 7o



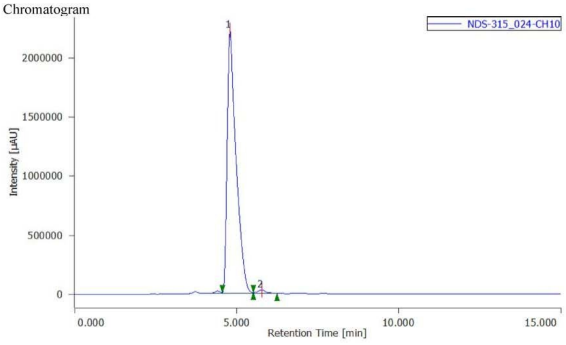
HPLC (percentage purity) of 7o

Benzimidazolederivatives_0914 NDS-315_024 9/16/2017 7:37:14 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis

Chromatogram



Chromatogram Information

User Name	Administrator
Date Modified	9/14/2017 7:11:45 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/14/2017 5:55:03 PM
Volume	20.00 [µL]
Sample #	23
Project Name	DST
Acquisition Time	15.0 [min]
Acquisition Sequence	
Control Method	15min6040meohbuffer1.0mlpermin
Peak ID Table	

Peak Information

#	Peak Name	CH	tR [min]	Area [µV sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.797	42213264	2224509	98.737	98.704	1757	2.070	1.870
2	Unknown	10	5.777	540124	29202	1.263	1.296	2613	N/A	N/A

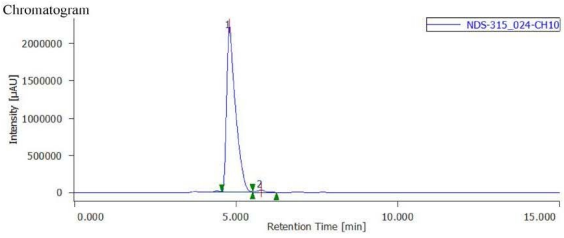
HPLC (peak purity) of 7o

Benzimidazolederivatives_0914 NDS-315_024 9/22/2017 10:56:48 AM

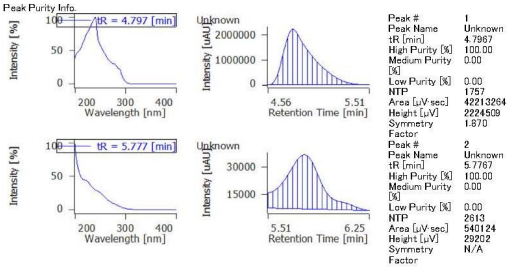
Institute of Pharmacy, Nirma University

Report - HPLC peak purity

Chromatogram

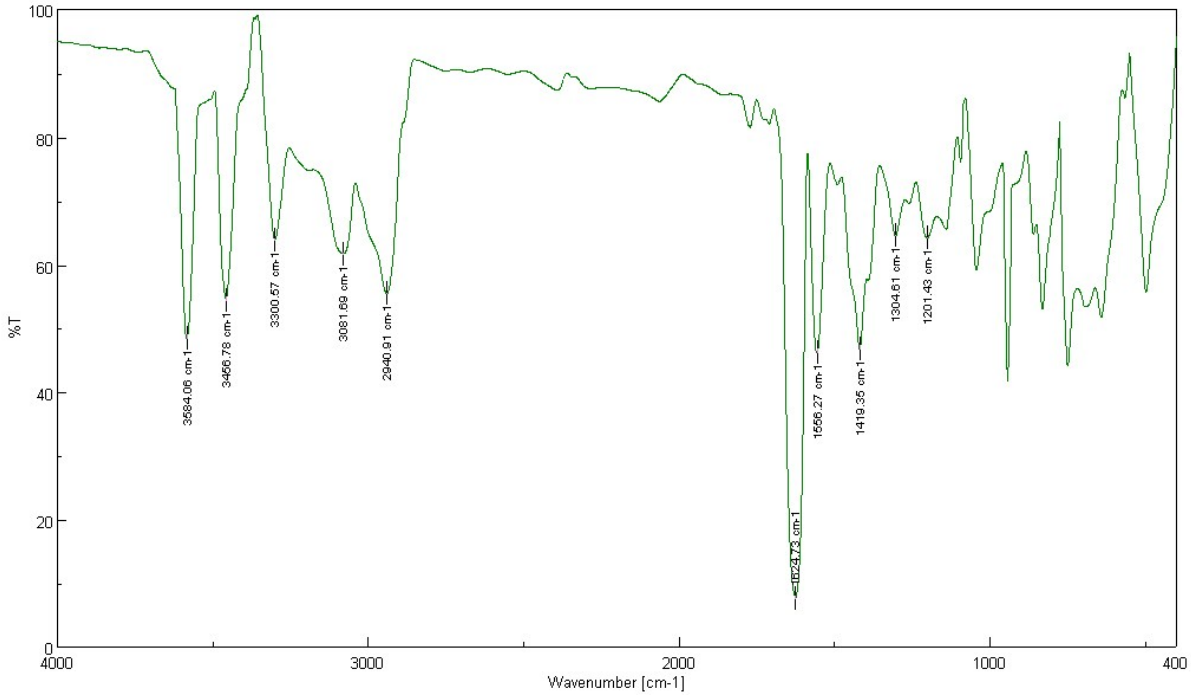


Peak Purity Info

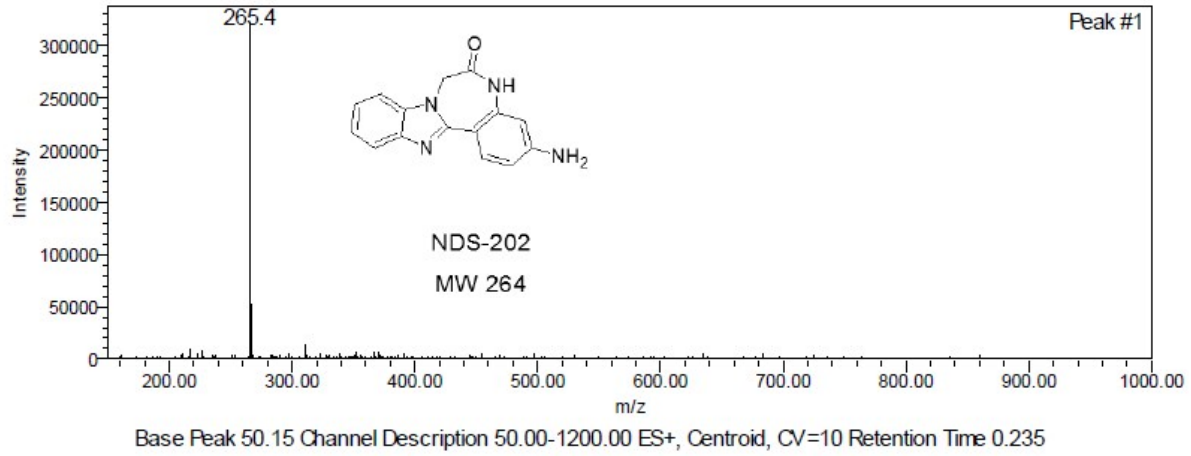


Spectral Data for Series 2

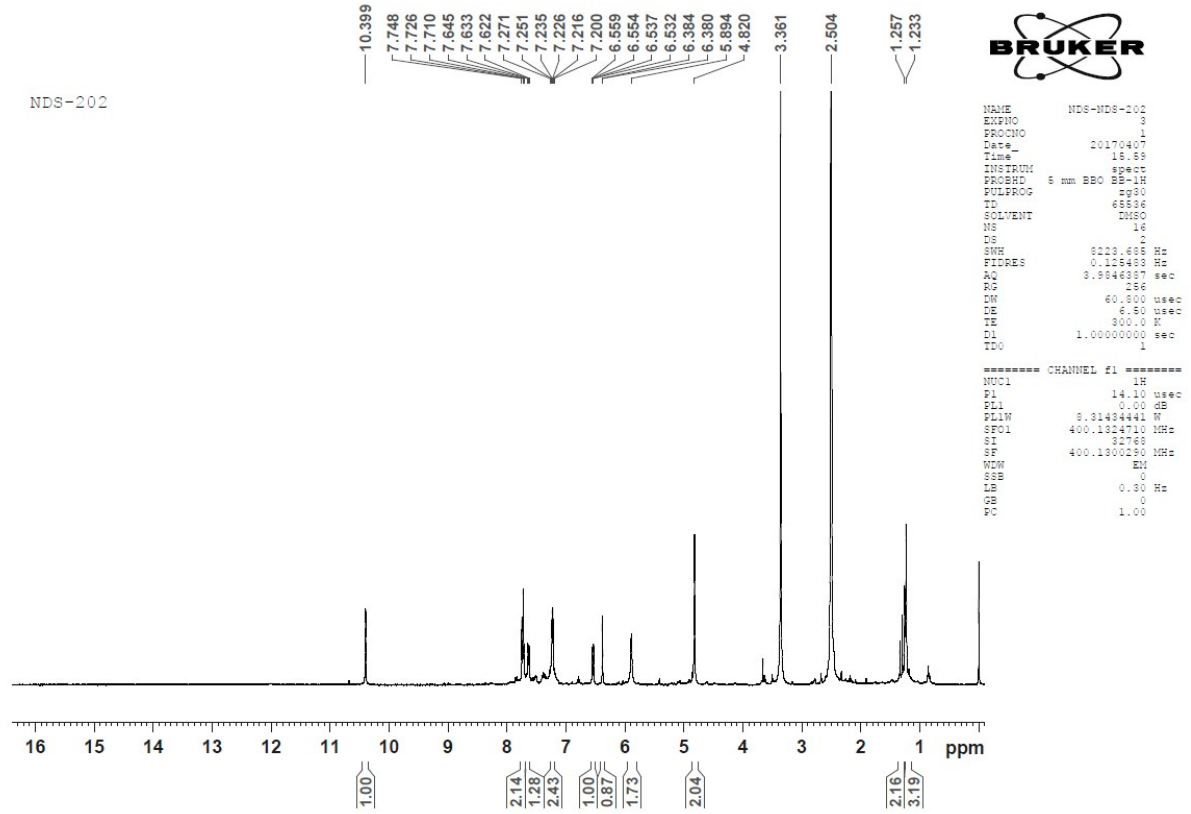
FTIR spectra of 16



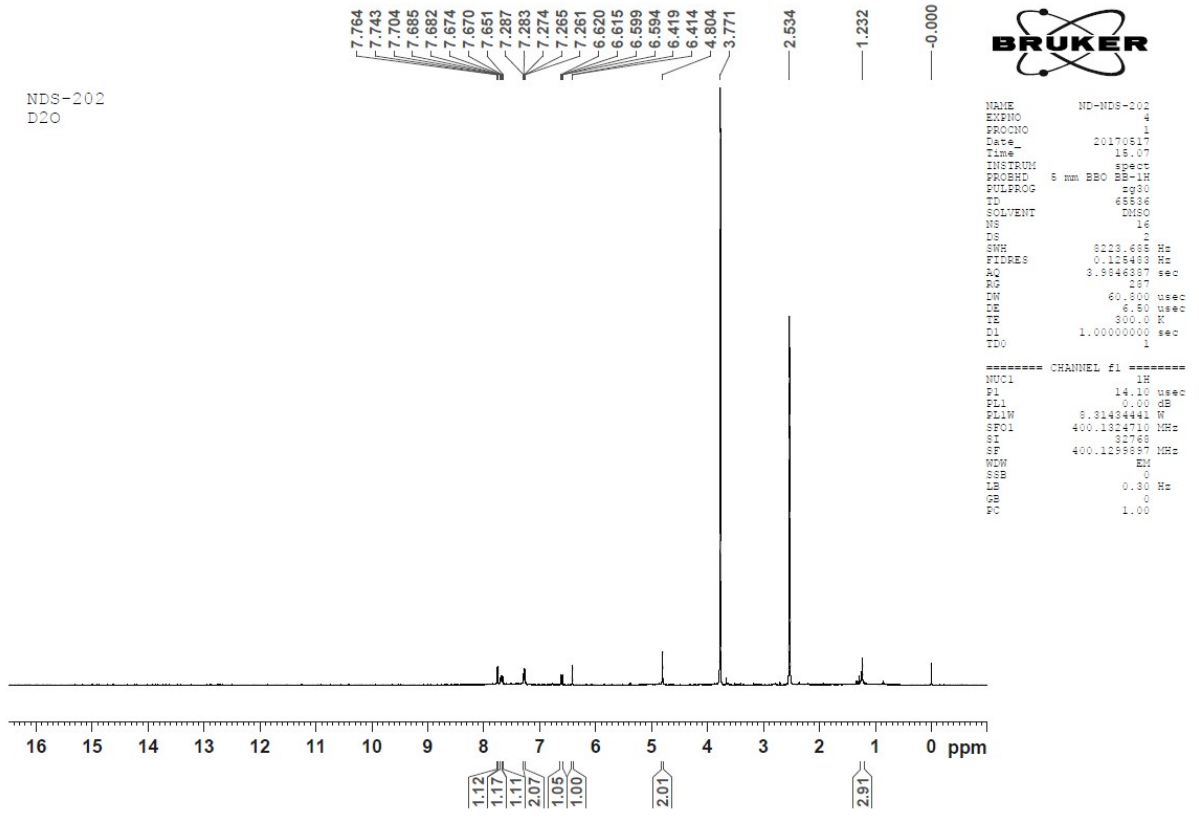
MASS Analysis of synthesized compound: 16 M+1: 265



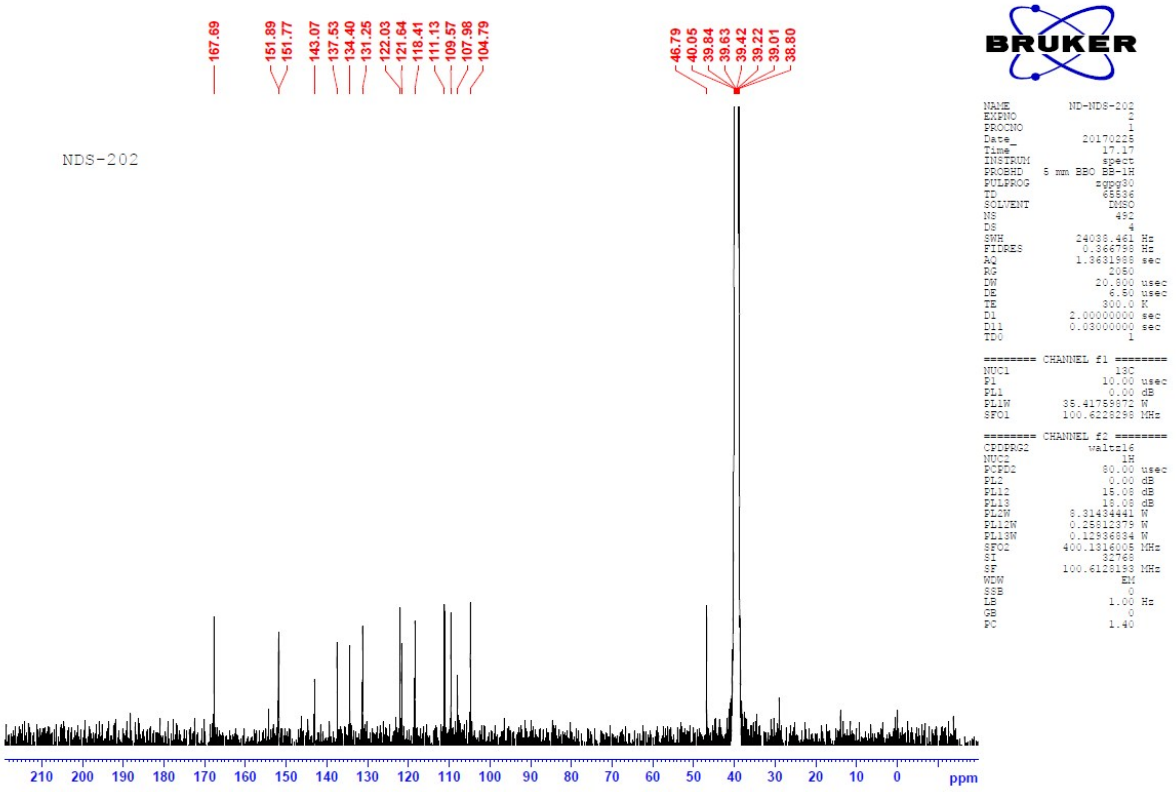
1H-NMR Analysis of synthesized compound: 16



1H-NMR-D2O exchange analysis of synthesized compound: 16



13C-NMR Analysis of synthesized compound: 16

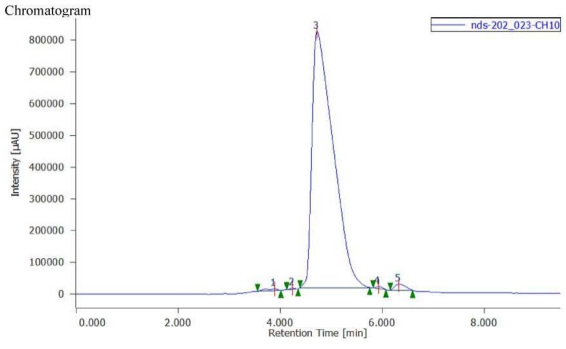


HPLC (percentage purity) of 16

Benzimidazole derivatives_0915 nds-202_023 9/16/2017 7:15:33 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

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Injection Date	9/15/2017 5:11:00 PM
Volume	20.00 [µL]
Sample #	20
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

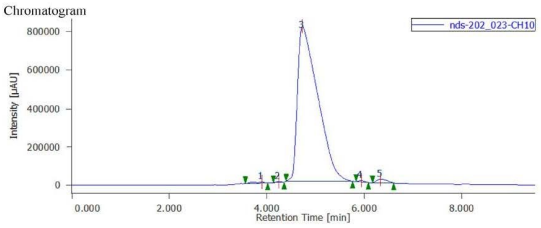
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.893	98792	6073	0.417	0.721	702	0.979	0.651
2	Unknown	10	4.247	26430	3927	0.111	0.466	7533	0.988	0.864
3	Unknown	10	4.727	23257571	807286	98.063	95.777	615	2.397	2.341
4	Unknown	10	5.933	56784	7054	0.239	0.837	10934	1.219	1.192
5	Unknown	10	6.333	277399	18543	1.170	2.200	3244	N/A	1.292

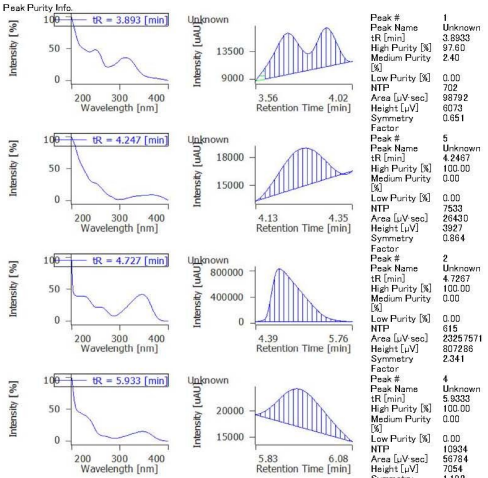
HPLC (peak purity) of 16

Benzimidazole derivatives_0915 nds-202_023 9/22/2017 10:23:11 AM

Institute of Pharmacy, Nirma University

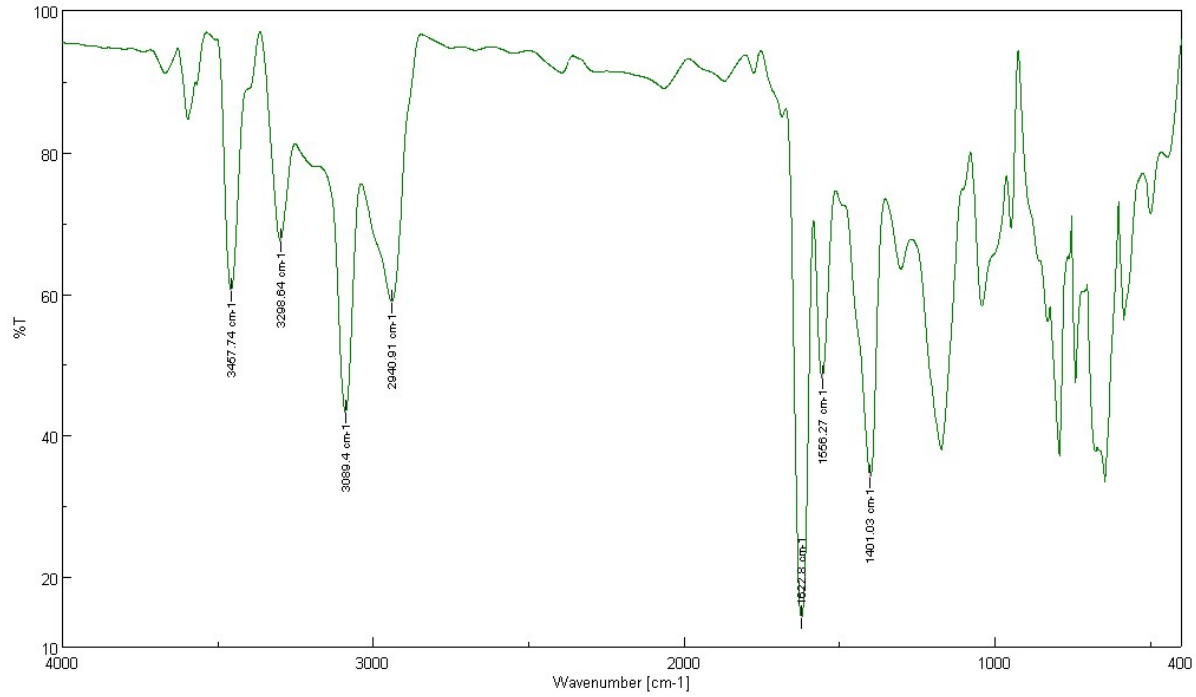
Report - HPLC peak purity



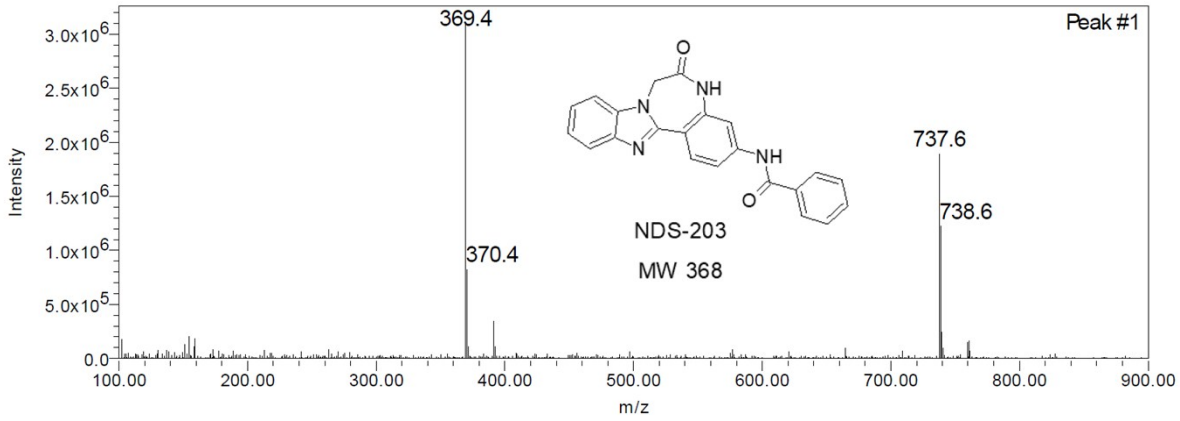


Peak #	1
Peak Name	Unknown
tR [min]	3.8933
High Purity [%]	97.60
Medium Purity [%]	2.40
Low Purity [%]	0.00
NTP	702
Area [µV·sec]	98792
Height [µV]	6073
Symmetry Factor	0.651
Peak #	5
Peak Name	Unknown
tR [min]	4.2467
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	7533
Area [µV·sec]	26430
Height [µV]	3927
Symmetry Factor	0.864
Peak #	2
Peak Name	Unknown
tR [min]	4.7267
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	615
Area [µV·sec]	23257571
Height [µV]	807286
Symmetry Factor	2.341
Peak #	4
Peak Name	Unknown
tR [min]	5.9333
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	10934
Area [µV·sec]	56784
Height [µV]	7054
Symmetry Factor	1.192

FTIR spectra of 17a

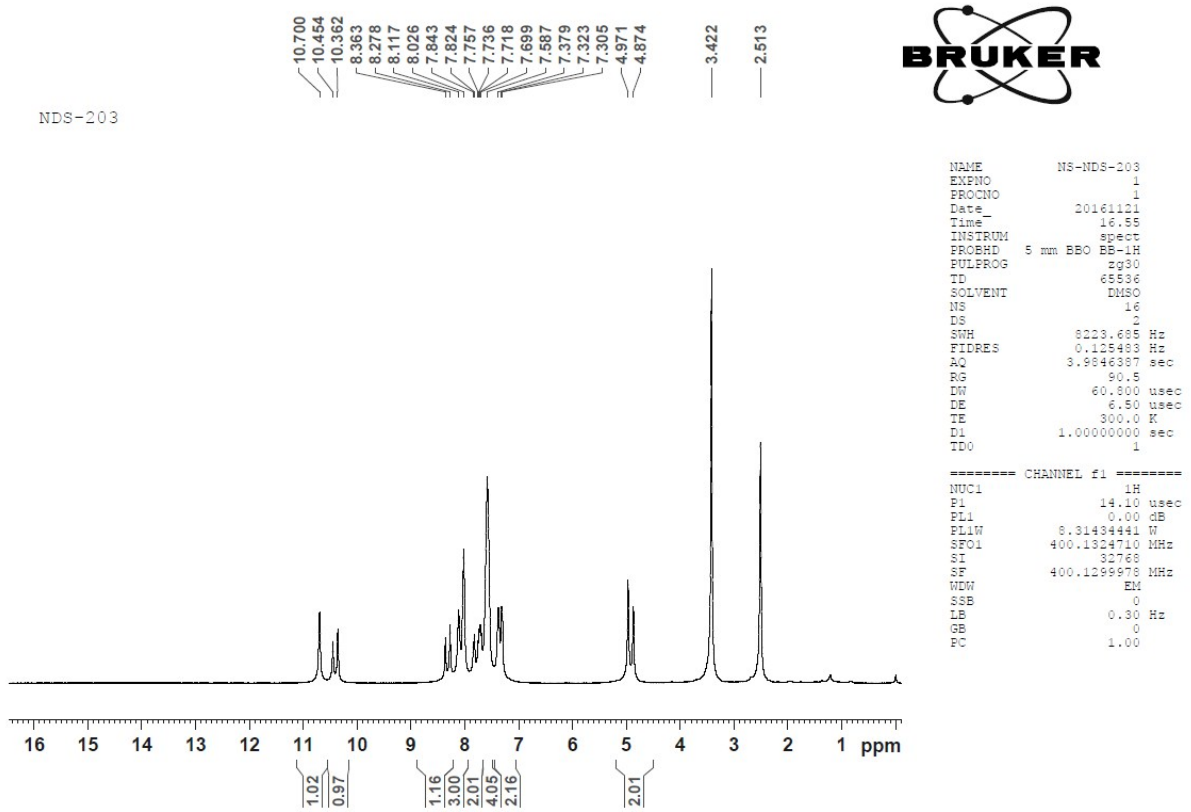


MASS Analysis of synthesized compound: 17a M+1: 369

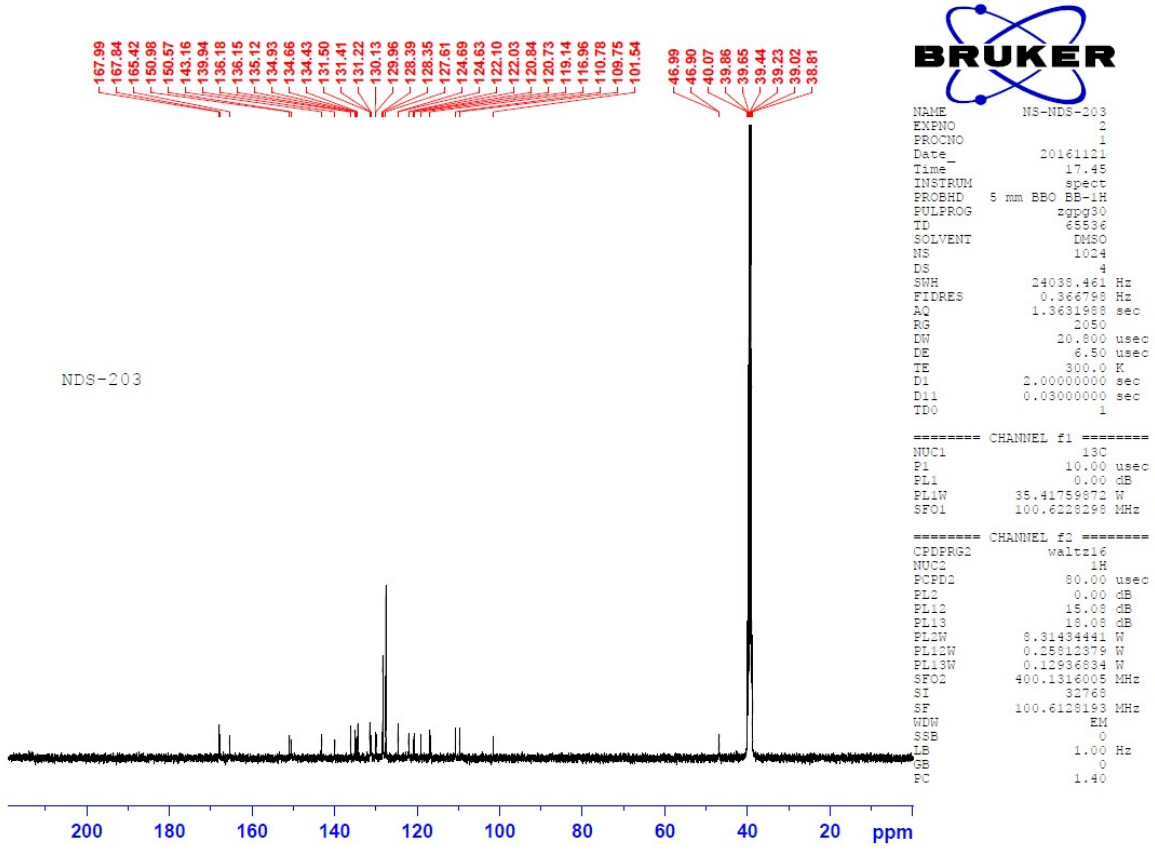


Base Peak 369.42 Channel Description 100.00-1200.00 ES+, Centroid, CV=10 Retention Time 0.232

1H-NMR Analysis of synthesized compound: 17a



13C-NMR Analysis of synthesized compound: 17a



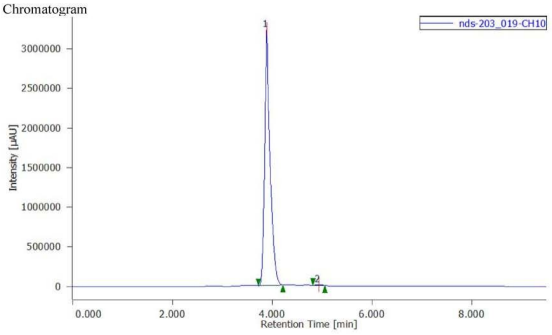
HPLC (percentage purity) of 17a

Benzimidazole derivatives_0915 nds-203_019 9/16/2017 7:14:38 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis

Chromatogram



Chromatogram Information

User Name	Administrator
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Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 4:20:35 PM
Volume	20.00 [µL]
Sample #	16
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.893	24081427	3229802	99.698	99.736	9684	4.888	1.440
2	Unknown	10	4.933	73008	8559	0.302	0.264	6089	N/A	1.069

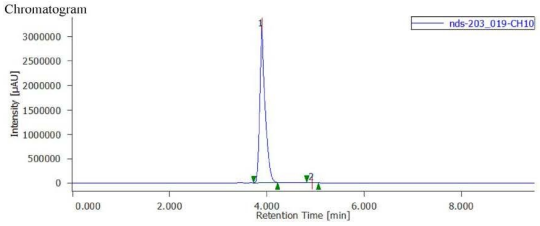
HPLC (peak purity) of 17a

Benzimidazole derivatives_0915 nds-203_019 9/22/2017 10:30:10 AM

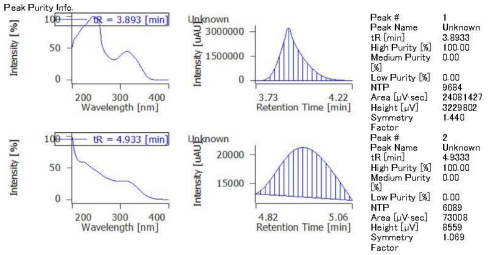
Institute of Pharmacy, Nirma University

Report - HPLC peak purity

Chromatogram

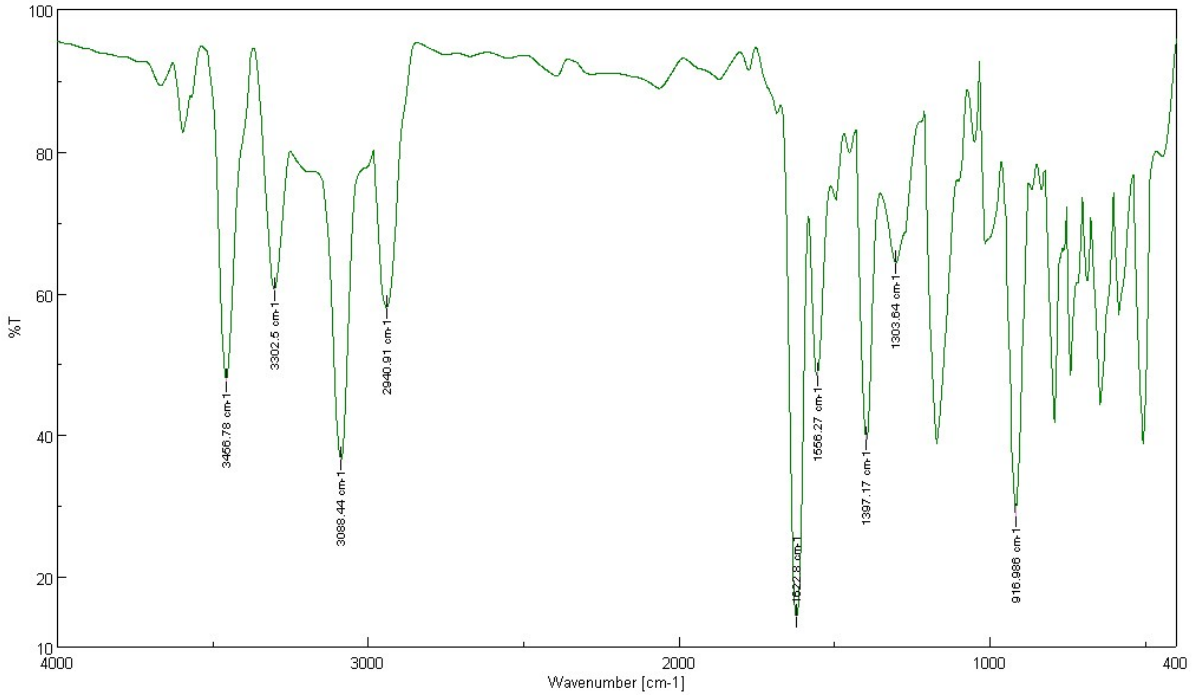


Peak Purity Info.

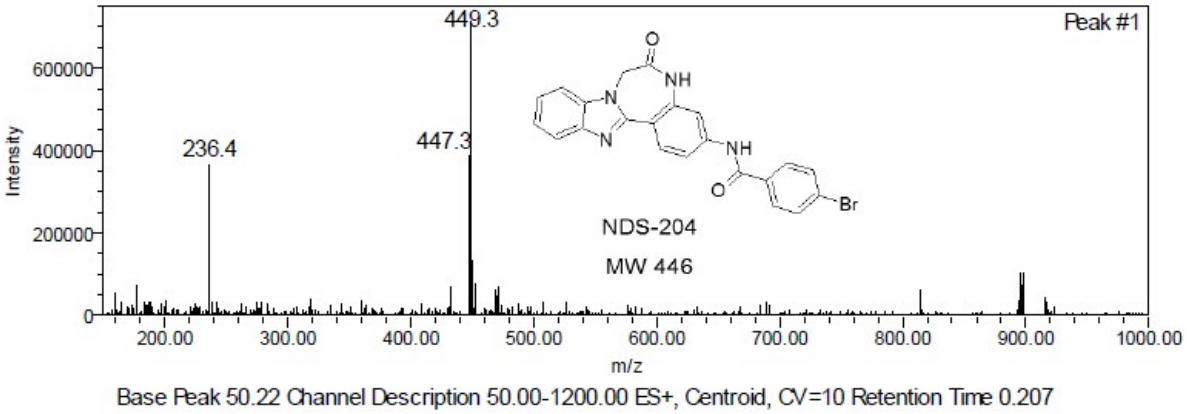


Peak #	1
Peak Name	Unknown
tR [min]	3.8933
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	9684
Area [µV·sec]	24081427
Height [µV]	3229802
Symmetry Factor	1.440
Peak #	2
Peak Name	Unknown
tR [min]	4.9333
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	6089
Area [µV·sec]	73008
Height [µV]	8559
Symmetry Factor	1.069

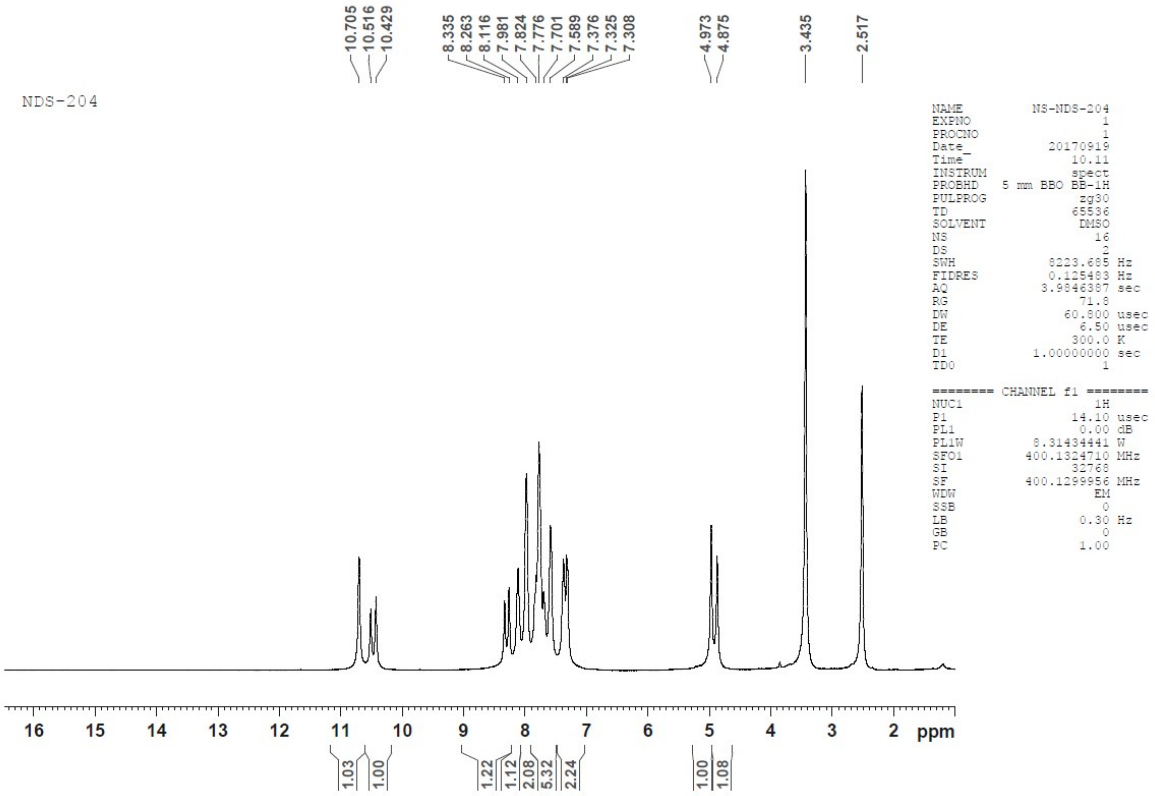
FTIR spectra of 17b



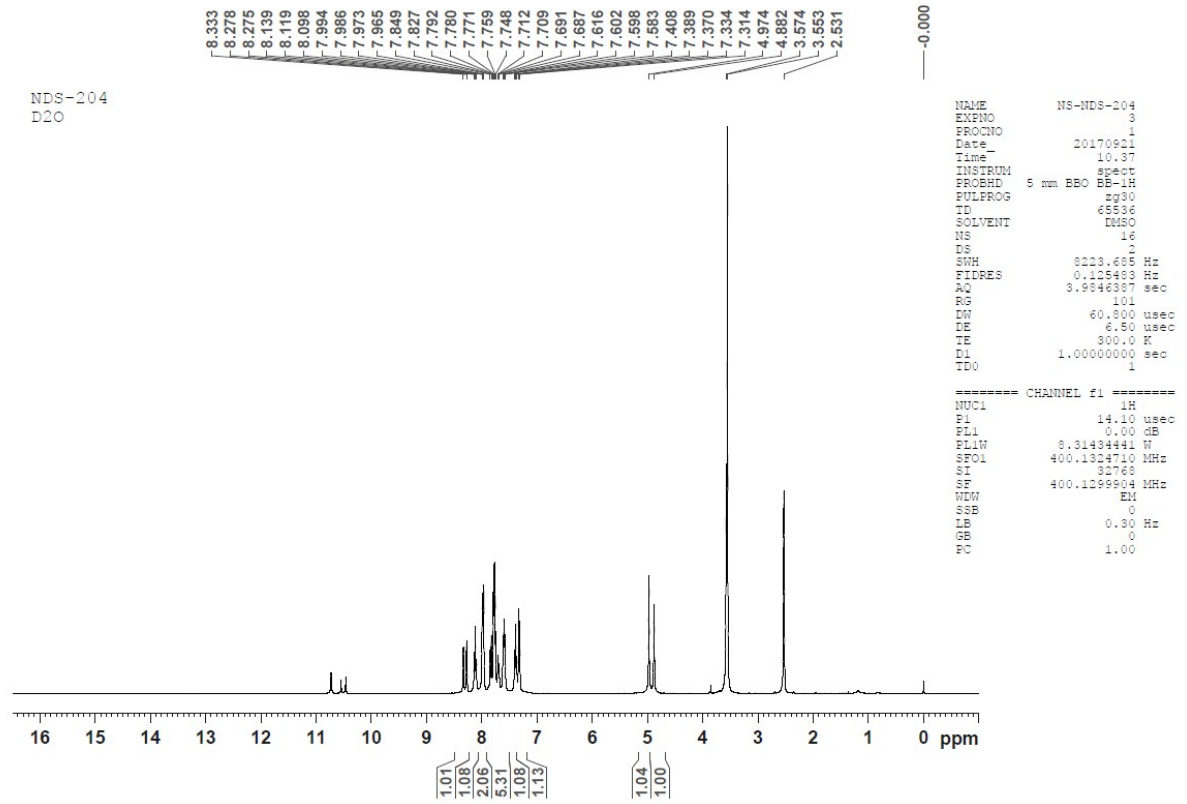
MASS Analysis of synthesized compound: 17b M+1: 447, M+3: 449



1H-NMR Analysis of synthesized compound: 17b



1H-NMR-D2O exchange analysis of synthesized compound: 17b

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NAME          NS-NDS-204
EXPNO                  3
PROCNO                 1
Date_           20170921
Time_              10.37
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            8223.685 Hz
FIDRES         0.125493 Hz
AQ             3.9846387 sec
RG                   101
DW              60.800 usec
DE               6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1               14.10 usec
PL1               0.00 dB
PL1W        8.31434441 W
SFO1       400.1324710 MHz
SI                 32768
SF         400.1299904 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
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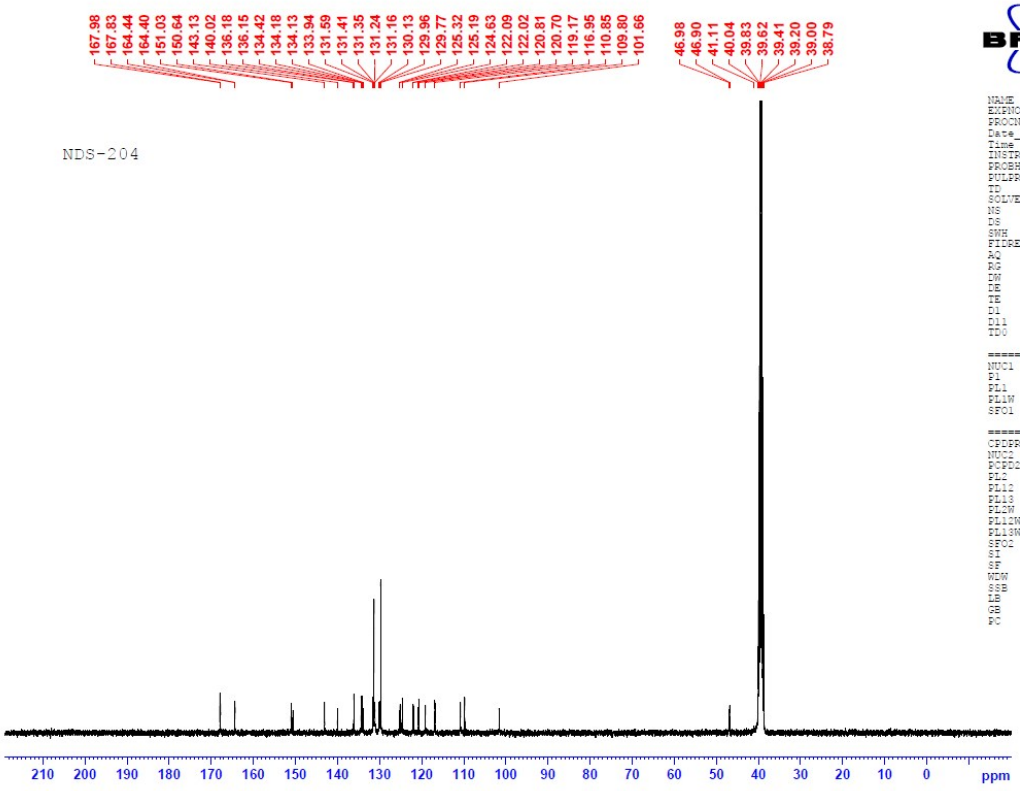
13C-NMR Analysis of synthesized compound: 17b



BRUKER

```
NAME          NS-NDS-204
EXPNO                  2
PROCNO                 1
Date_           20170918
Time_              11.10
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  2050
DW              20.800 usec
DE               6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1               10.00 usec
PL1               0.00 dB
PL1W       35.41758272 W
SFO1       100.6228298 MHz

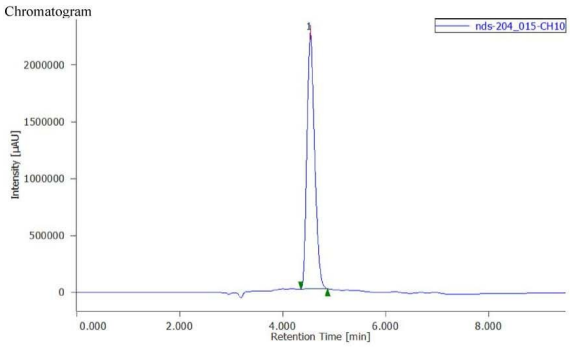
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            80.00 usec
PL2               0.00 dB
PL12             15.08 dB
PL13             15.08 dB
PL2W        8.31434441 W
PL12W       0.26812379 W
PL13W       0.12936834 W
SFO2       400.1316005 MHz
SI                 32768
SF         100.6128193 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

HPLC (percentage purity) of 17b

Benzimidazole derivatives_0915 nds-204_015 9/16/2017 7:18:38 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

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Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 3:05:48 PM
Volume	20.00 [µL]
Sample #	12
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

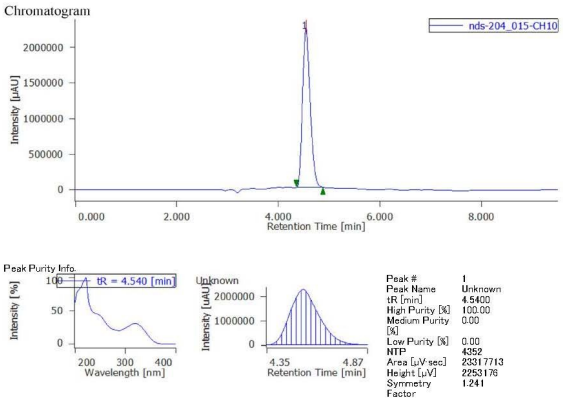
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.540	23317713	2253176	100.000	100.000	4352	N/A	1.241

HPLC (peak purity) of 17b

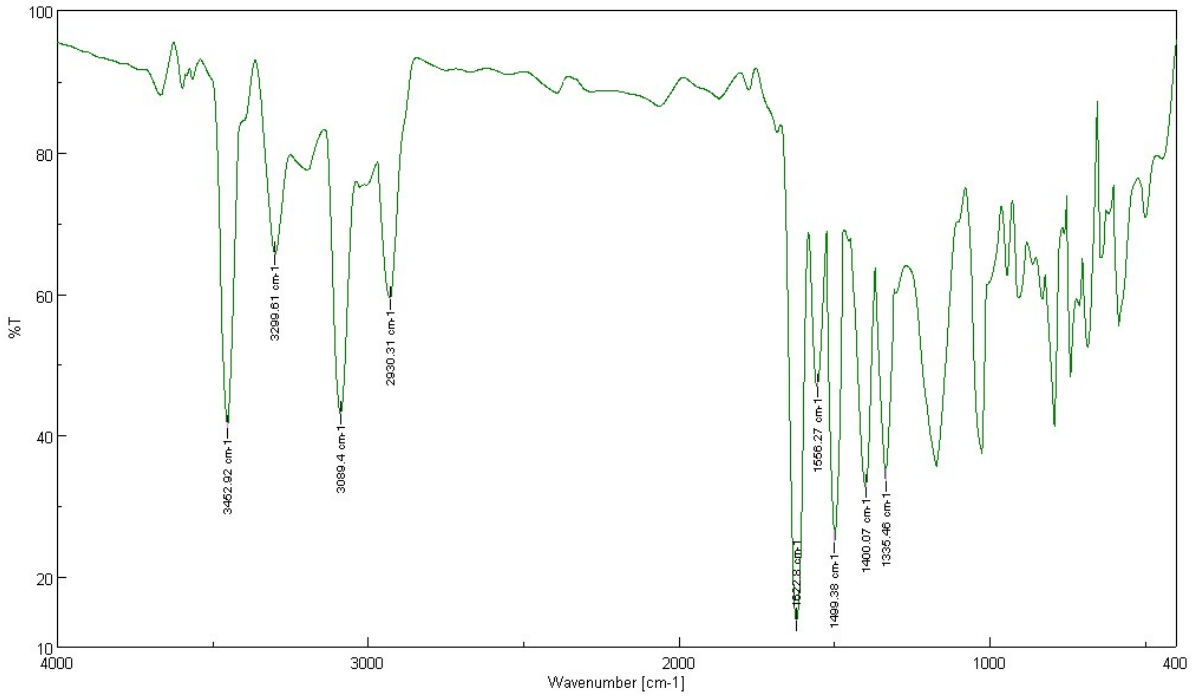
Benzimidazole derivatives_0915 nds-204_015 9/22/2017 10:29:35 AM

Institute of Pharmacy, Nirma University

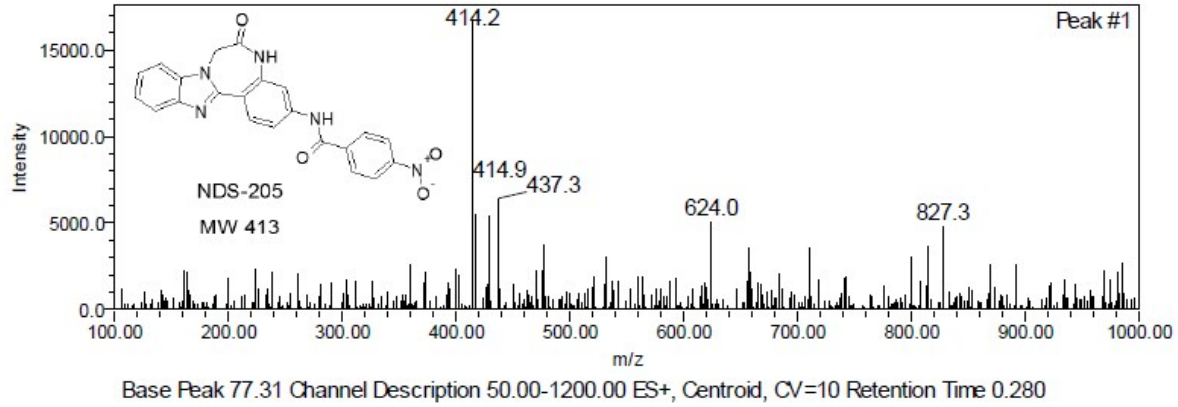
Report - HPLC peak purity



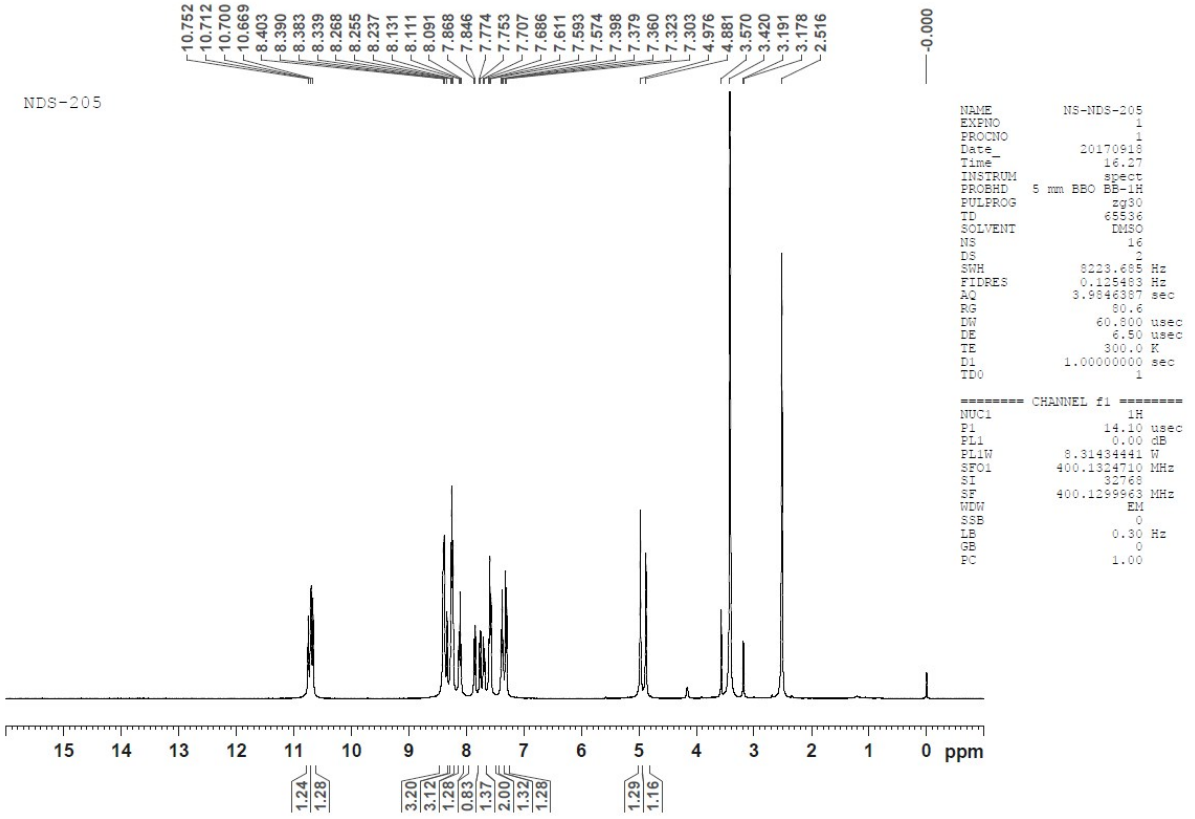
FTIR spectra of 17c



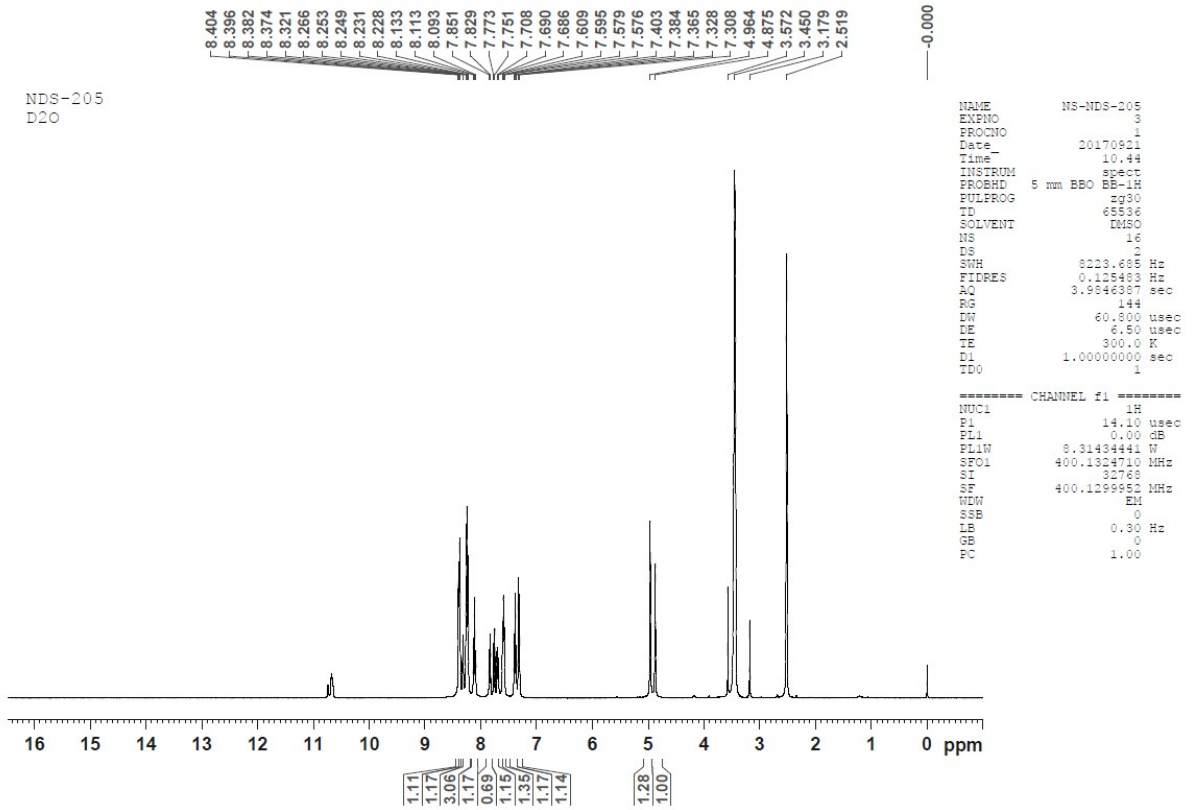
MASS Analysis of synthesized compound: 17c M+1: 414



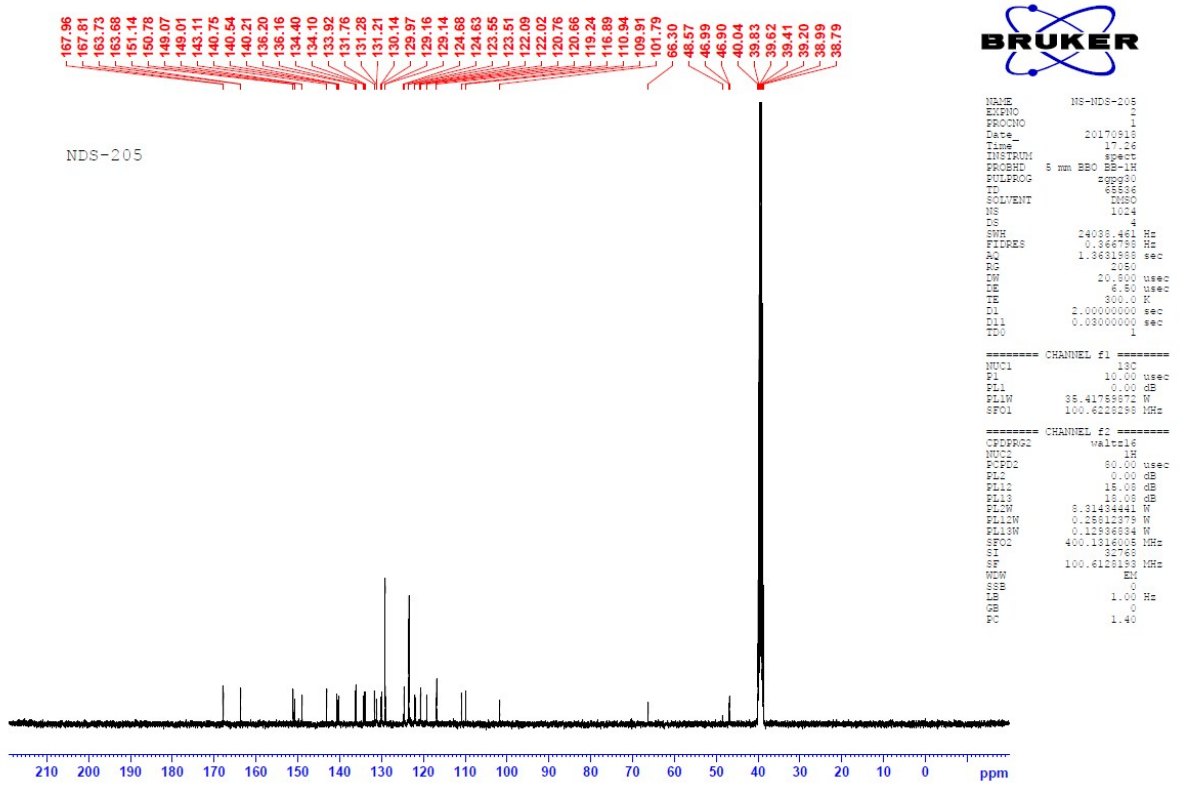
1H-NMR Analysis of synthesized compound: 17c



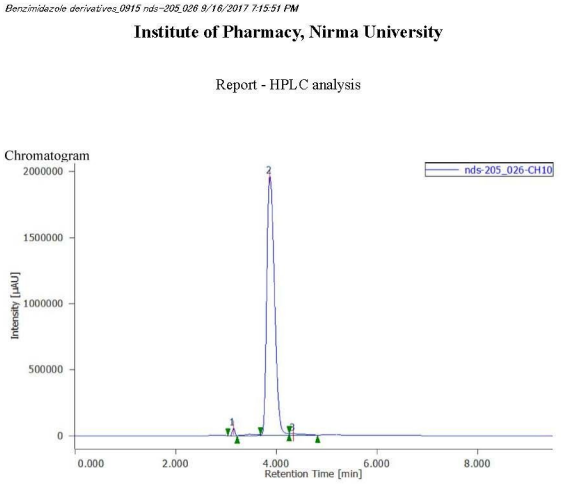
1H-NMR-D2O exchange analysis of synthesized compound: 17c



13C-NMR Analysis of synthesized compound: 17c



HPLC (percentage purity) of 17c



Chromatogram Information

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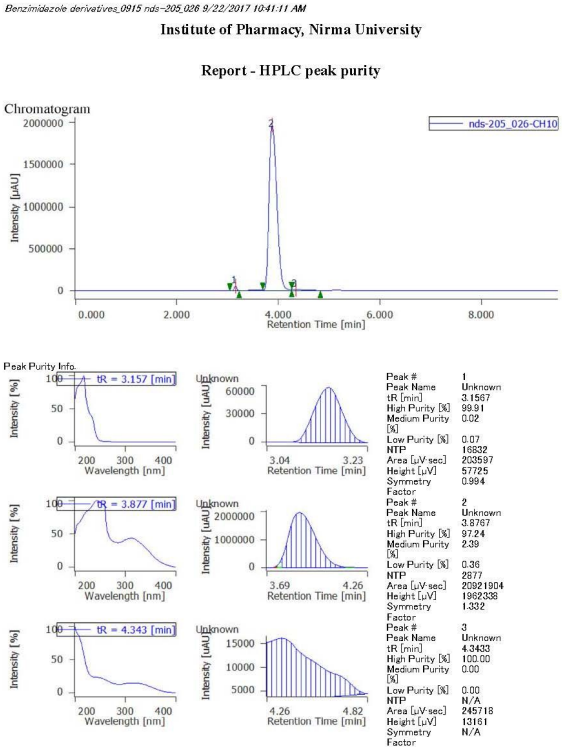
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 5:57:13 PM
Volume	20.00 [µL]
Sample #	23
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

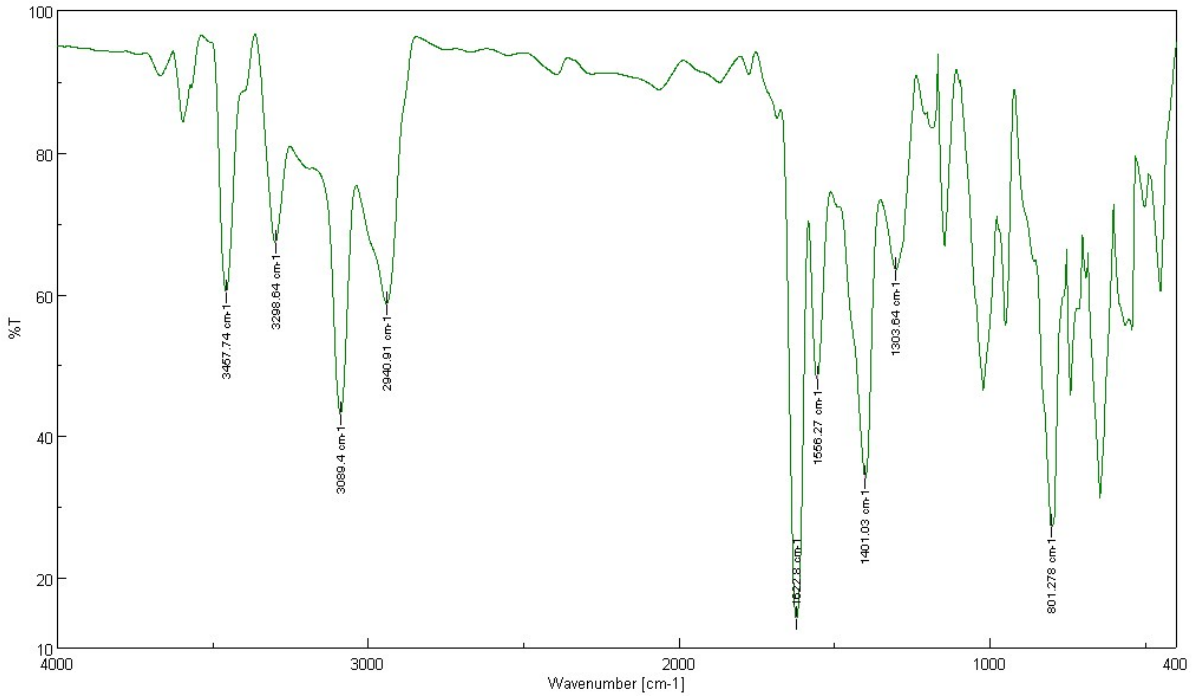
Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.157	203597	57725	0.953	2.839	16832	3.774	0.994
2	Unknown	10	3.877	20921904	1962338	97.898	96.514	2877	N/A	1.332
3	Unknown	10	4.343	245718	13161	1.150	0.647	N/A	N/A	N/A

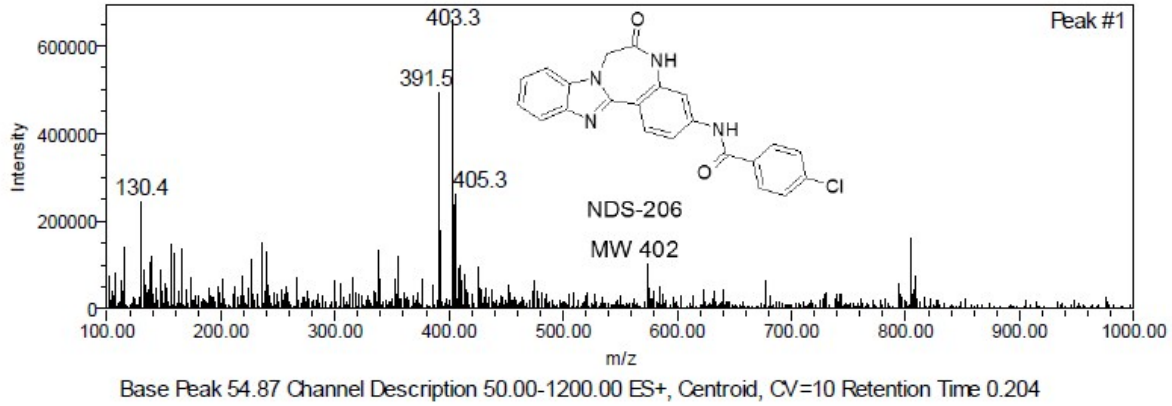
HPLC (peak purity) of 17c



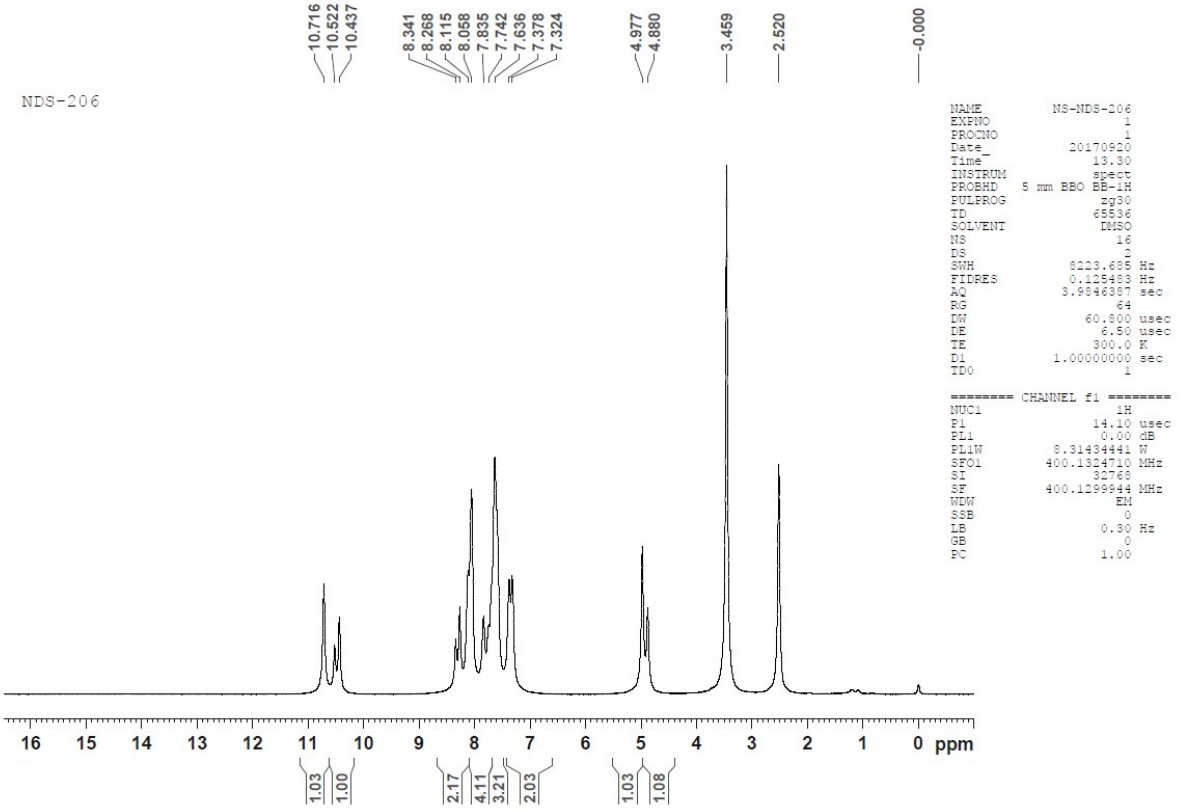
FTIR spectra of 17d



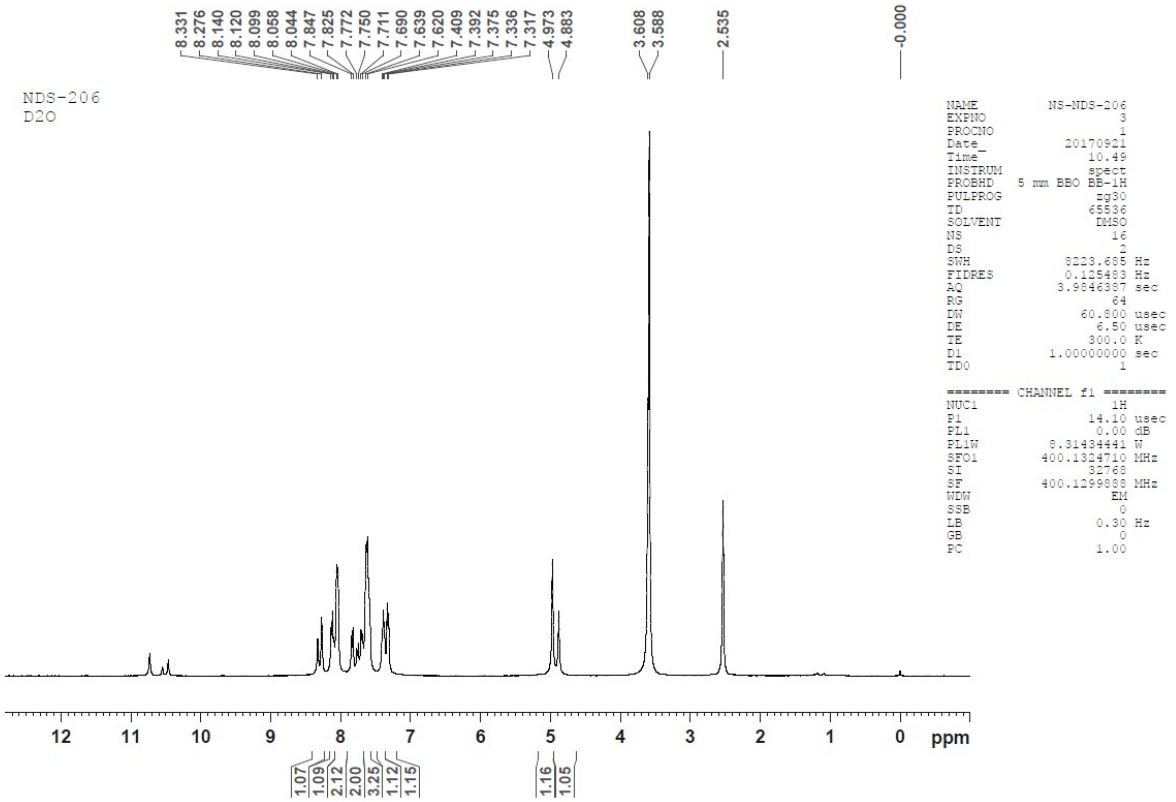
MASS Analysis of synthesized compound: 17d M+1: 403, M+3: 405



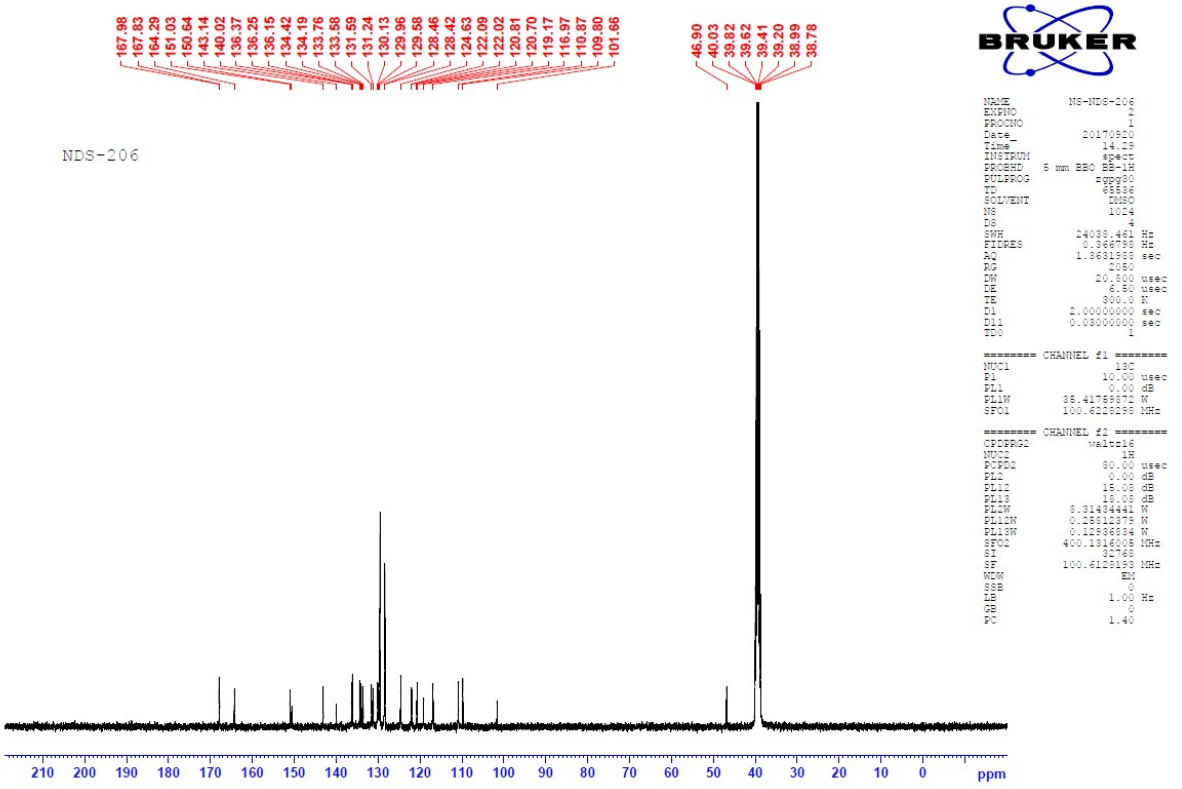
1H-NMR Analysis of synthesized compound: 17d



1H-NMR-D2O exchange analysis of synthesized compound: 17d



13C-NMR Analysis of synthesized compound: 17d

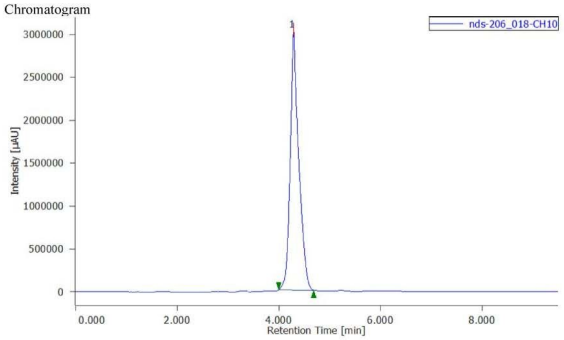


HPLC (percentage purity) of 17d

Benzimidazole derivatives_0915 nds-206_018 9/16/2017 7:14:01 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

User Name	Administrator
Date Modified	9/15/2017 7:15:13 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 4:00:13 PM
Volume	20.00 [µL]
Sample #	15
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

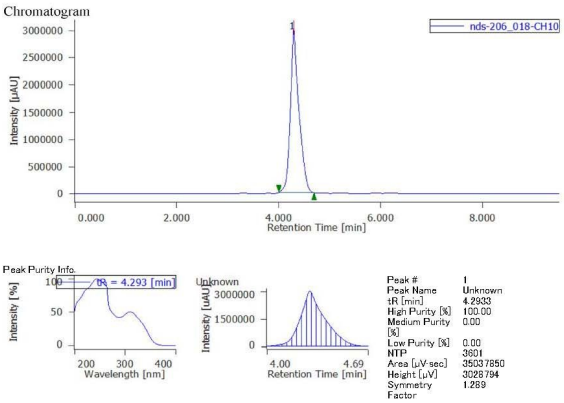
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.293	35037850	3028794	100.000	100.000	3601	N/A	1.289

HPLC (peak purity) of 17d

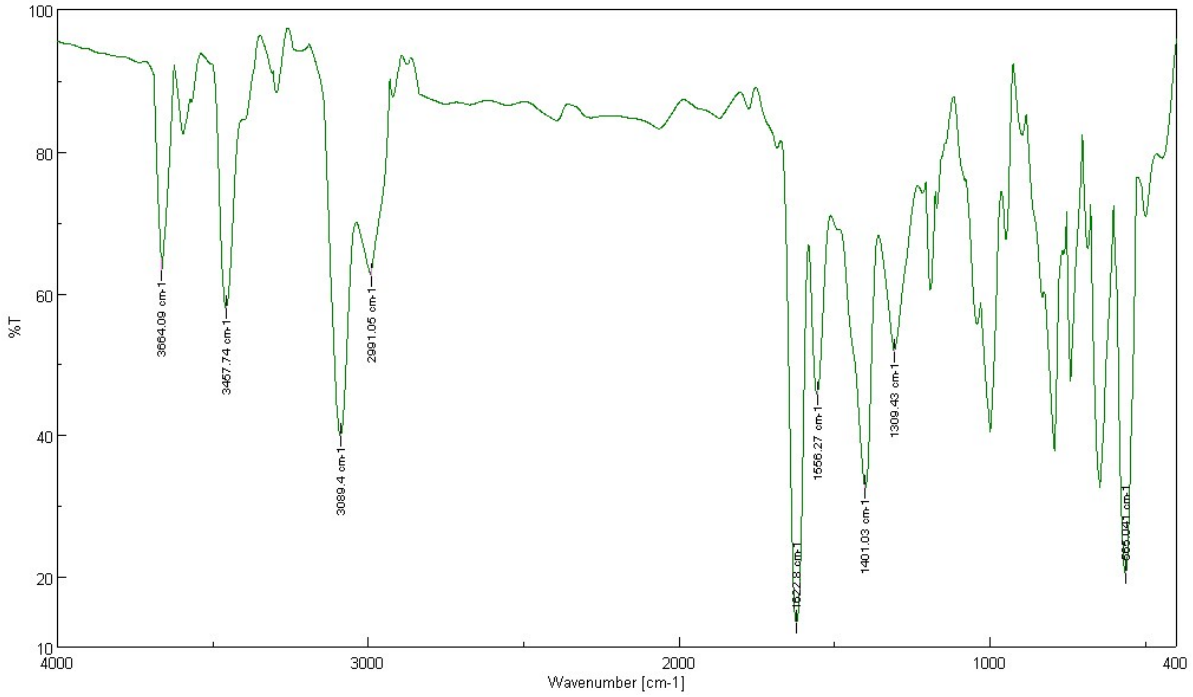
Benzimidazole derivatives_0915 nds-206_018 9/22/2017 10:29:52 AM

Institute of Pharmacy, Nirma University

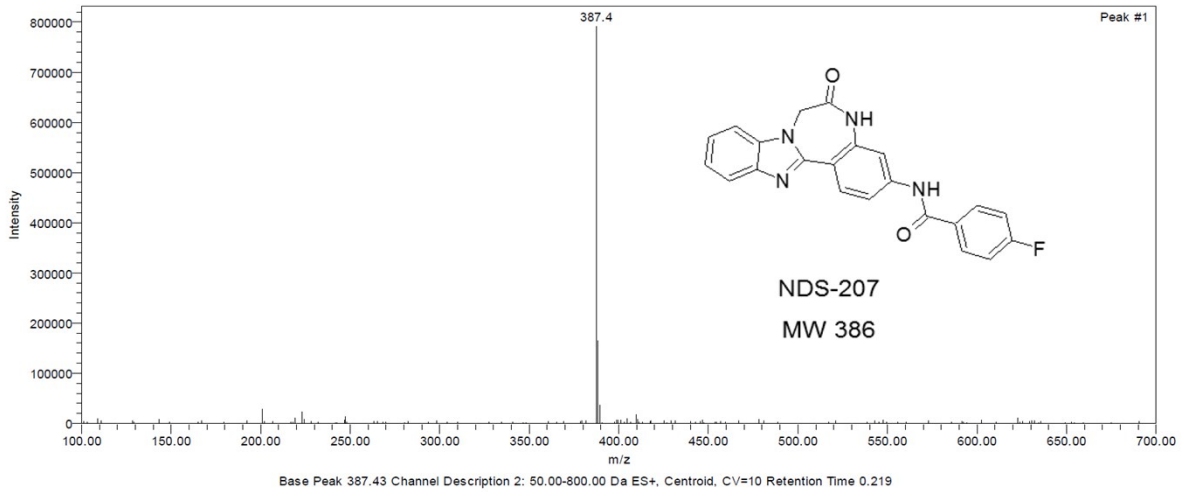
Report - HPLC peak purity



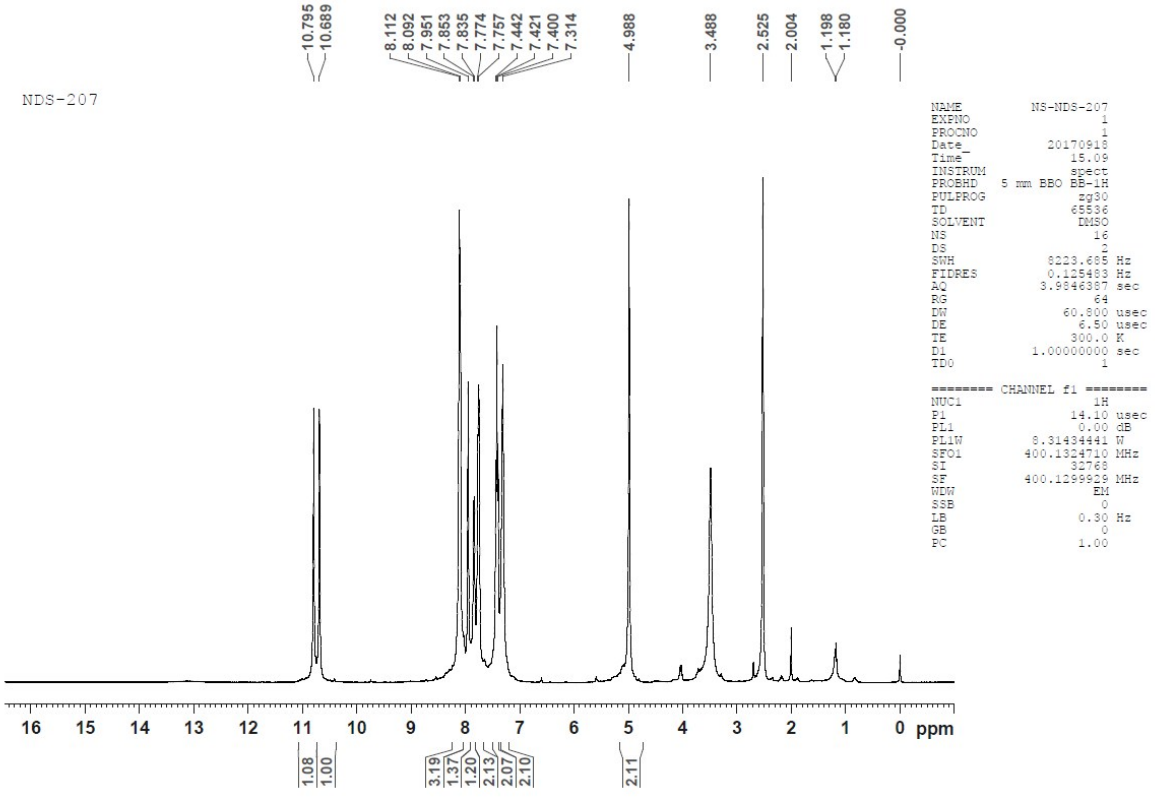
FTIR spectra of 17e



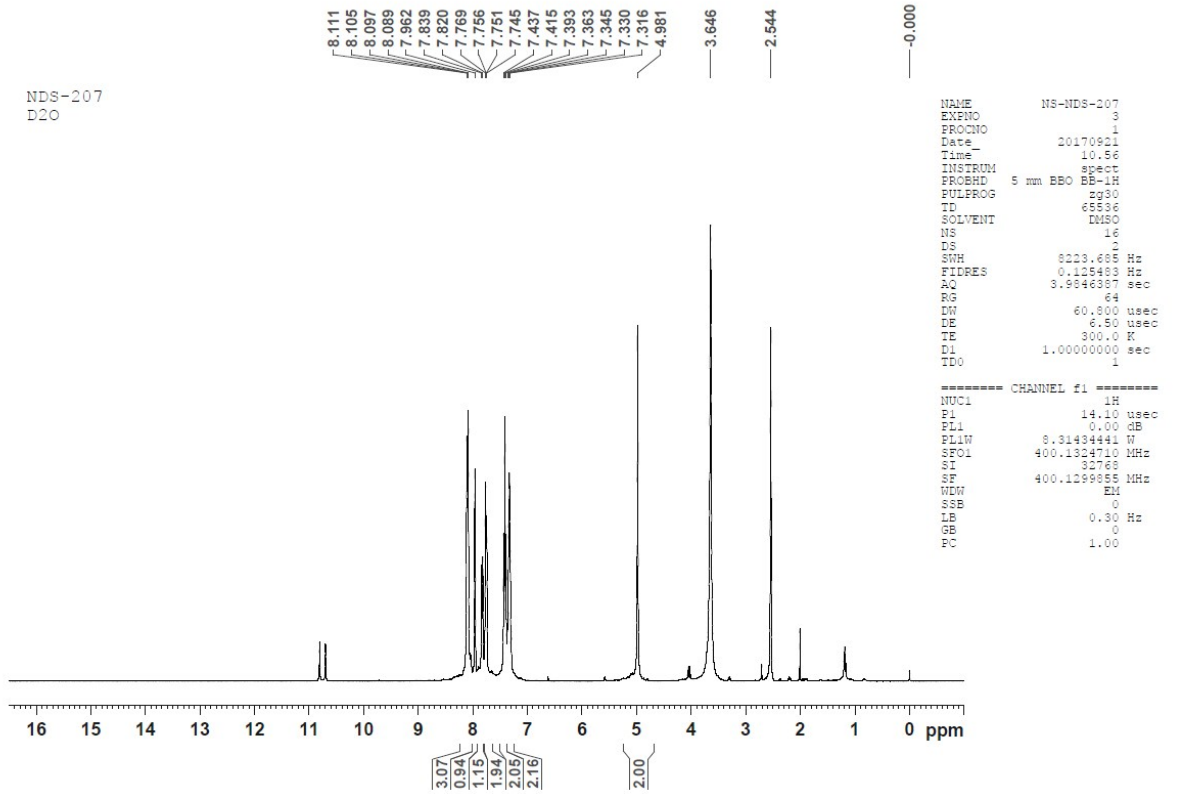
MASS Analysis of synthesized compound: 17e M+1: 387



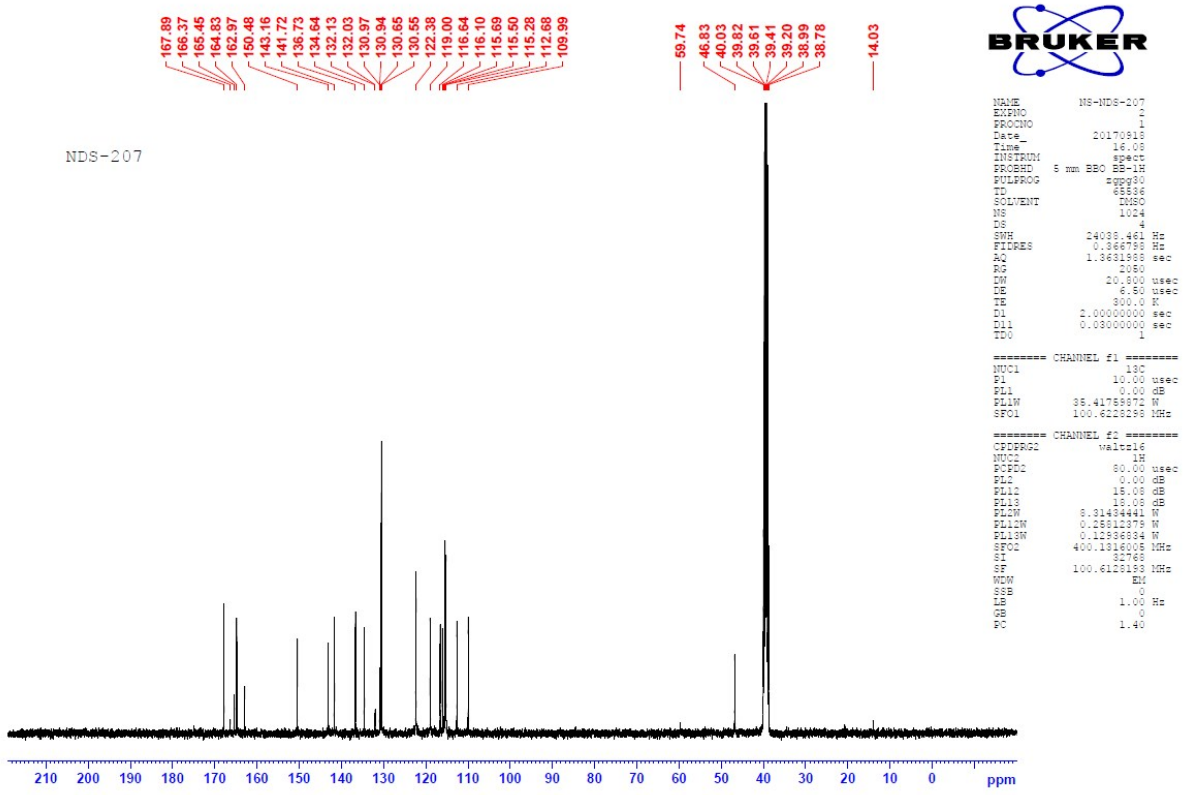
1H-NMR Analysis of synthesized compound: 17e



1H-NMR-D2O exchange analysis of synthesized compound: 17e



13C-NMR Analysis of synthesized compound: 17e

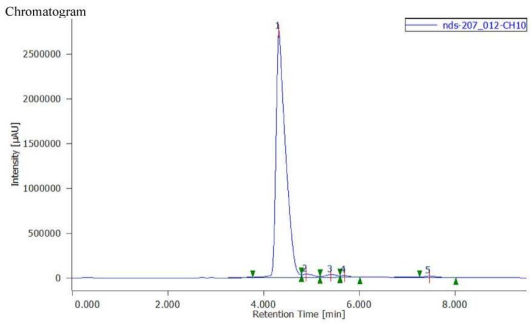


HPLC (percentage purity) of 17e

Benzimidazole derivatives_0915 nds-207_012 9/16/2017 7:17:39 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

User Name	Administrator
Date Modified	9/15/2017 7:15:03 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 2:01:09 PM
Volume	20.00 [µL]
Sample #	9
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

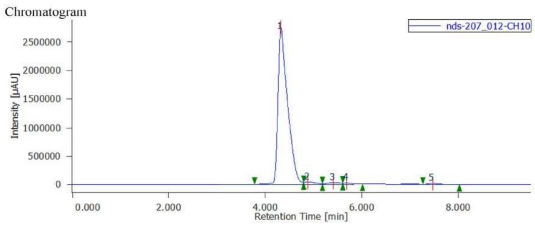
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.323	3792777	2751846	95.701	96.349	2650	N/A	1.821
2	Unknown	10	4.887	620159	35862	1.565	1.256	N/A	N/A	N/A
3	Unknown	10	5.410	555668	29657	1.402	1.038	N/A	N/A	N/A
4	Unknown	10	5.687	247102	21696	0.624	0.760	N/A	N/A	N/A
5	Unknown	10	7.460	280552	17076	0.708	0.598	5601	N/A	N/A

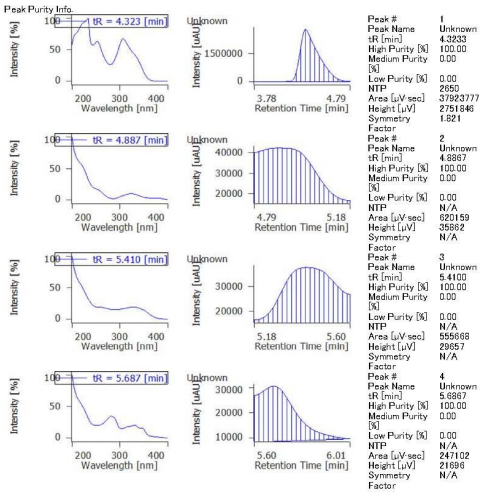
HPLC (peak purity) of 17e

Benzimidazole derivatives_0915 nds-207_012 9/22/2017 10:28:33 AM

Institute of Pharmacy, Nirma University

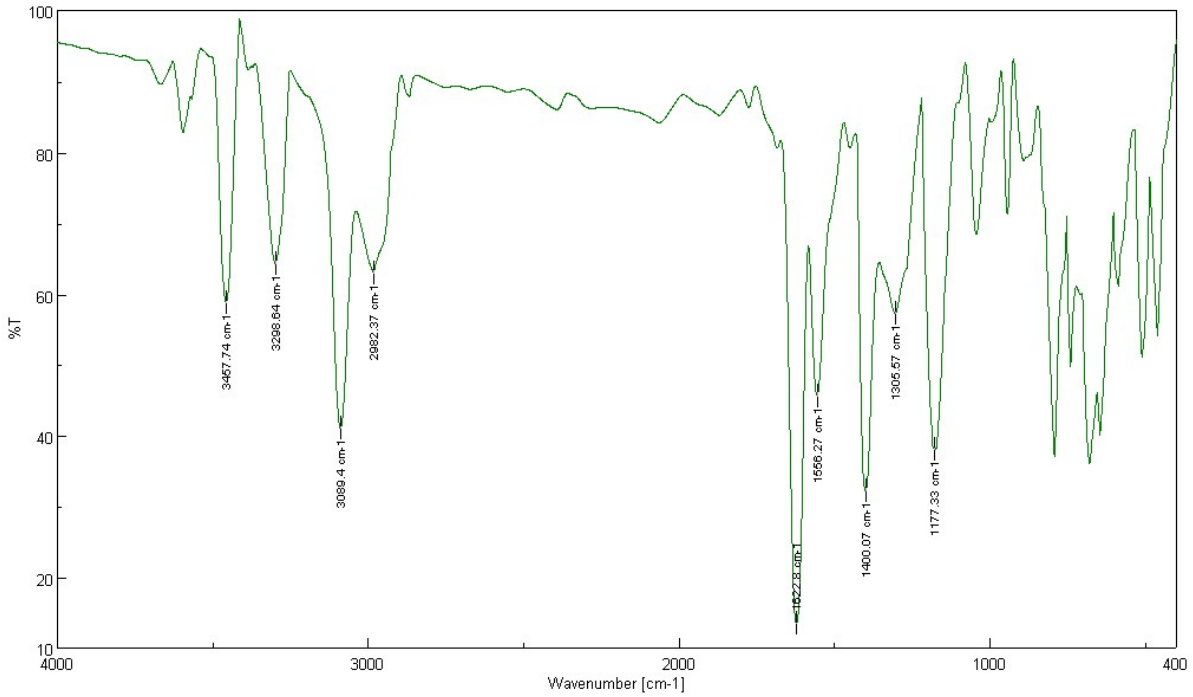
Report - HPLC peak purity



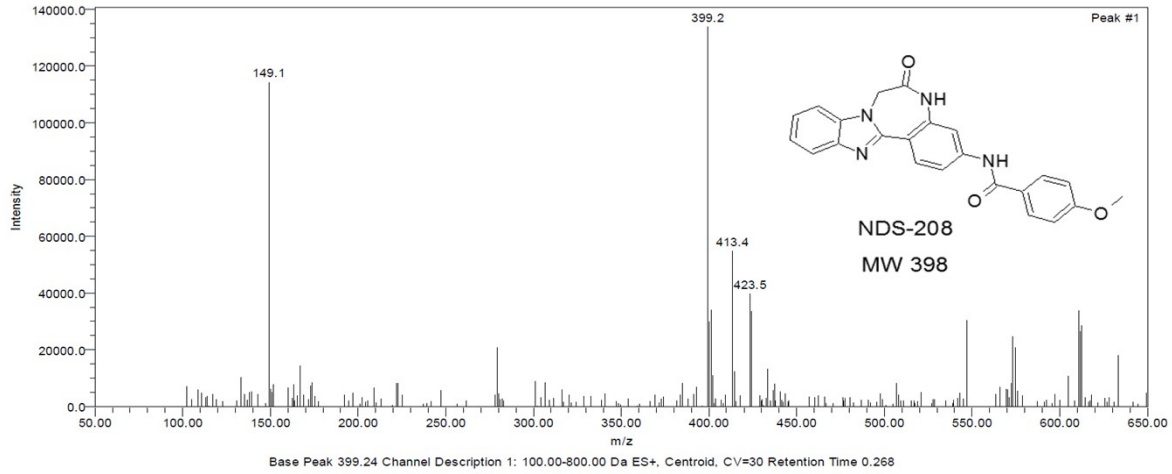


Peak #	1	Peak #	2	Peak #	3	Peak #	4
Peak Name	Unknown	Peak Name	Unknown	Peak Name	Unknown	Peak Name	Unknown
tR [min]	4.3233	tR [min]	4.8867	tR [min]	5.4100	tR [min]	5.6867
High Purity [%]	100.00	High Purity [%]	100.00	High Purity [%]	100.00	High Purity [%]	100.00
Medium Purity [%]	0.00	Medium Purity [%]	0.00	Medium Purity [%]	0.00	Medium Purity [%]	0.00
Low Purity [%]	0.00	Low Purity [%]	0.00	Low Purity [%]	0.00	Low Purity [%]	0.00
NTP	2650	NTP	N/A	NTP	N/A	NTP	N/A
Area [µV·sec]	3792777	Area [µV·sec]	620159	Area [µV·sec]	555668	Area [µV·sec]	247102
Height [µV]	2751846	Height [µV]	35862	Height [µV]	29657	Height [µV]	21696
Symmetry Factor	1.821	Symmetry Factor	N/A	Symmetry Factor	N/A	Symmetry Factor	N/A

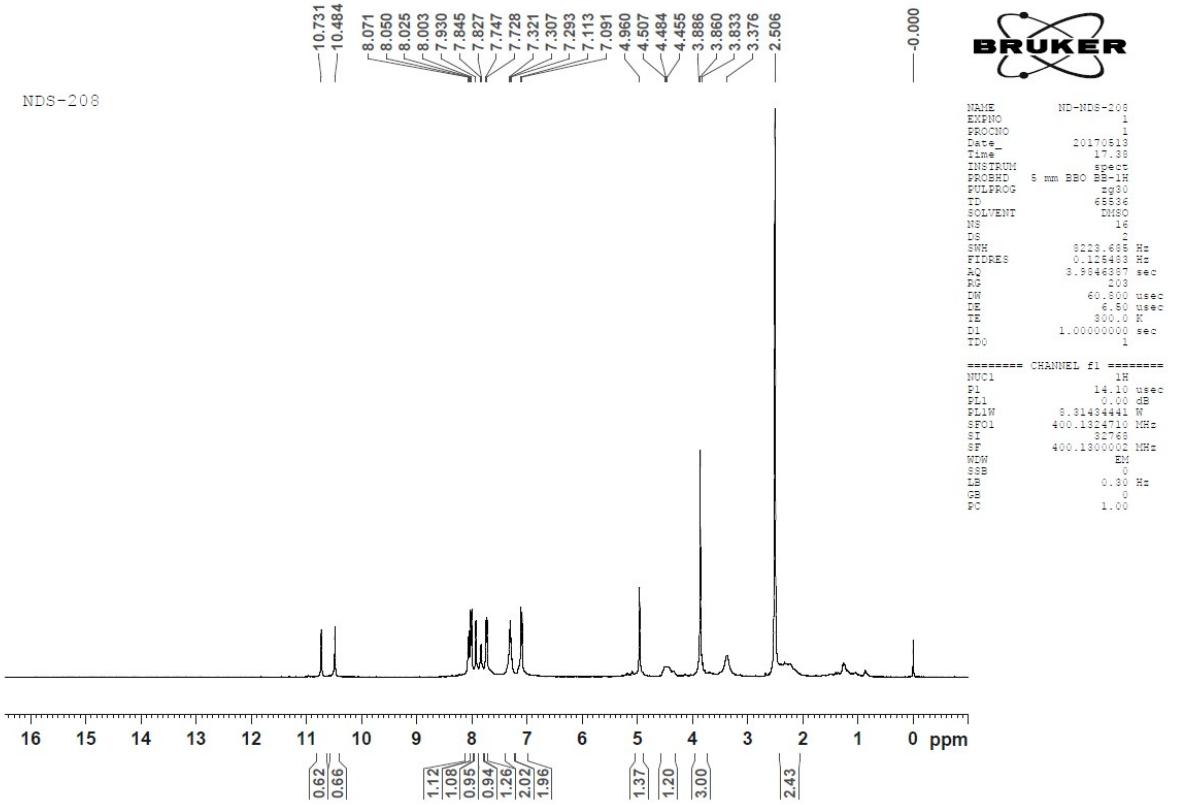
FTIR spectra of 17f



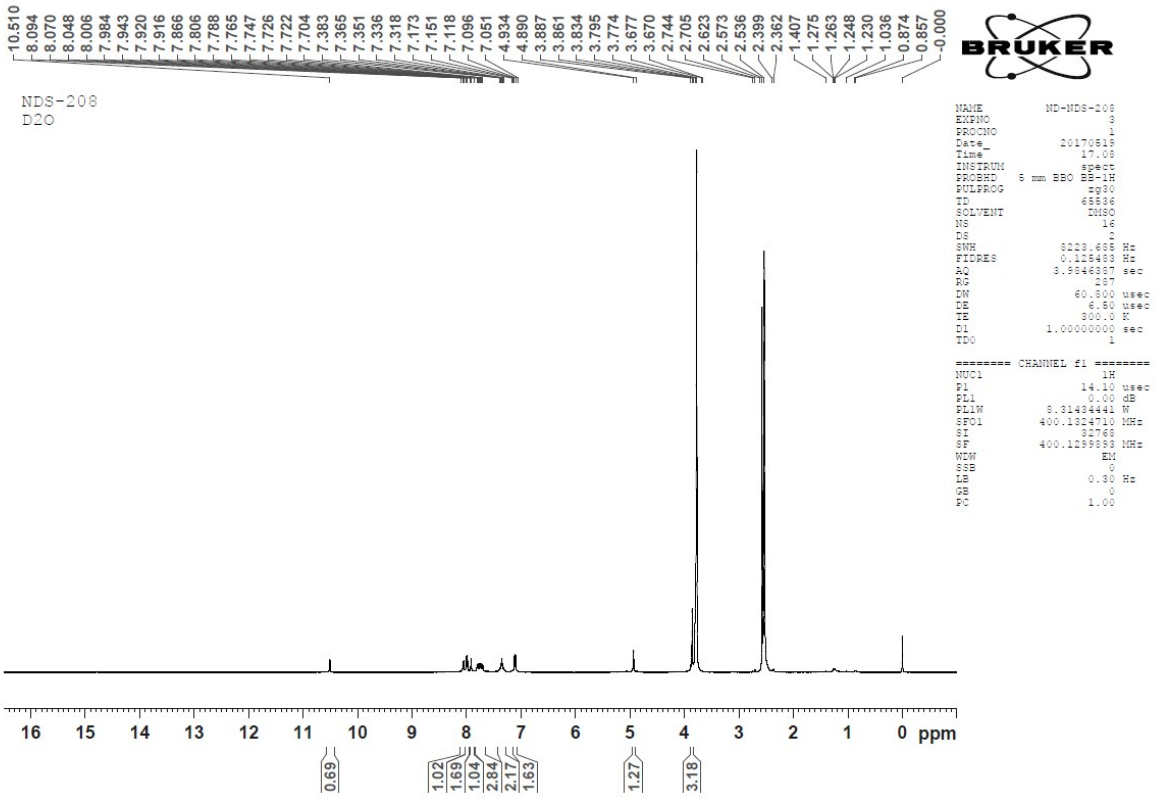
MASS Analysis of synthesized compound: 17f M+1: 399



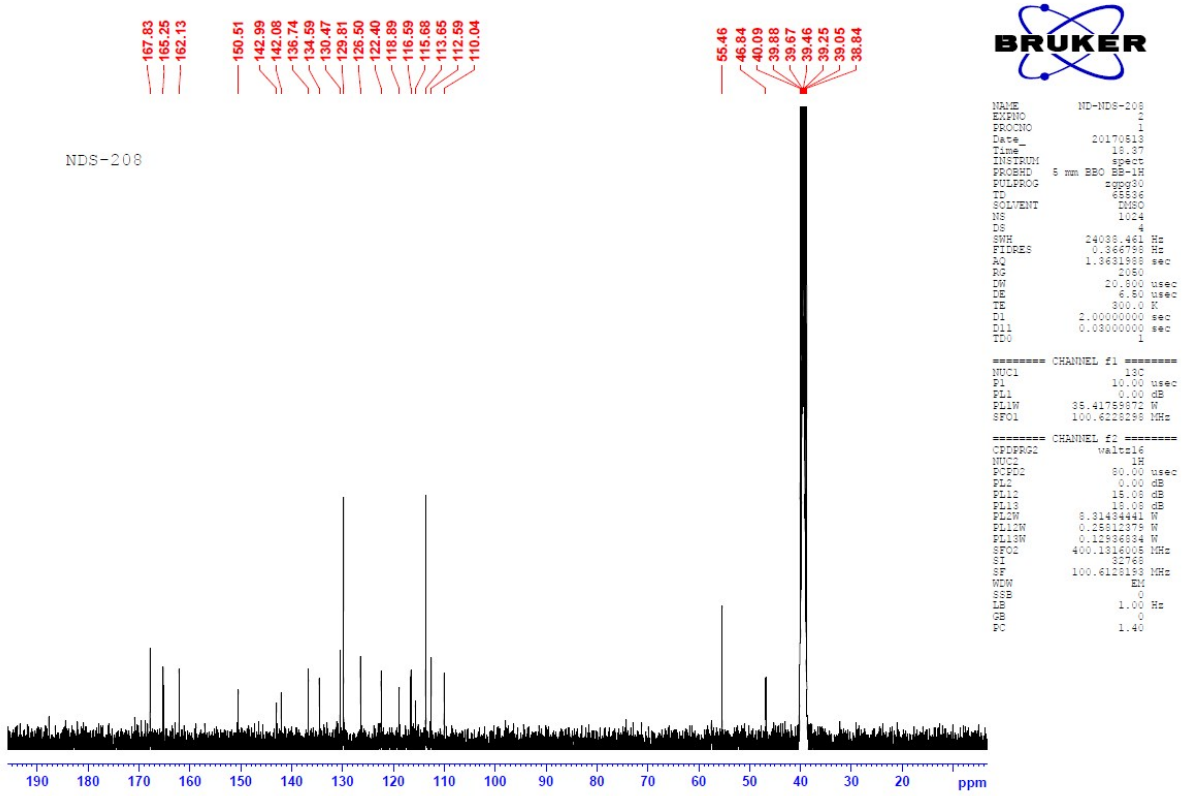
1H-NMR Analysis of synthesized compound: 17f



1H-NMR-D2O exchange analysis of synthesized compound: 17f



13C-NMR Analysis of synthesized compound: 17f

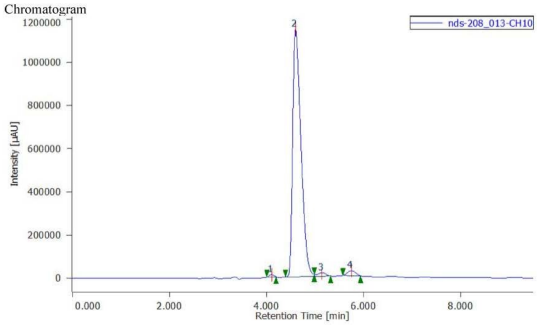


HPLC (percentage purity) of 17f

Benzimidazole derivatives_0915 nds-208_013 9/16/2017 7:17:53 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

User Name	Administrator
Date Modified	9/15/2017 7:15:05 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 2:12:36 PM
Volume	20.00 [µL]
Sample #	10
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

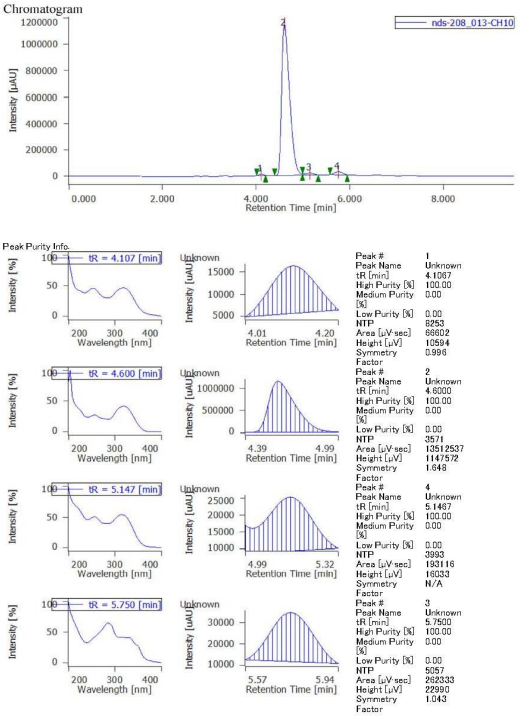
#	Peak Name	CH	tR [min]	Area [µV sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.107	66602	10594	0.475	0.885	8253	2.015	0.996
2	Unknown	10	4.600	13512537	1147572	96.280	95.856	3571	N/A	1.648
3	Unknown	10	5.147	193116	16033	1.376	1.339	3993	N/A	N/A
4	Unknown	10	5.750	262333	22990	1.869	1.920	5057	N/A	1.043

HPLC (peak purity) of 17f

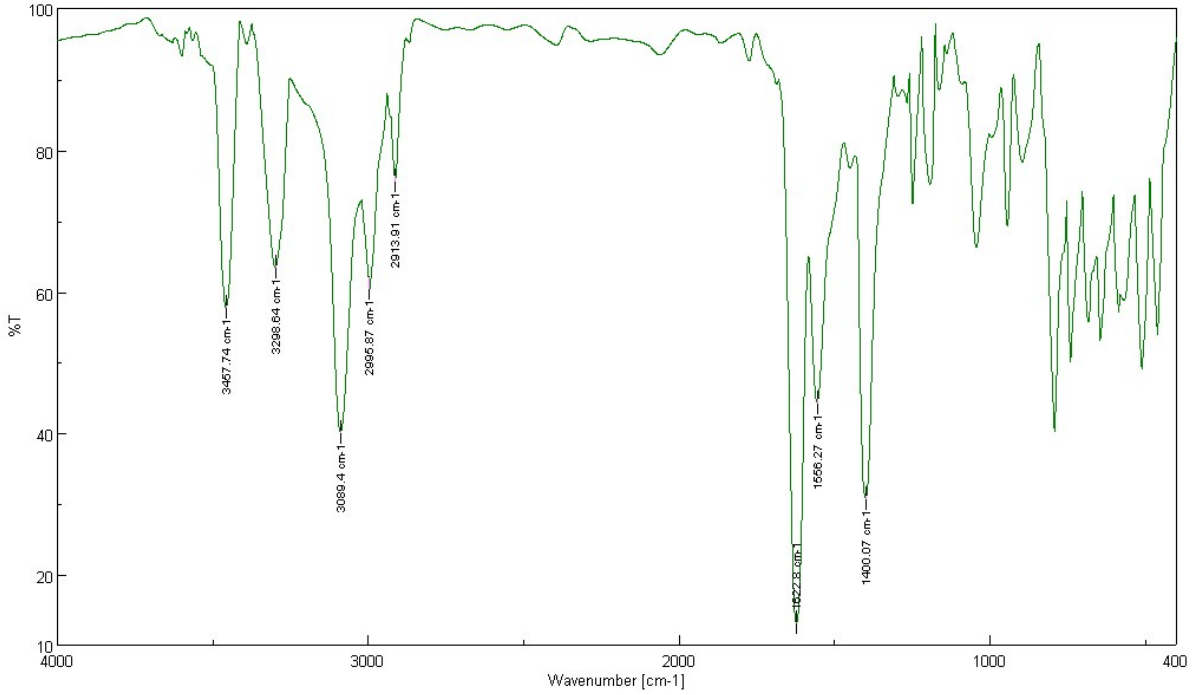
Benzimidazole derivatives_0915 nds-208_013 9/22/2017 10:23:53 AM

Institute of Pharmacy, Nirma University

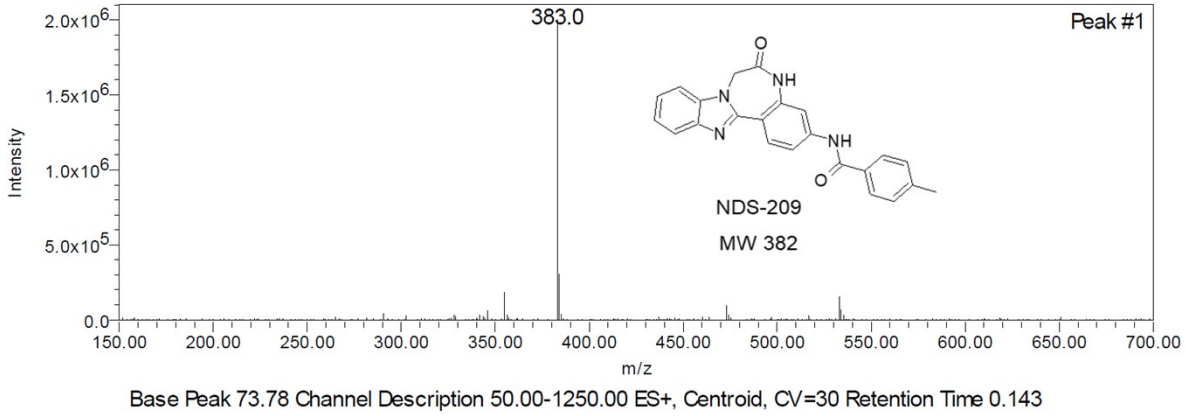
Report - HPLC peak purity



FTIR spectra of 17g

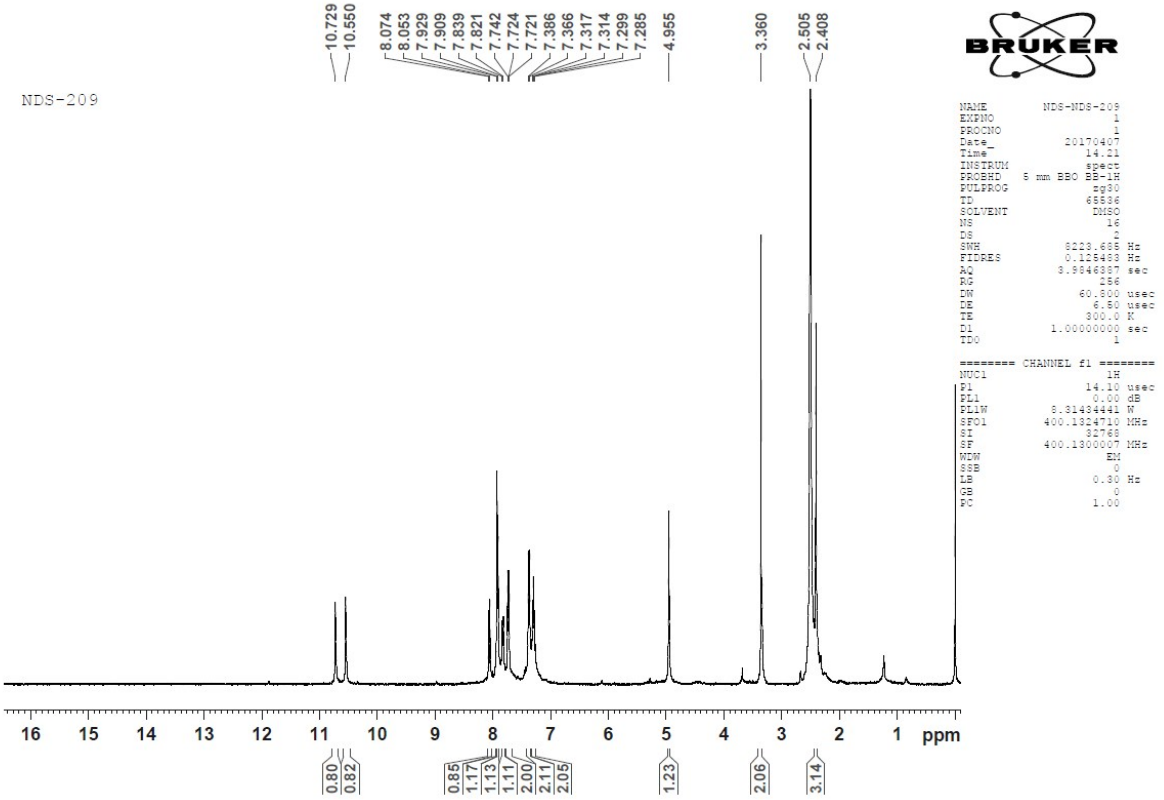


MASS Analysis of synthesized compound: 17g M+1: 383

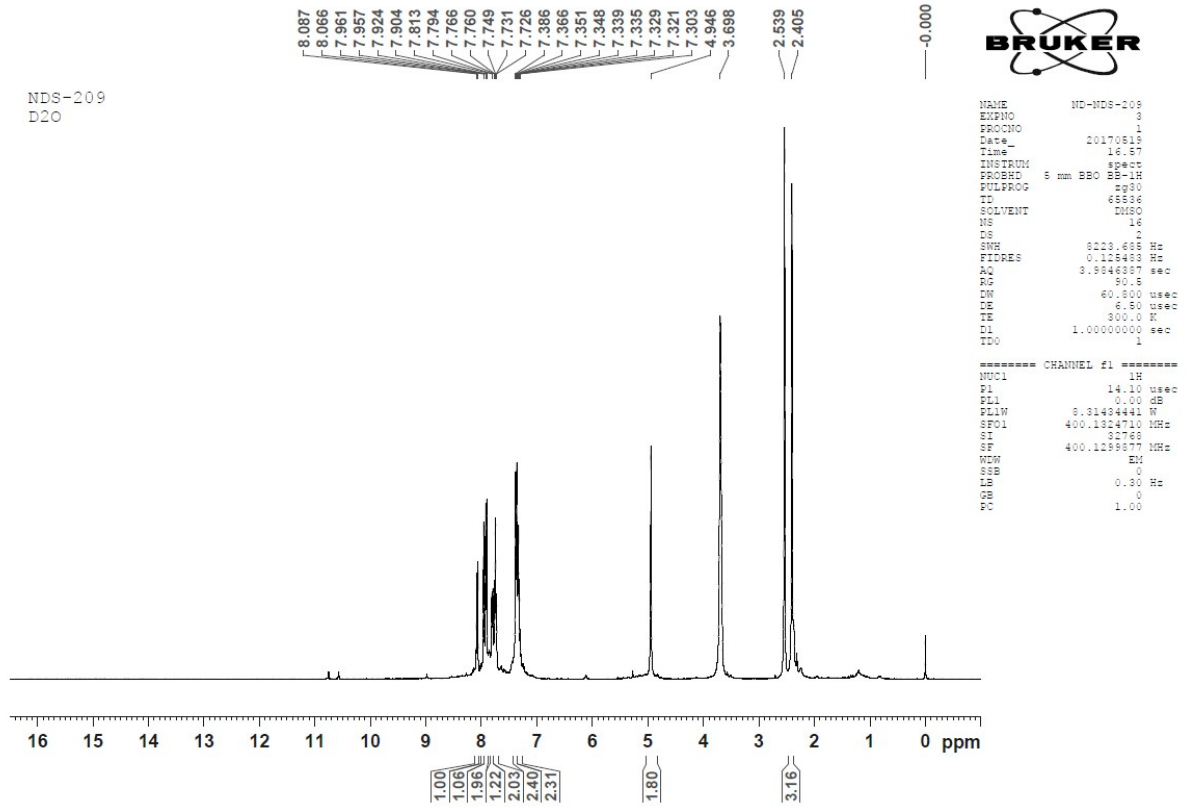


Base Peak 73.78 Channel Description 50.00-1250.00 ES+, Centroid, CV=30 Retention Time 0.143

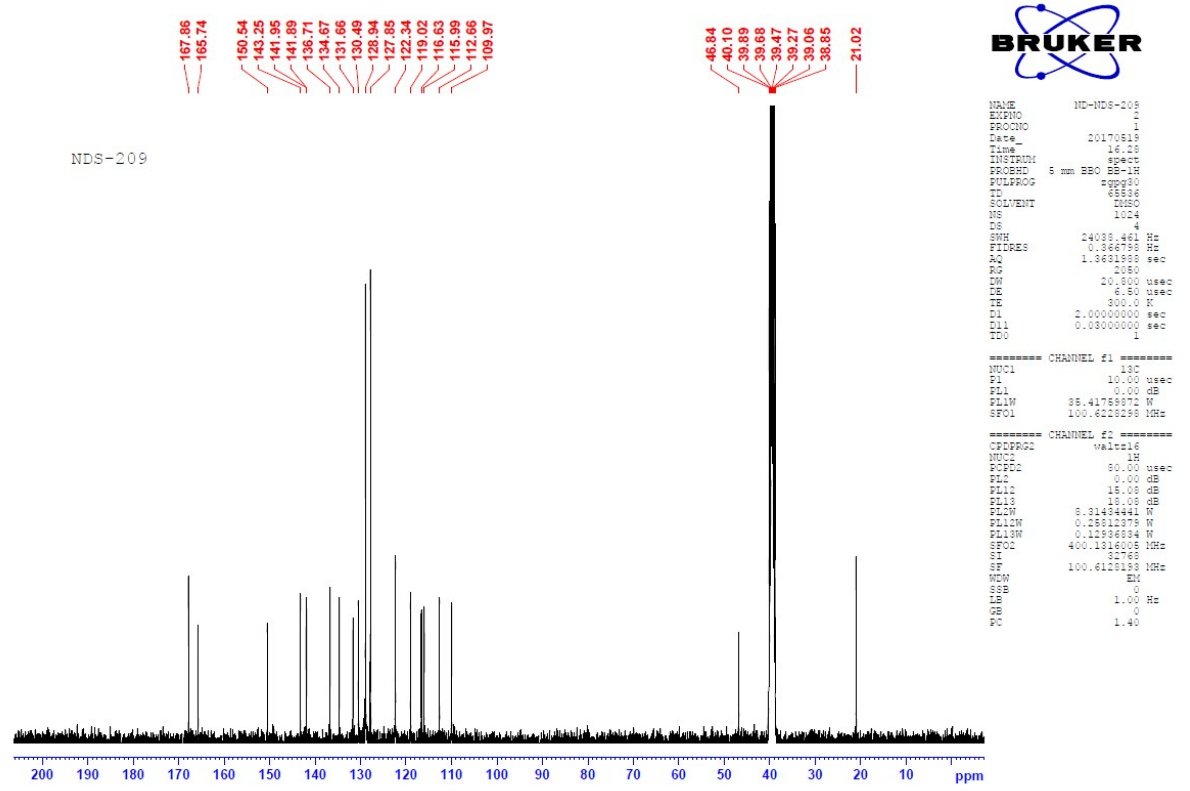
1H-NMR Analysis of synthesized compound: 17g



1H-NMR-D2O exchange analysis of synthesized compound: 17g



13C-NMR Analysis of synthesized compound: 17g



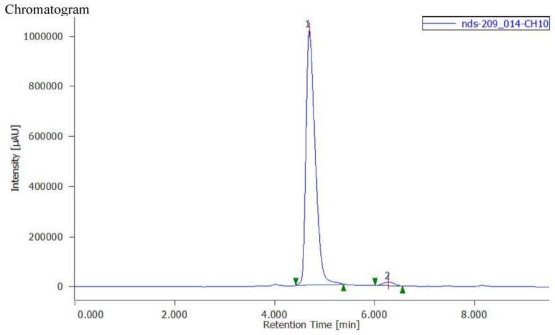
HPLC (percentage purity) of 17g

Benzimidazole derivatives_0815 nds-209_014 9/16/2017 7:18:19 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis

Chromatogram



Chromatogram Information

User Name	Administrator
Date Modified	9/15/2017 7:15:08 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 2:24:55 PM
Volume	20.00 [µL]
Sample #	11
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	4.697	13050351	1018424	98.330	98.579	3282	4.241	1.535
2	Unknown	10	6.283	221682	14682	1.670	1.421	3512	N/A	0.978

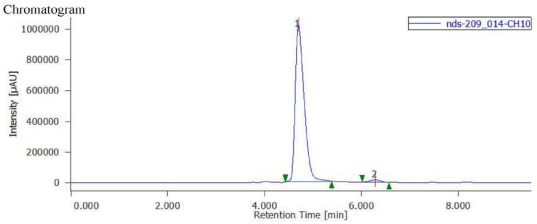
HPLC (peak purity) of 17g

Benzimidazole derivatives_0815 nds-209_014 9/22/2017 10:29:15 AM

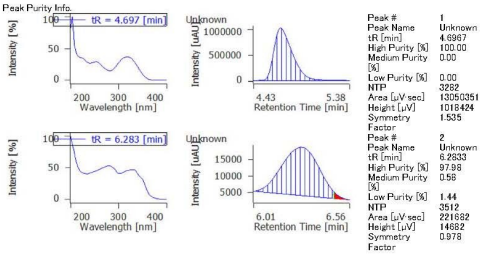
Institute of Pharmacy, Nirma University

Report - HPLC peak purity

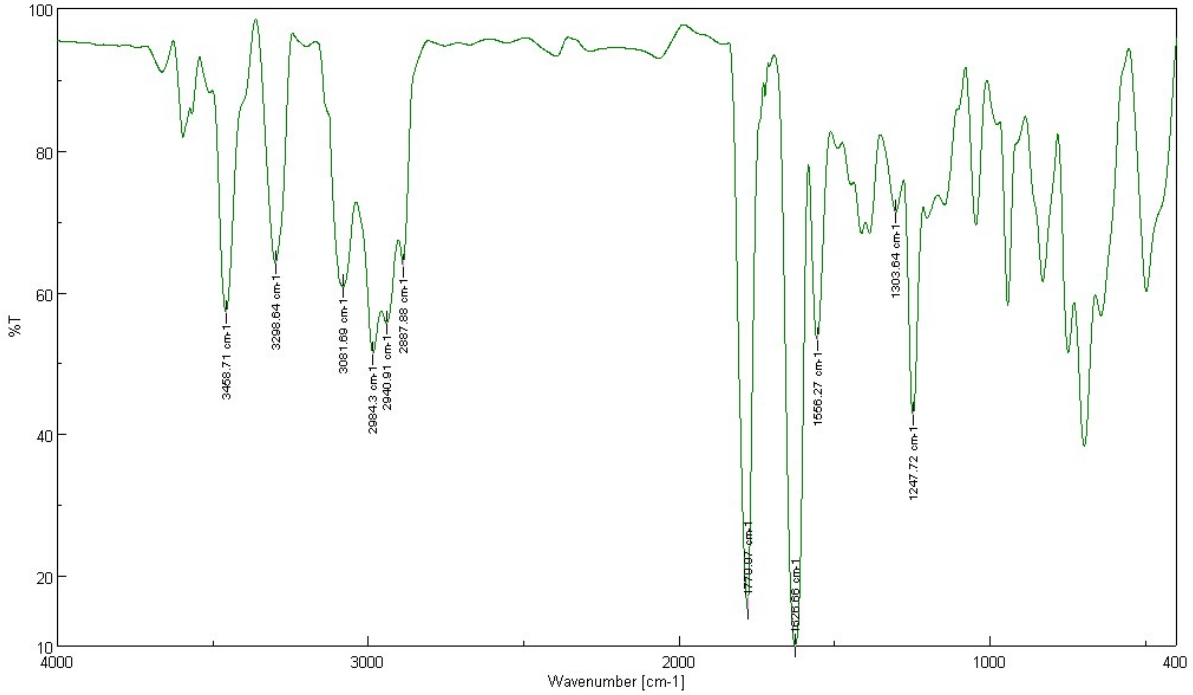
Chromatogram



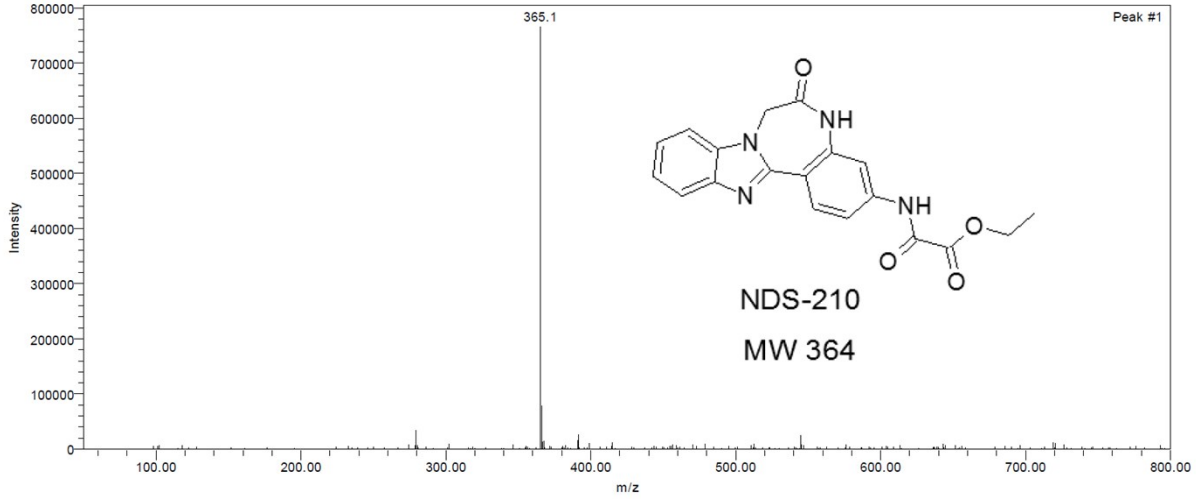
Peak Purity Info.



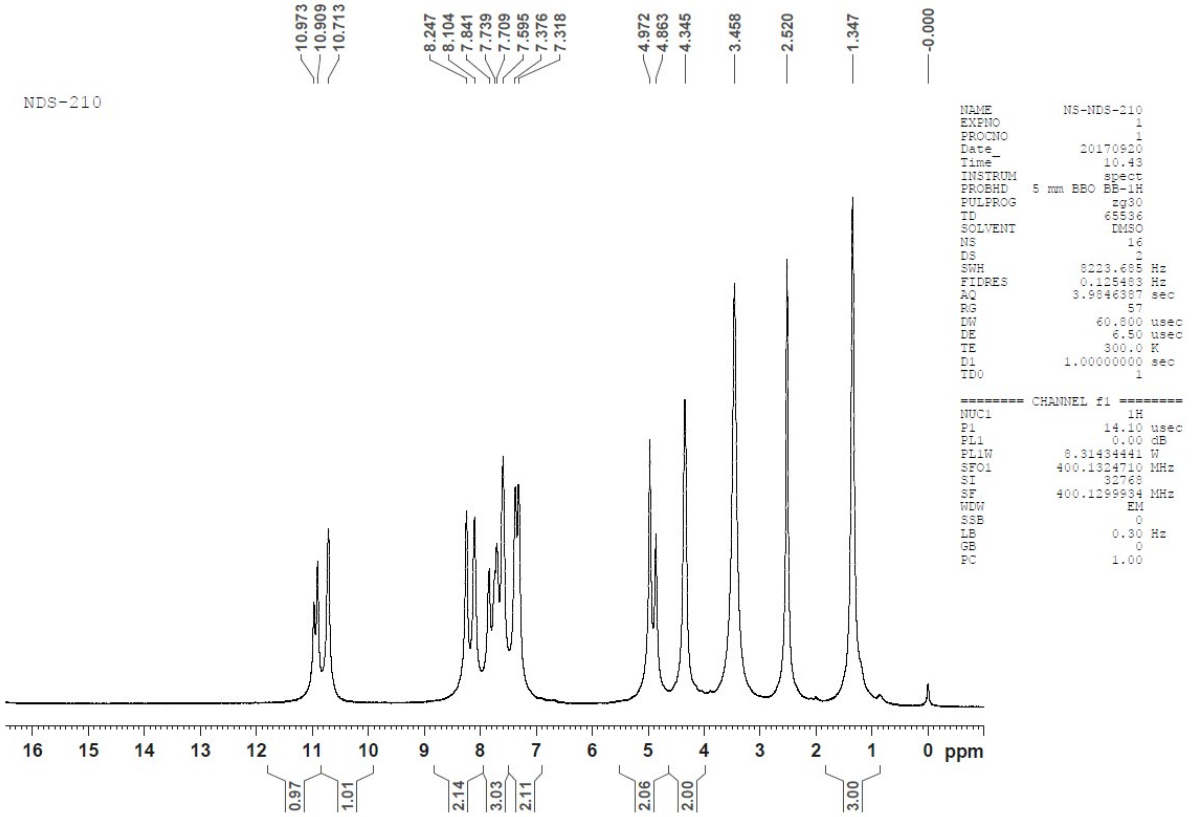
FTIR spectra of 17h



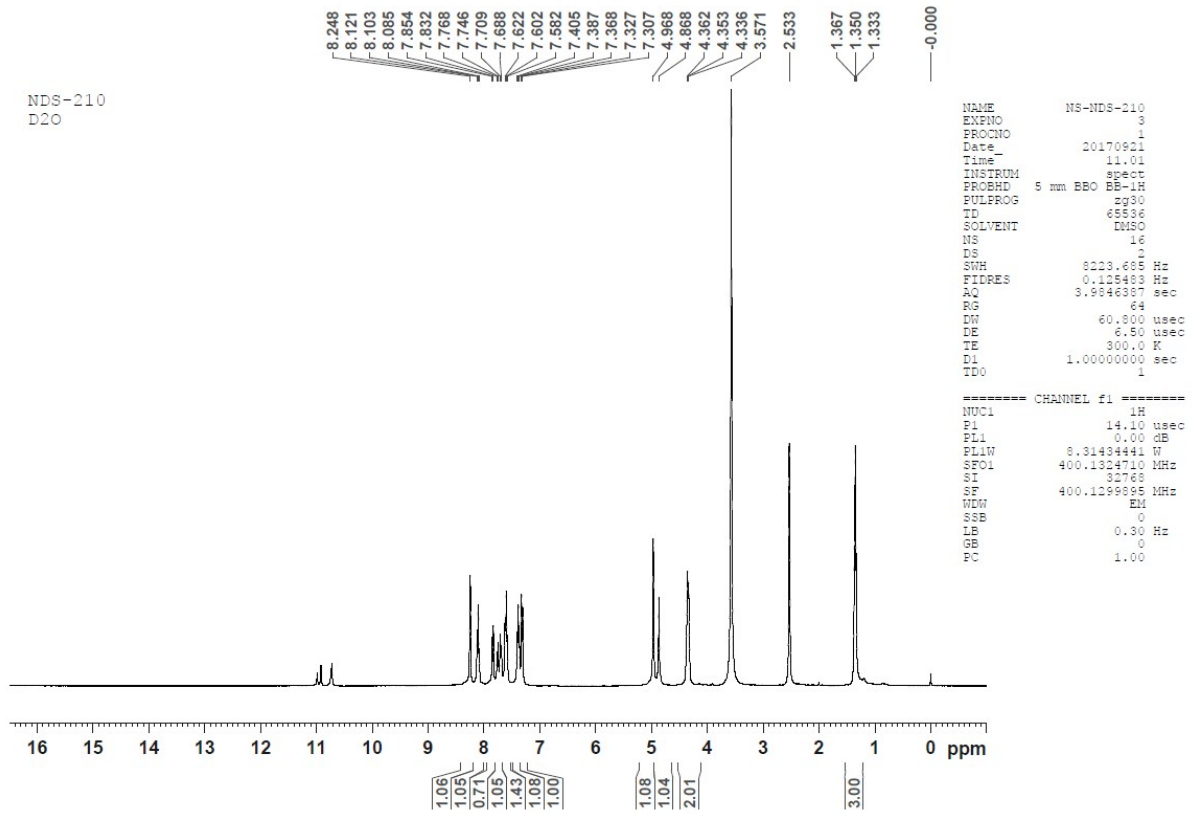
MASS Analysis of synthesized compound: 17h M+1: 365



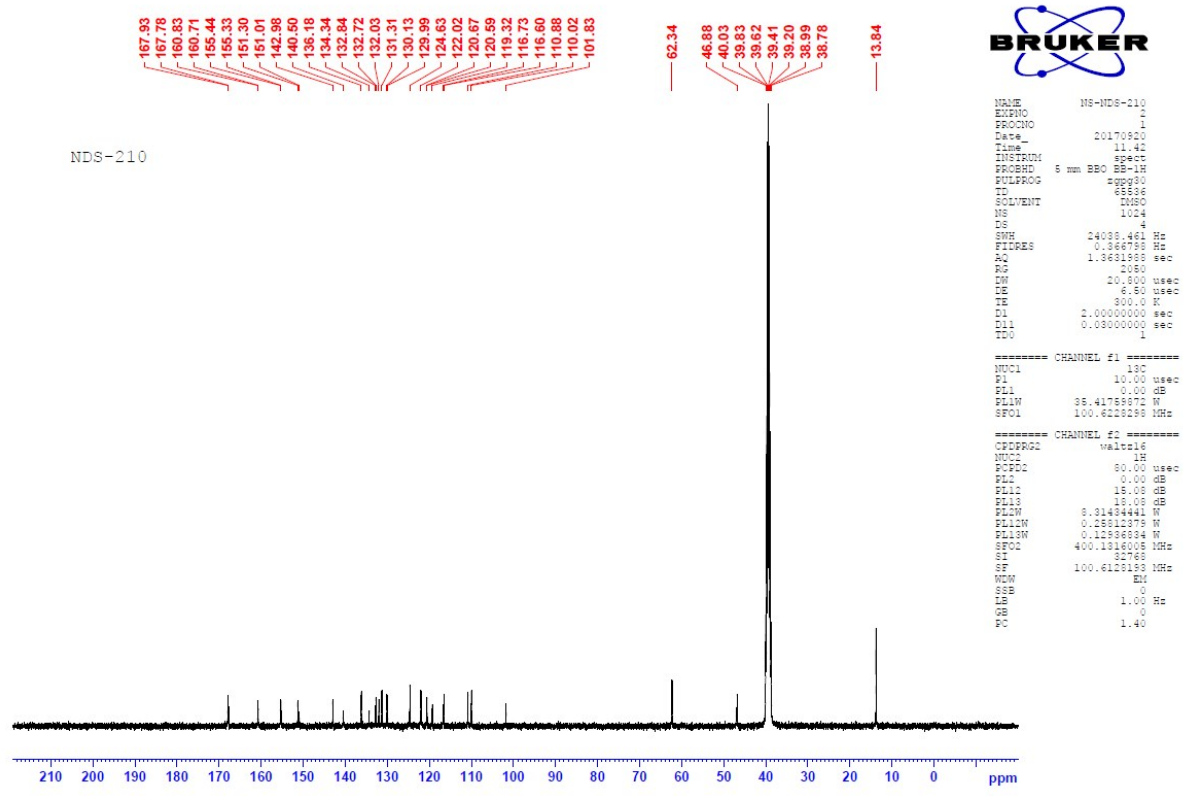
1H-NMR Analysis of synthesized compound: 17h



1H-NMR-D2O exchange analysis of synthesized compound: 17h



13C-NMR Analysis of synthesized compound: 17h

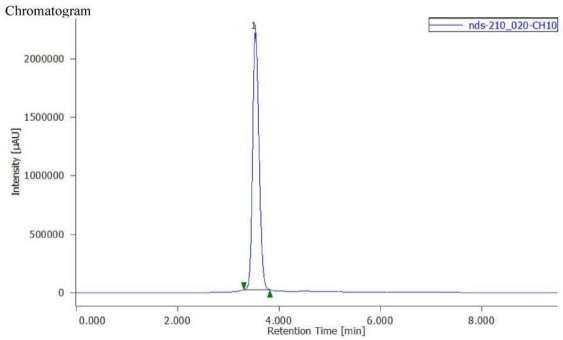


HPLC (percentage purity) of 17h

Benzimidazole derivatives_0915 nds-210_020 9/16/2017 7:14:53 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information	
User Name	Administrator
Date Modified	9/15/2017 7:15:18 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 4:32:26 PM
Volume	20.00 [µL]
Sample #	17
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

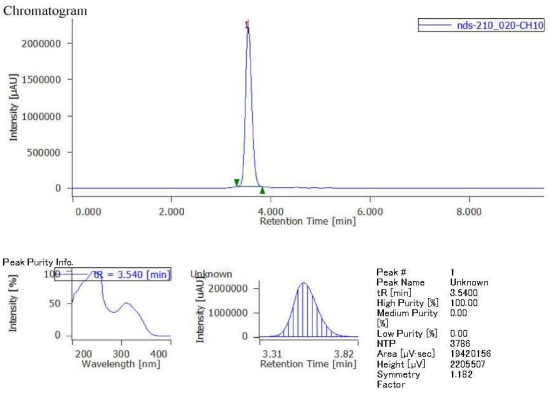
#	Peak Name	CH	tR [min]	Area [µV*sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.540	19420156	2205507	100.000	100.000	3786	N/A	1.182

HPLC (peak purity) of 17h

Benzimidazole derivatives_0915 nds-210_020 9/22/2017 10:30:29 AM

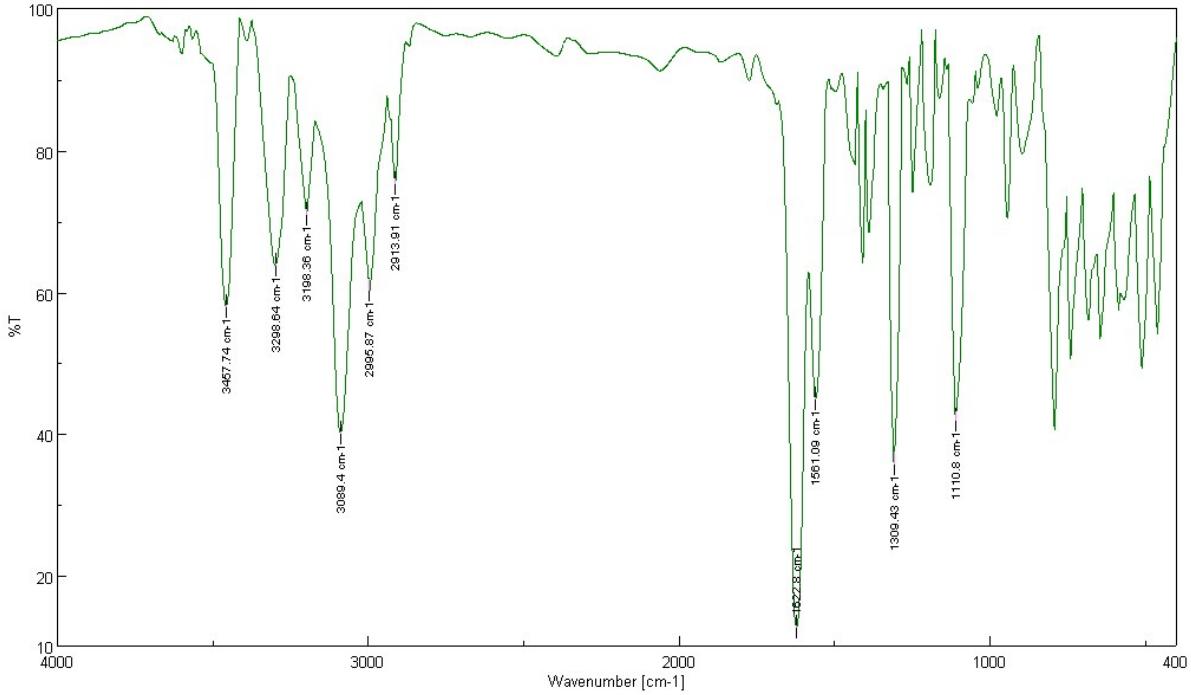
Institute of Pharmacy, Nirma University

Report - HPLC peak purity

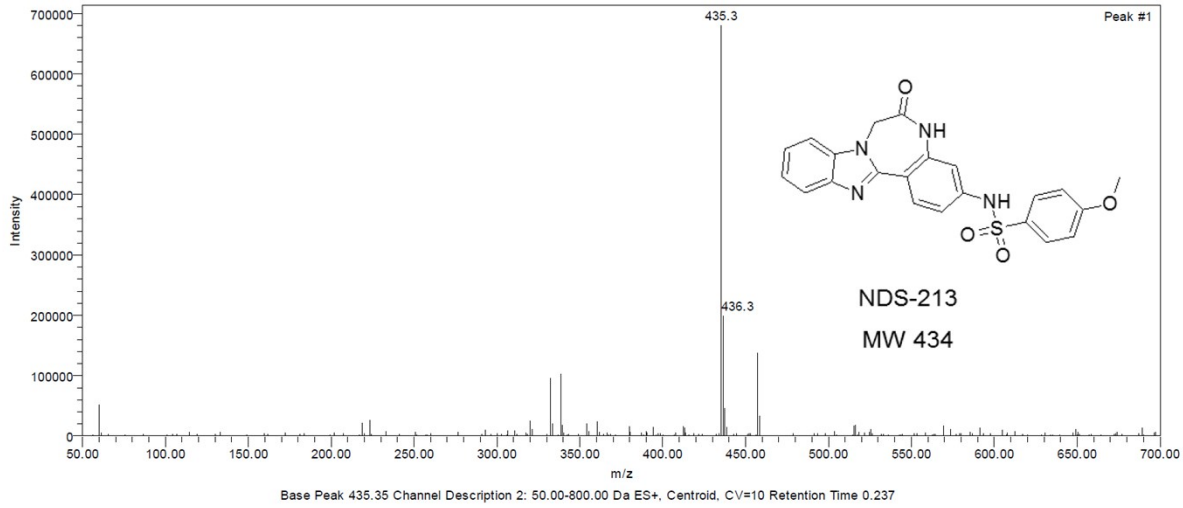


Peak #	1
Peak Name	Unknown
tR [min]	3.5400
High Purity [%]	100.00
Medium Purity [%]	0.00
Low Purity [%]	0.00
NTP	3786
Area [µV*sec]	19420156
Height [µV]	2205507
Symmetry Factor	1.182

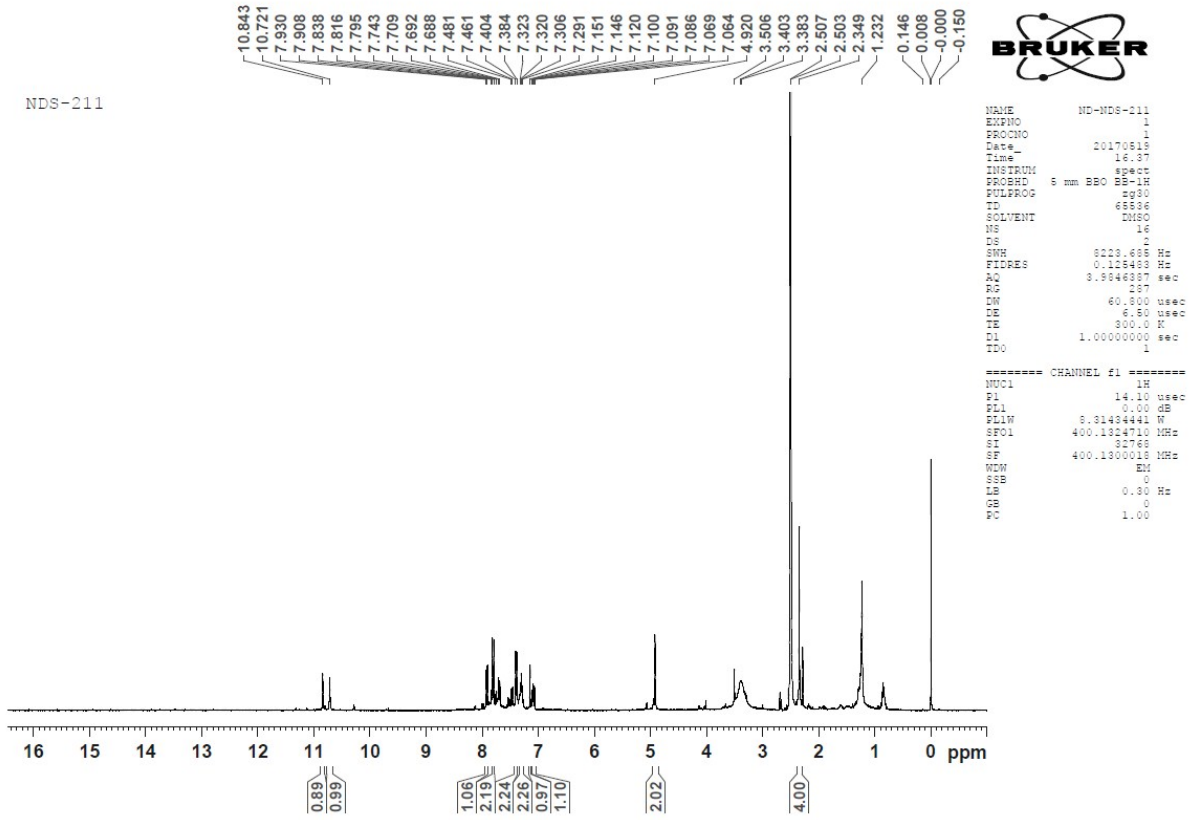
FTIR spectra of 17i



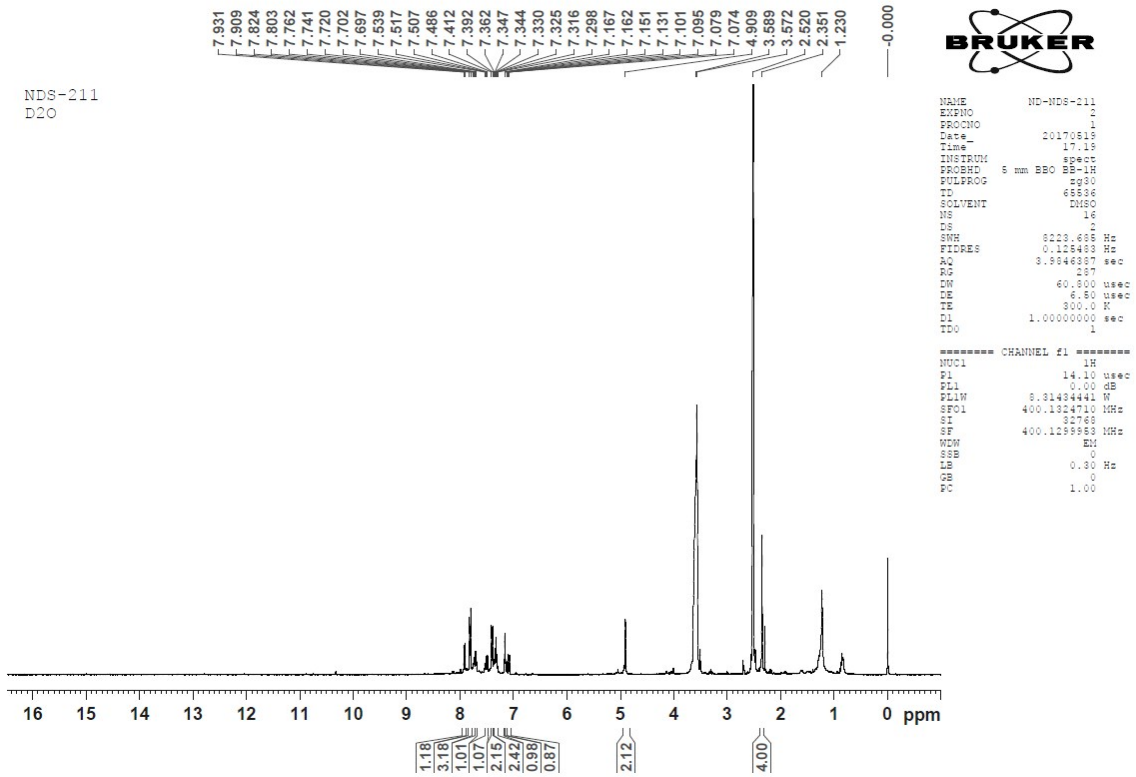
MASS Analysis of synthesized compound: 17i M+1: 435



1H-NMR Analysis of synthesized compound: 17i



1H-NMR-D2O exchange analysis of synthesized compound: 17i

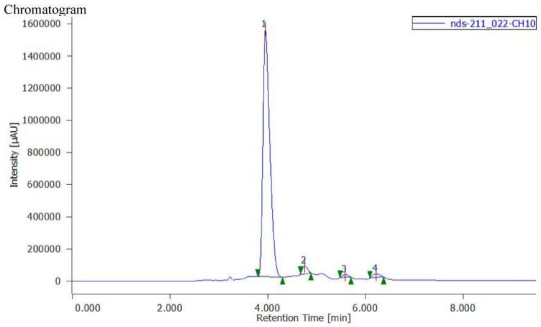


HPLC (percentage purity) of 17i

Benzimidazole derivatives_0915 nds-211_022 9/16/2017 7:15:16 PM

Institute of Pharmacy, Nirma University

Report - HPLC analysis



Chromatogram Information

User Name	Administrator
Date Modified	9/15/2017 7:15:20 PM
Description	
HPLC System Name	Jasco HPLC-4000
Injection Date	9/15/2017 4:53:22 PM
Volume	20.00 [µL]
Sample #	19
Project Name	DST
Acquisition Time	9.5 [min]
Acquisition Sequence	
Control Method	10min8020meohbuffer1mlpermin
Peak ID Table	

Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	NTP	Resolution	Symmetry Factor
1	Unknown	10	3.957	15110610	1538162	95.308	94.496	3864	3.429	1.514
2	Unknown	10	4.763	369143	49509	2.326	3.042	7891	3.659	N/A
3	Unknown	10	5.590	146076	17778	0.921	1.092	8203	2.251	1.045
4	Unknown	10	6.223	228722	22311	1.443	1.371	6571	N/A	1.076

HPLC (peak purity) of 17i

Benzimidazole derivatives_0915 nds-211_022 9/22/2017 10:43:17 AM

Institute of Pharmacy, Nirma University

Report - HPLC peak purity