Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Synthesis of D-D-A-type small organic molecules with enlarged linker system towards organic solar cells and effect of co-adsorbents on cell performance

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CORRESPONDING AUTHOR FOOTNOTE

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Supporting information S1

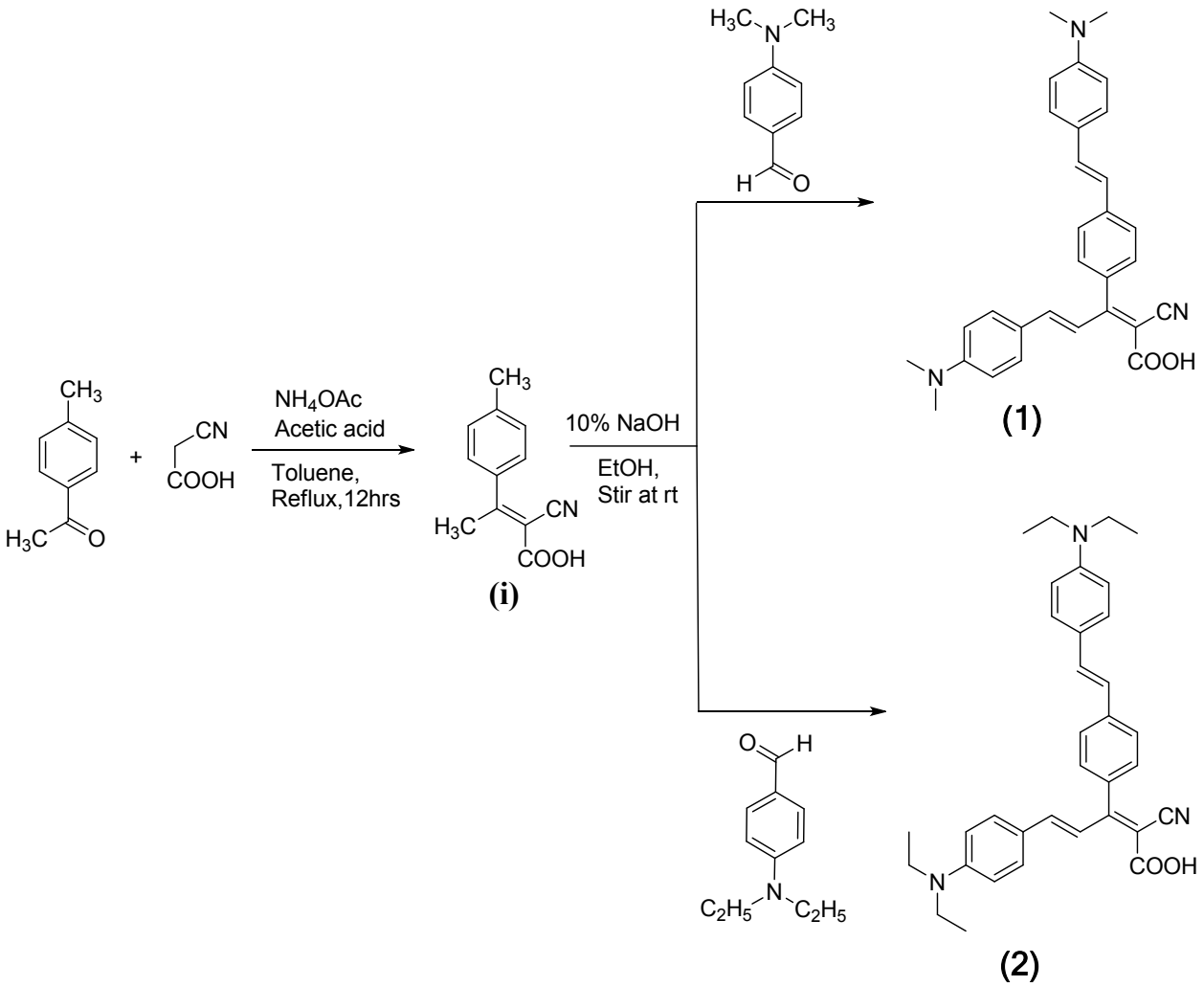


Fig S1. Scheme 1. Synthetic route for (a) Compound 1 (b) Compound 2

Supporting information S2

IR, ^{1}H NMR, ^{13}C NMR, Mass and LC-HR-MS spectra of Compound (i), 1 and compound 2

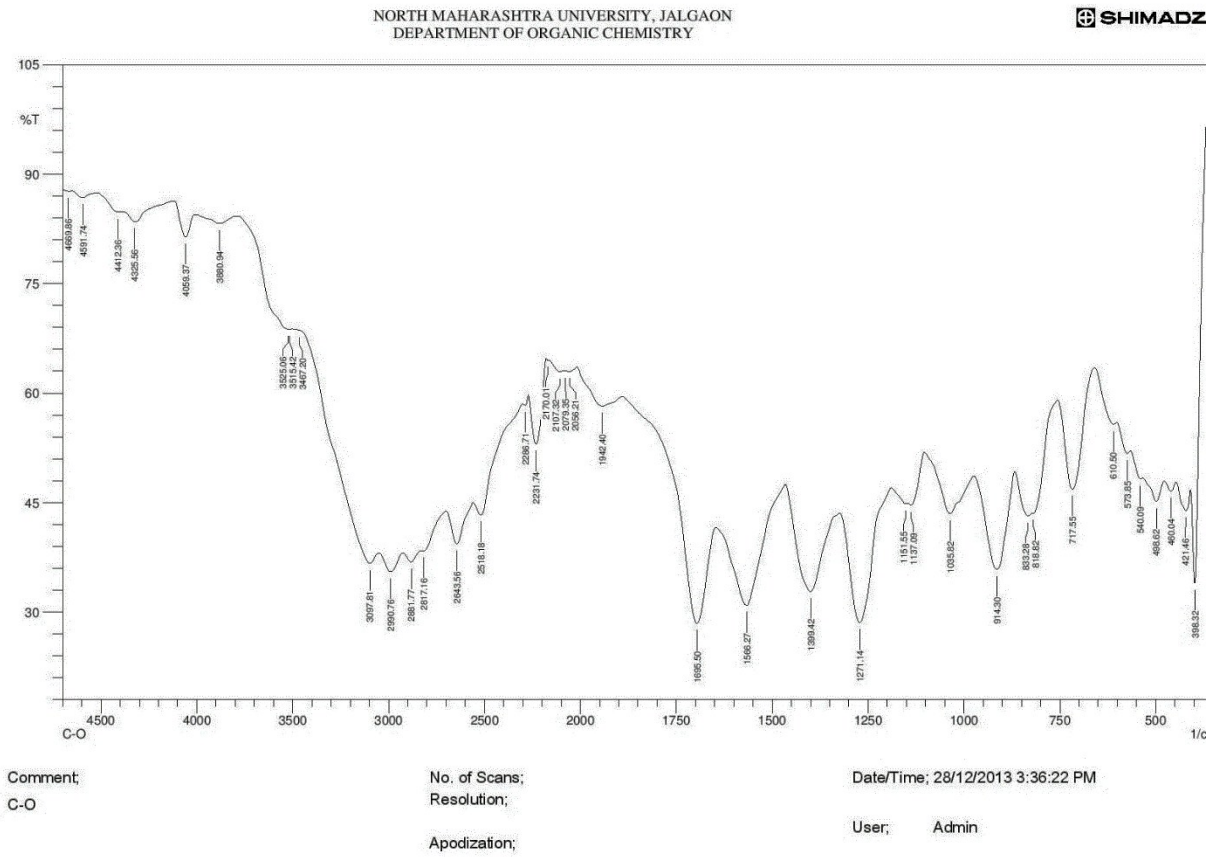


Fig S2.1. IR spectrta of Compound (i)

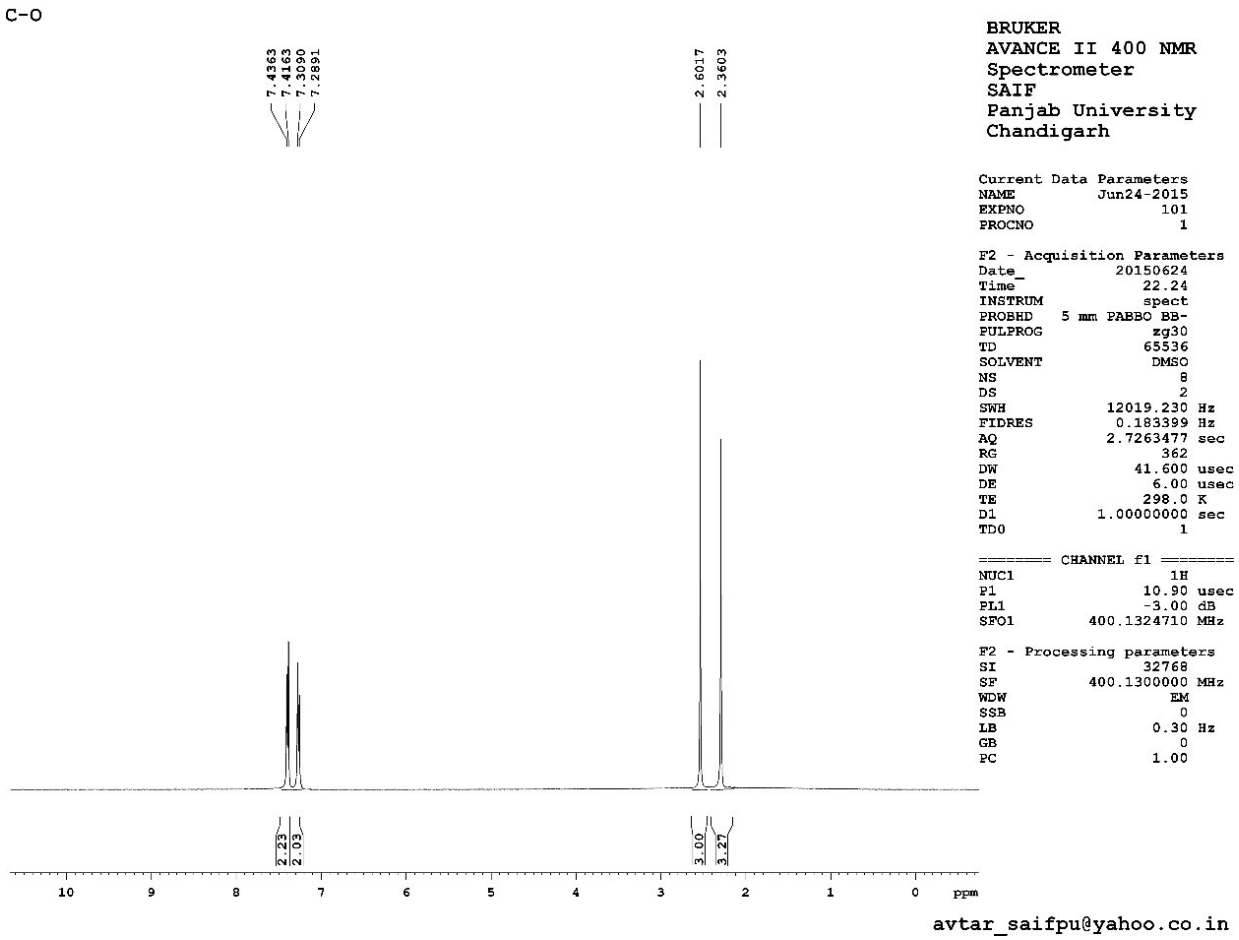


Fig S2.2. ^{1}H NMR spectra of Compound (i)

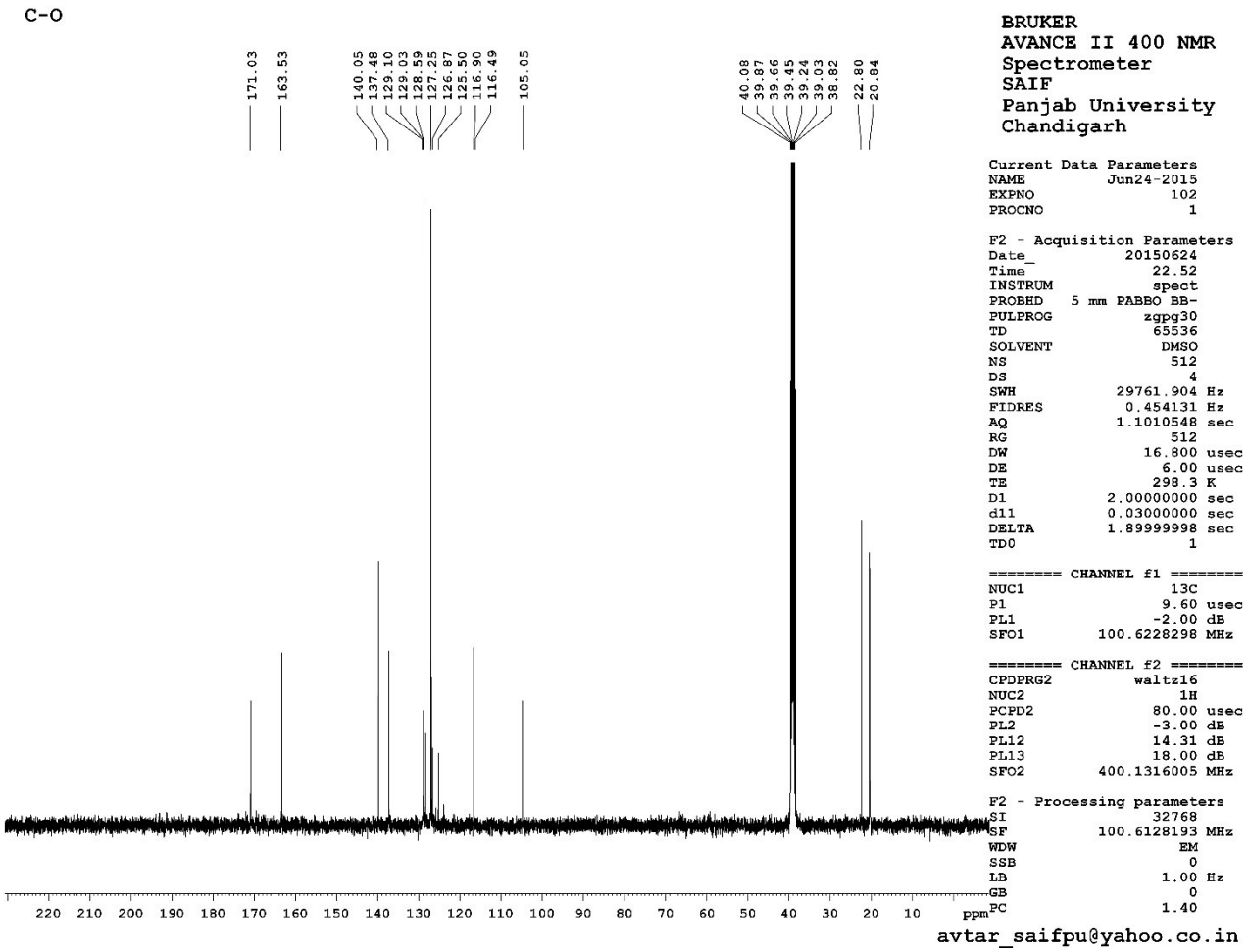


Fig S2.3. ^{13}C NMR spectra of Compound (i)

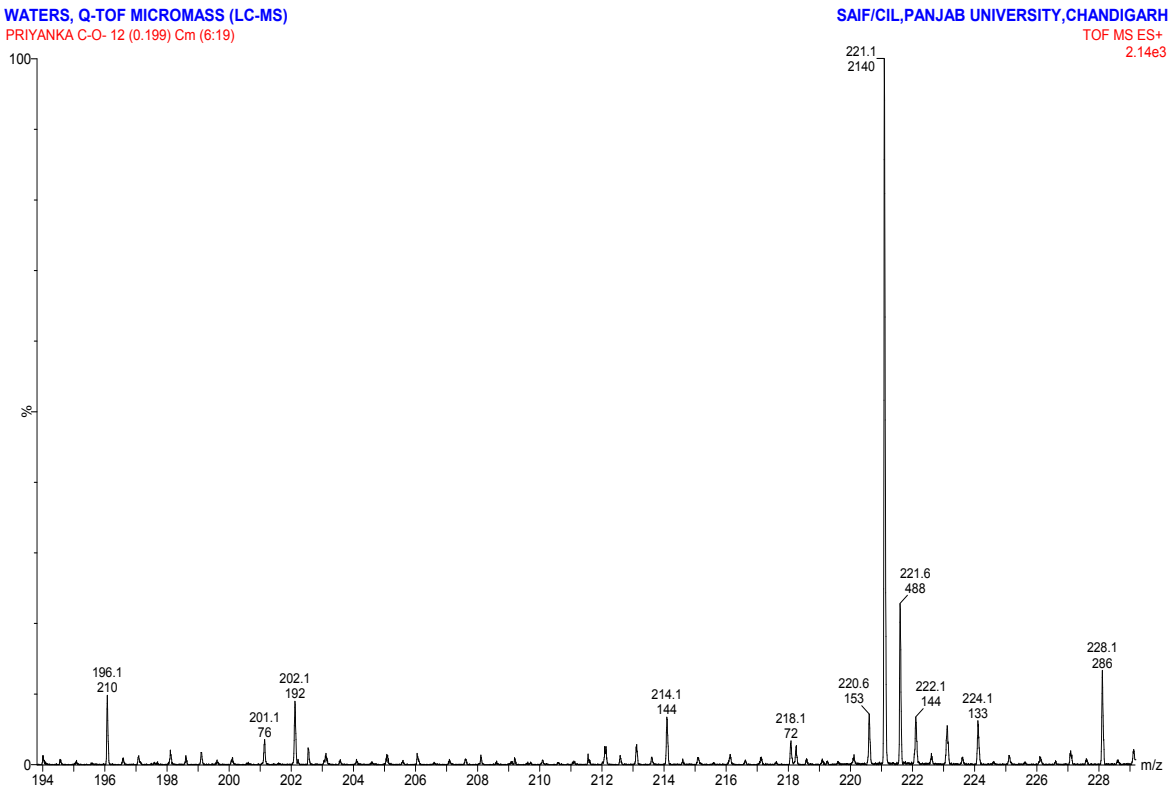


Fig S2.4. Mass spectra of Compound (i)

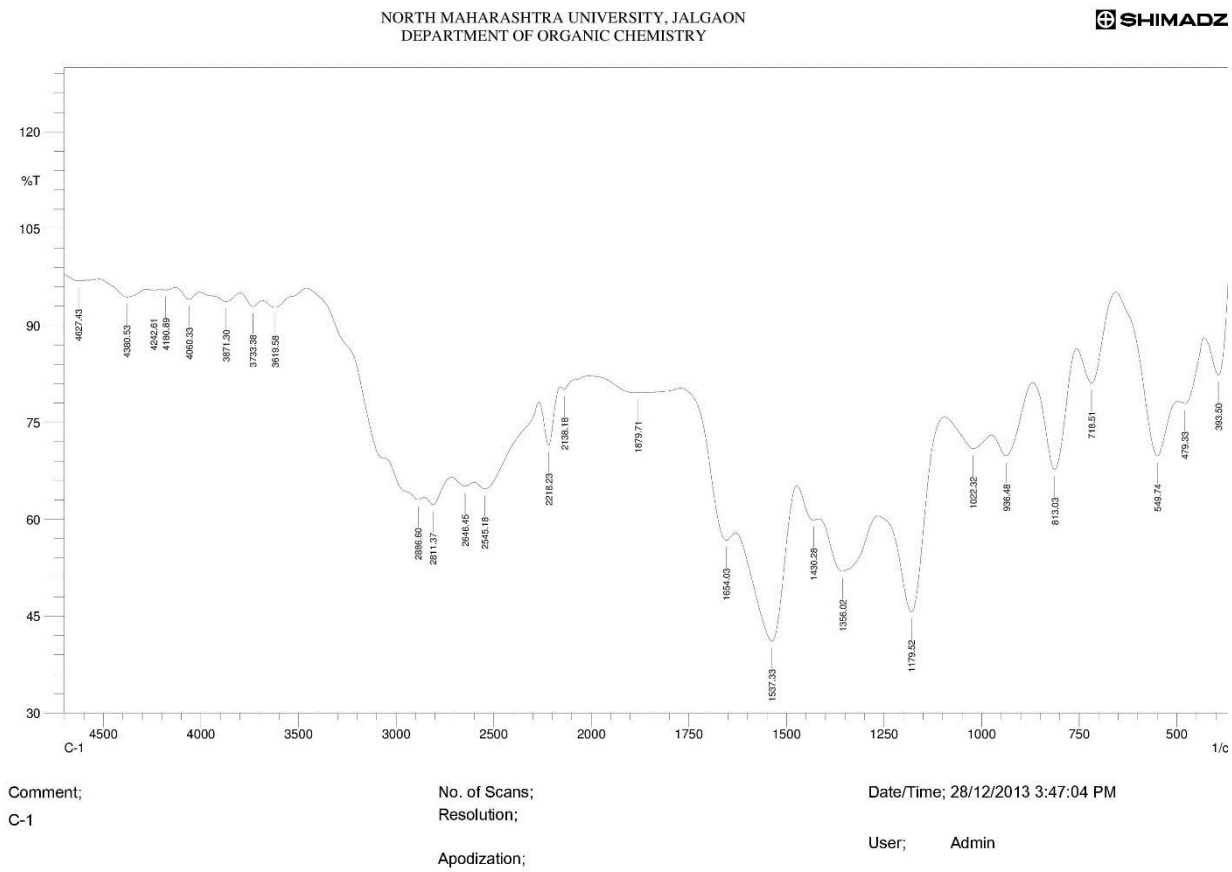
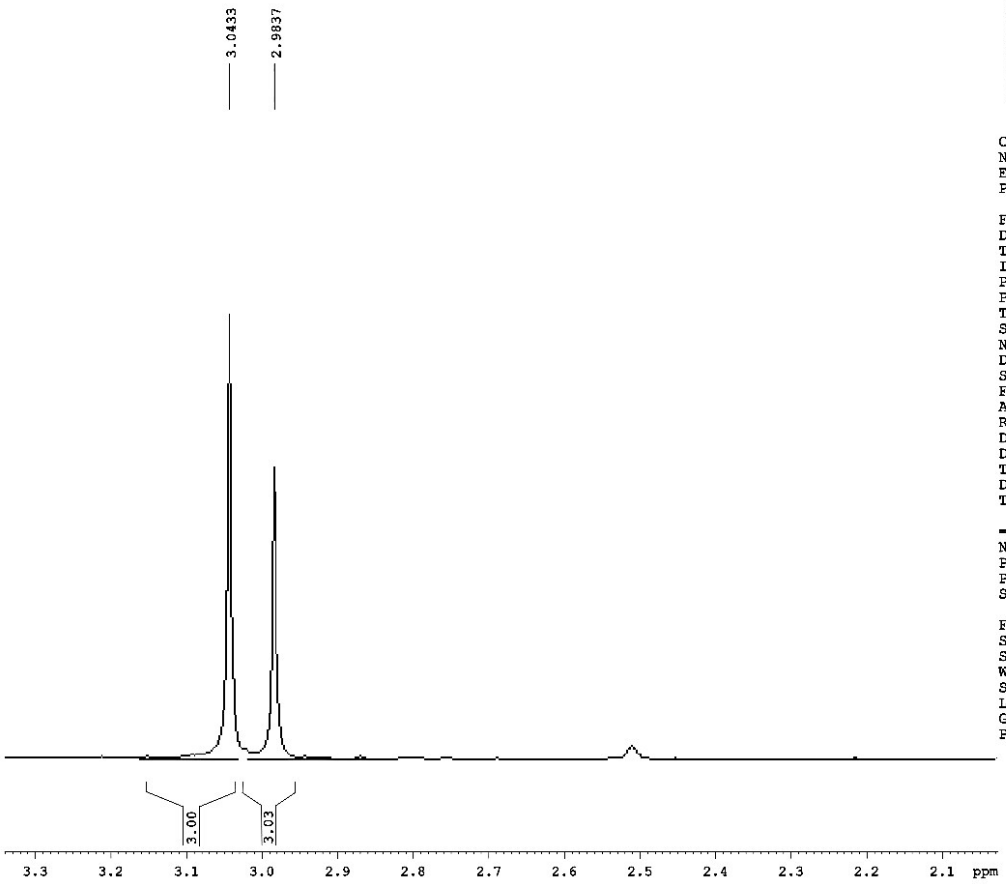


Fig S2.5. IR spectrta of Compound 1

C-1



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

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PROCNO	1
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PC	1.00

avtar_saifpu@yahoo.co.in

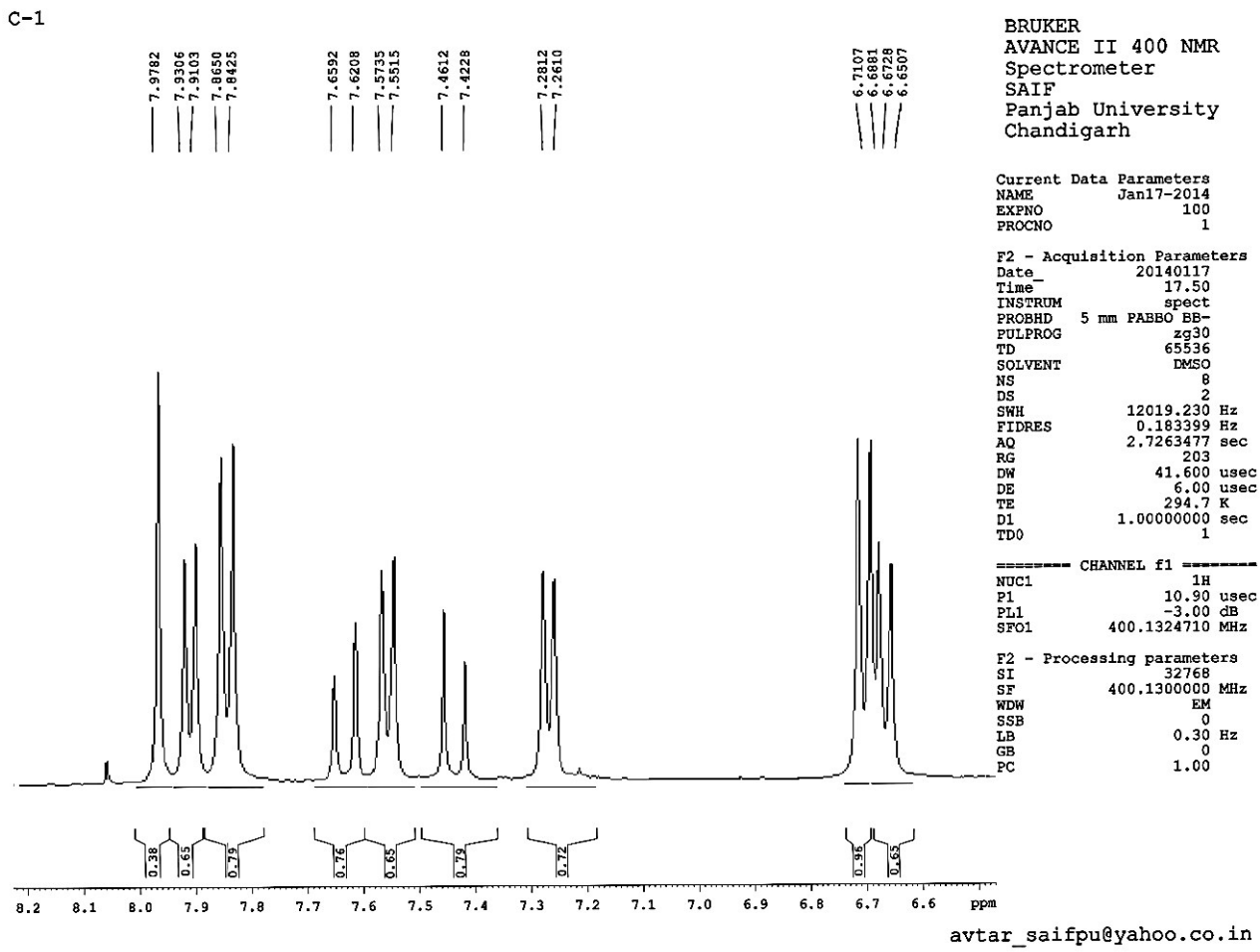

Fig S2.6. ^{1}H NMR spectra of Compound 1

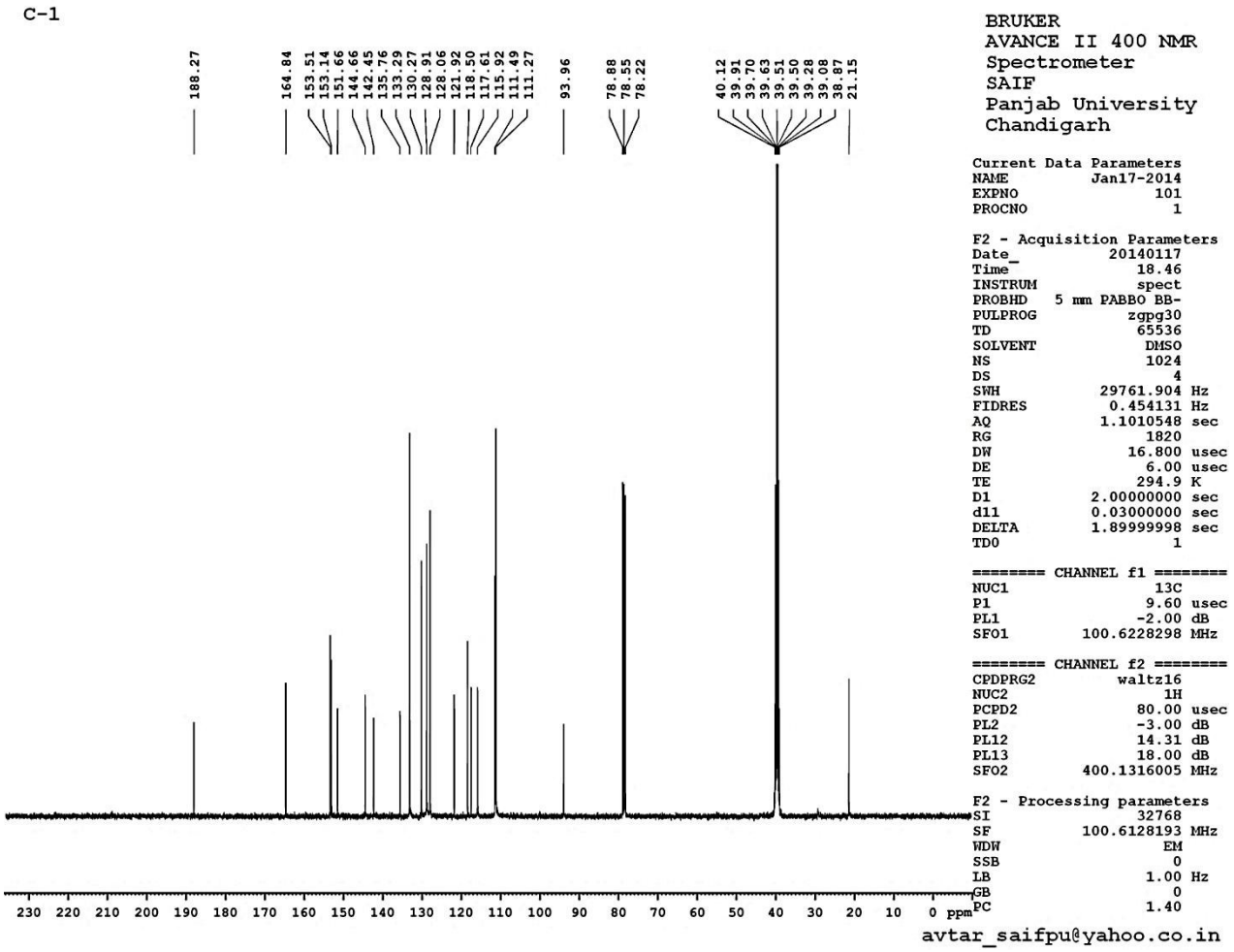

Fig S2.7. ^{13}C NMR spectra of Compound 1

Qualitative Compound Report

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IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C30 H29 N3 O2	0.144	463.2279	299	C30 H29 N3 O2	463.226	4.17	C30 H29 N3 O2	C30 H29 N3 O2

Compound Label	*m/z*	RT	Algorithm	Mass
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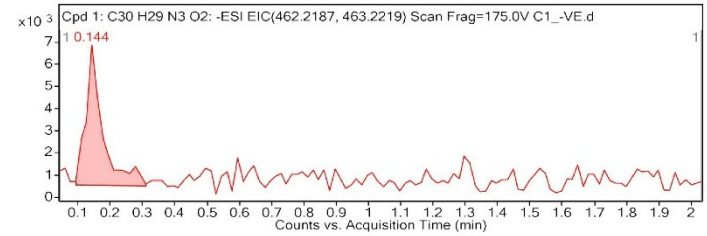
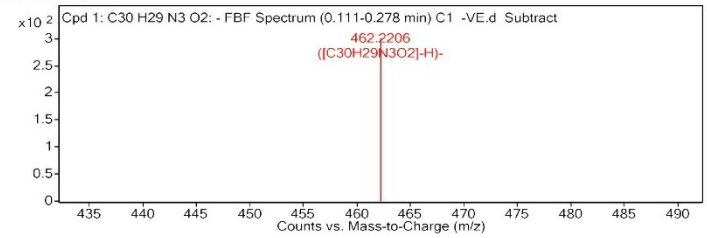


MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
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--- End Of Report ---

Fig S2.8. LC-HR-MS of Compound 1

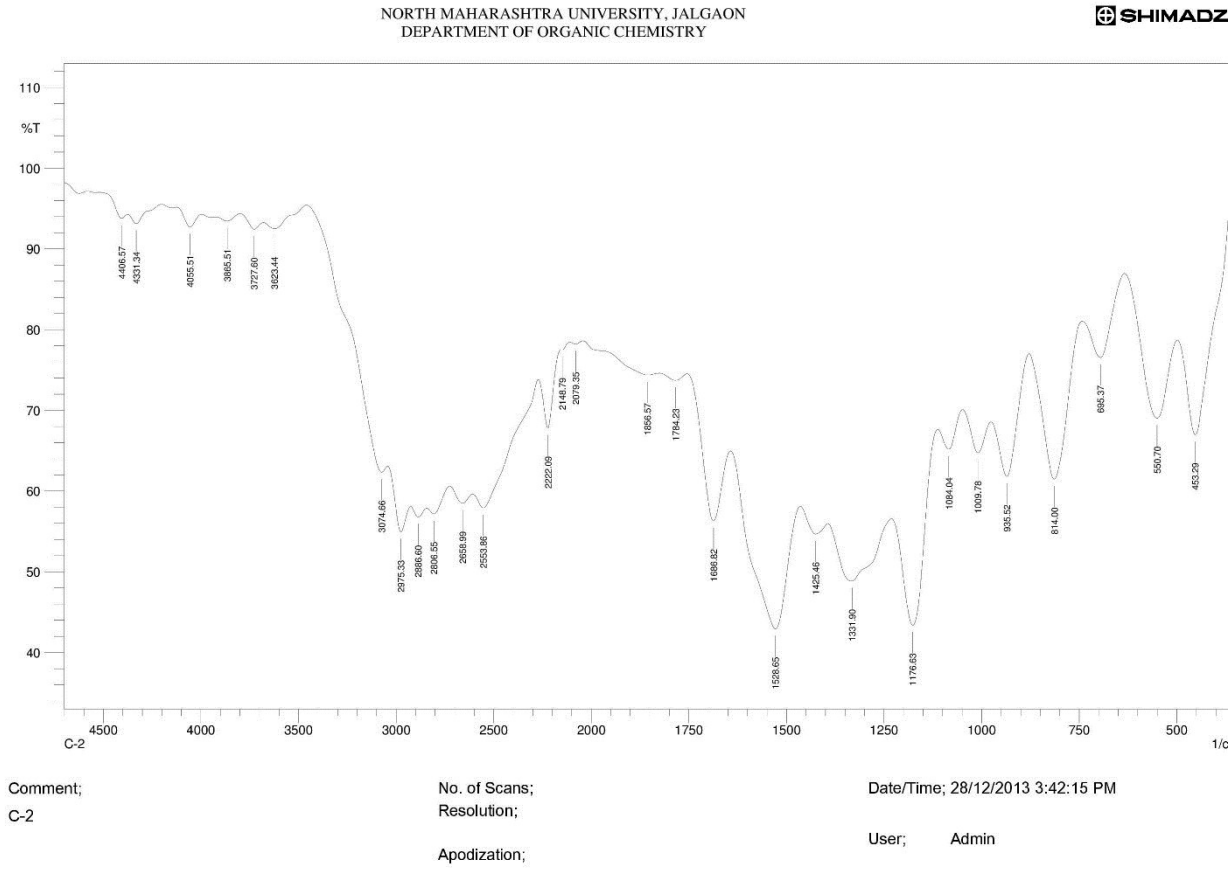
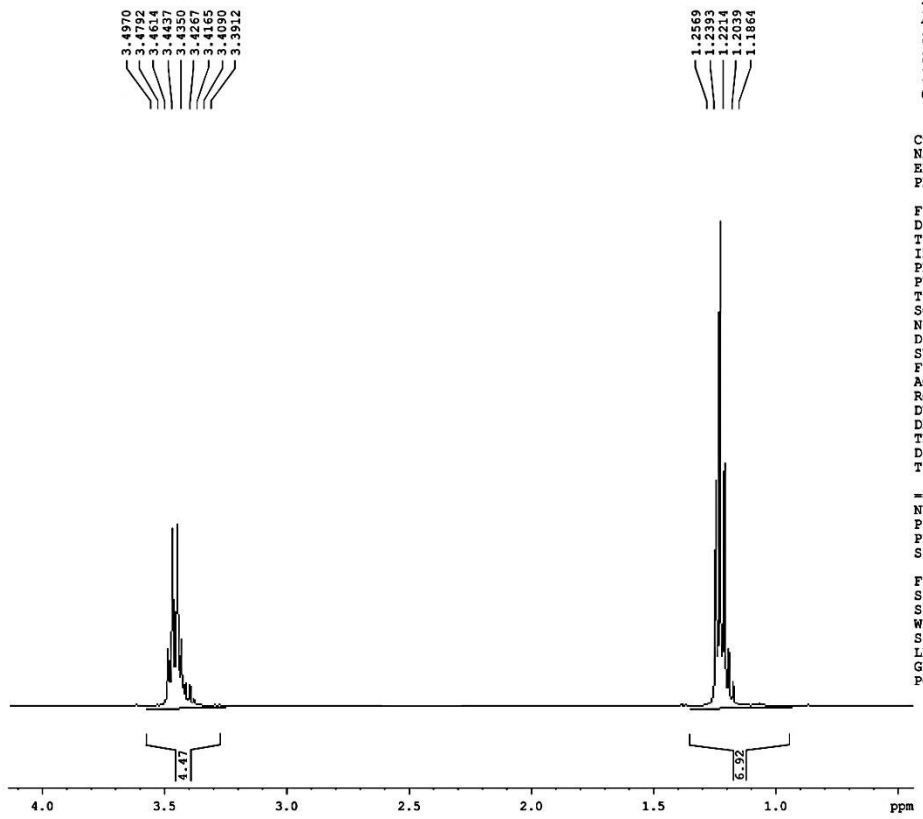


Fig S2.9. IR spectrta of Compound 2

C-2



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

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PROCNO	1
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FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	456
DW	41.600 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
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P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
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SF	400.1300083 MHz
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GB	0
PC	1.00

avtar_saifpu@yahoo.co.in

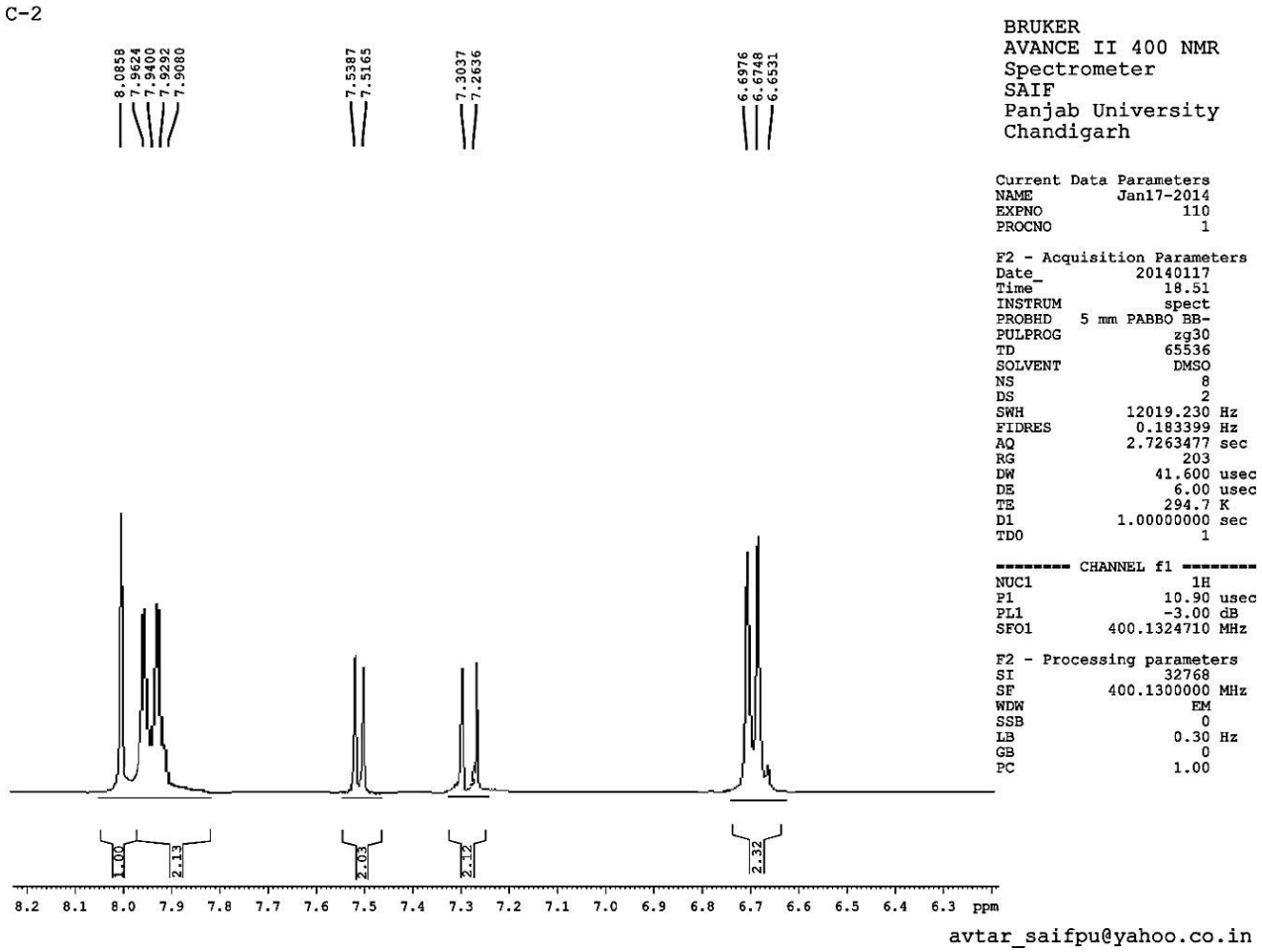

Fig S2.10. ^{1}H NMR spectrta of Compound 2

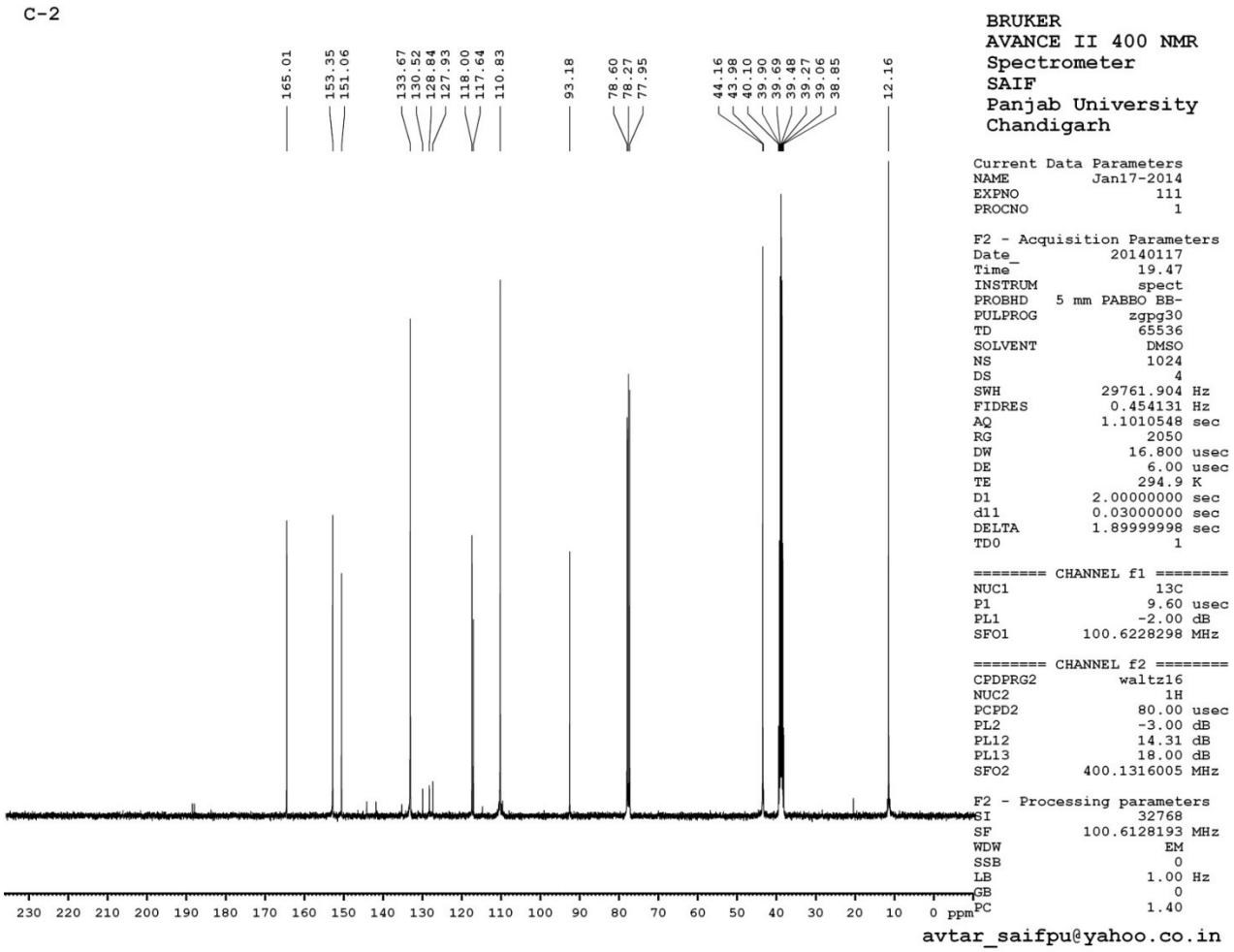

Fig S2.11. ^{13}C NMR spectrta of Compound 2

Qualitative Compound Report

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Sample Type	Sample	**Position**	P1C4
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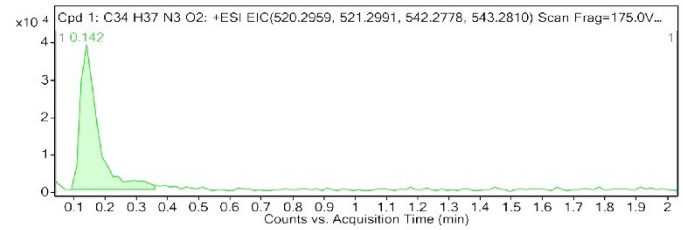
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)		

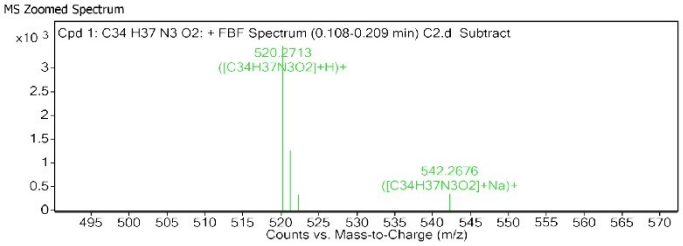
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C34 H37 N3 O2	0.142	519.2656	3473	C34 H37 N3 O2	519.2886	-44.25	C34 H37 N3 O2	C34 H37 N3 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C34 H37 N3 O2	520.2713	0.142	Find By Formula	519.2656



MS Zoomed Spectrum



MS Spectrum Peak List

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521.2765	1	1257.72	C34H37N3O2	(M+H)+
522.2812	1	315.92	C34H37N3O2	(M+H)+
542.2676	1	345.28	C34H37N3O2	(M+Na)+

--- End Of Report ---

Fig S2.12. LC-HR-MS of Compound 2

Supporting information S3

Estimation of the optical band gap for TiO_2

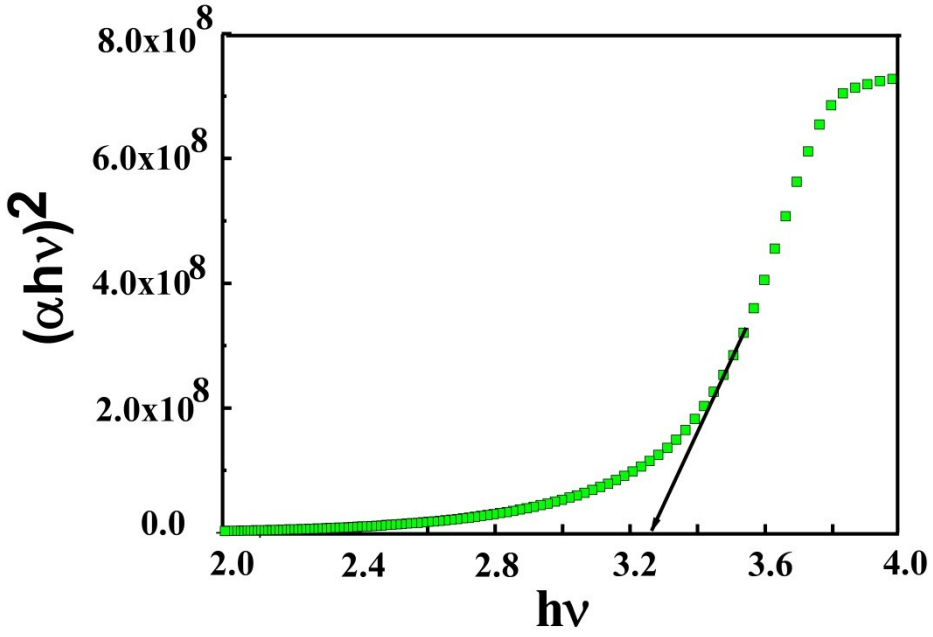


Fig S3. Plot of $(\alpha h\nu)^2$ vs. $(h\nu)$ for the estimation of the band gap energy value

(400^oC annealed TiO_2 coating)

Supporting information S4

Estimation of the optical band gap for synthesised organic compounds

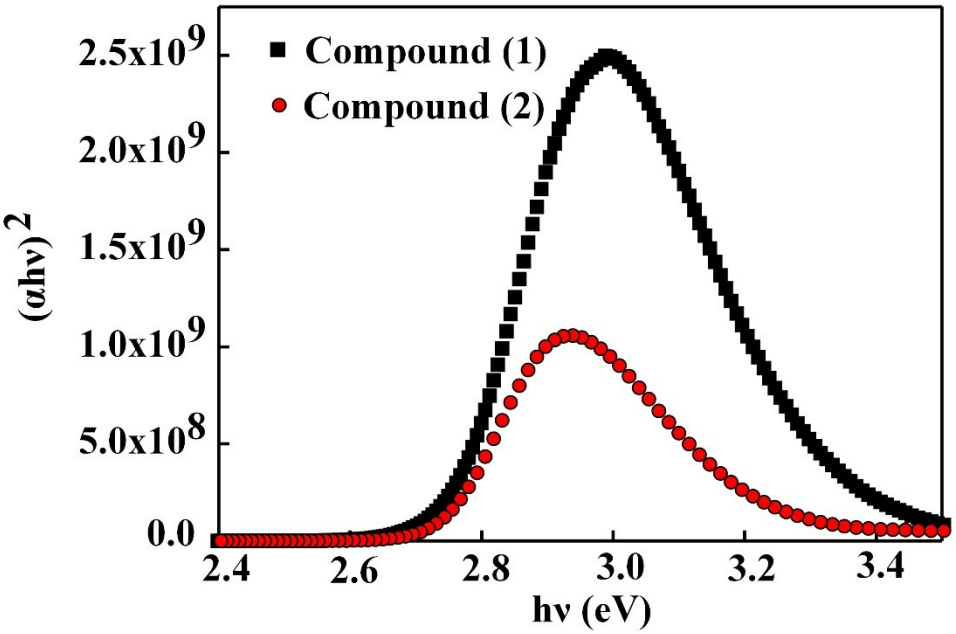


Fig S4. Optical band gap for synthesised organic compounds

Supporting information S5

FE-SEM Images

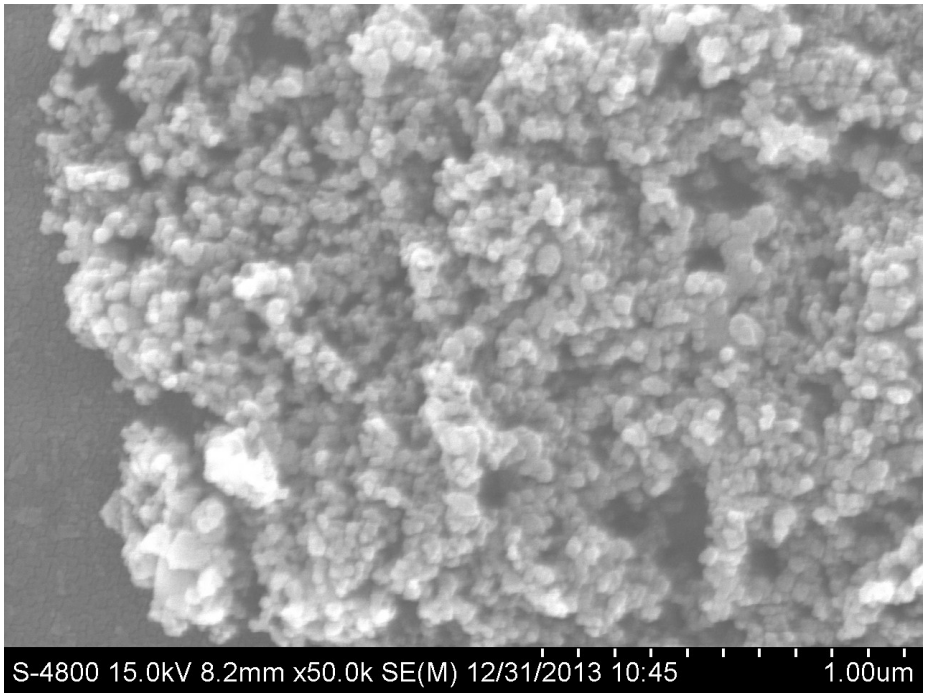


Fig S5.1. FE-SEM image for TiO_2 thin film

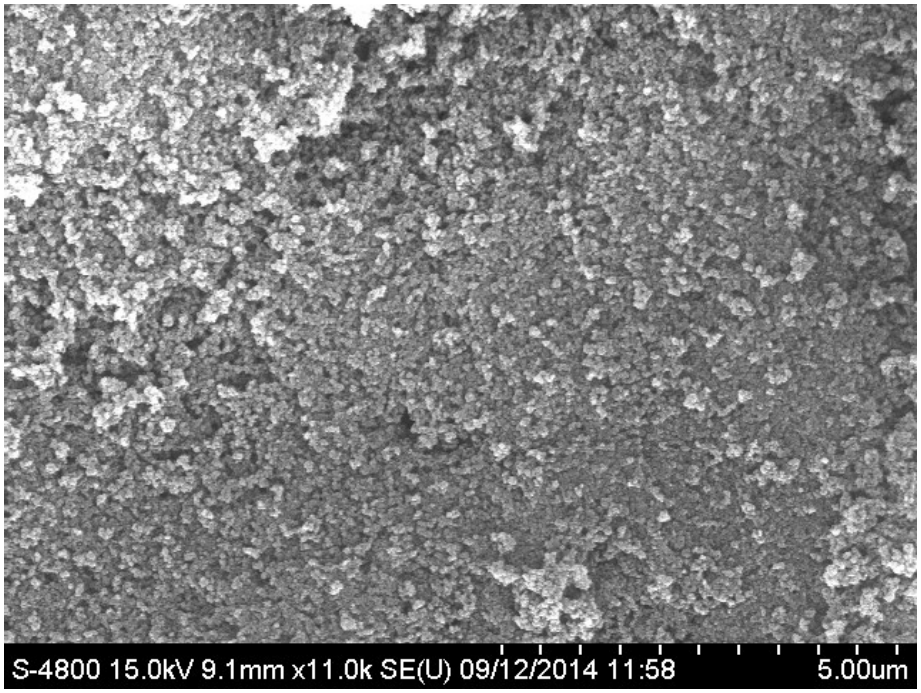


Fig S5.2. FE-SEM image for Compound 1 without Cholic Acid coated on TiO_2 film

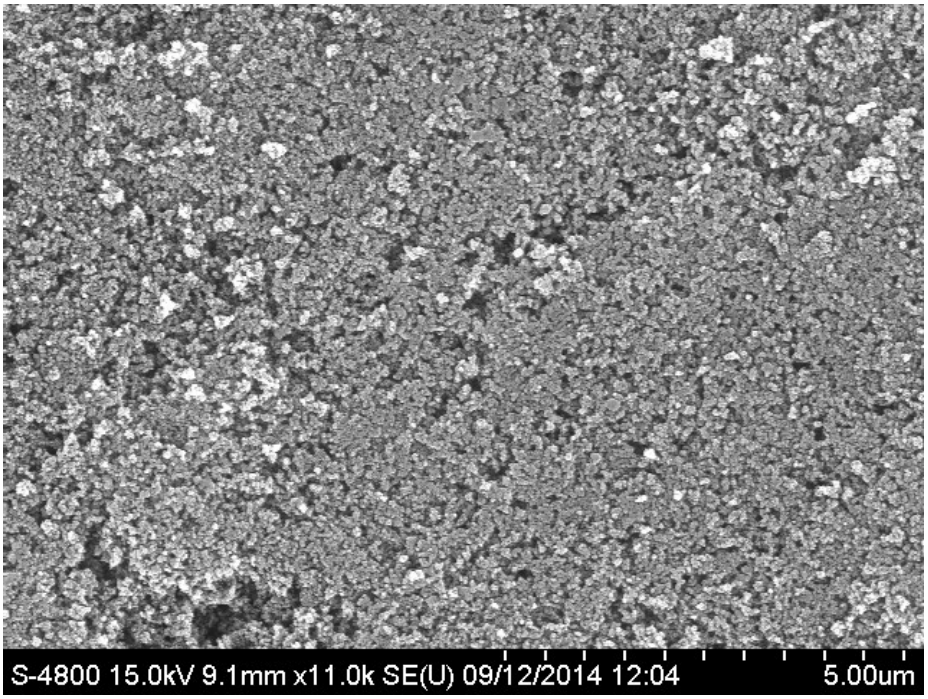


Fig S5.3. FE-SEM image for Compound 2 without Cholic Acid coated on TiO_2 film

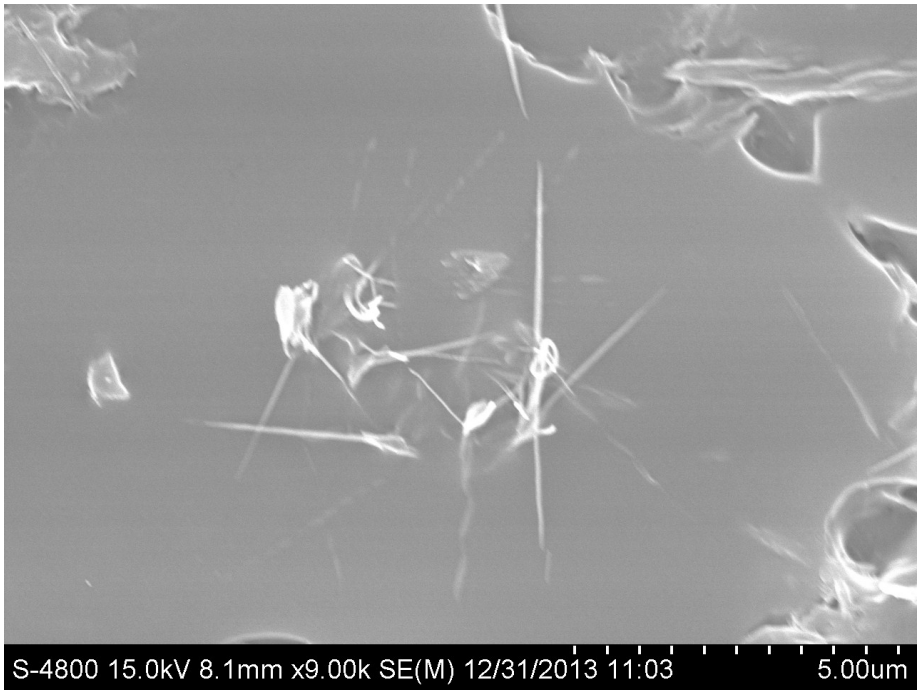


Fig S5.4. FE-SEM image for Compound 1 with Cholic Acid as co-adsorbent coated on TiO_2 film

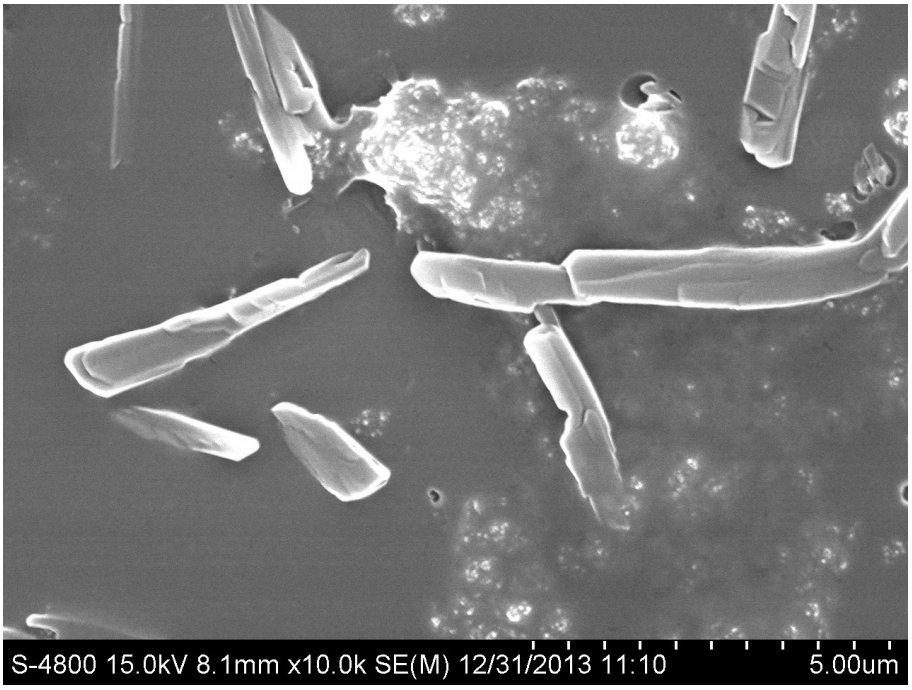
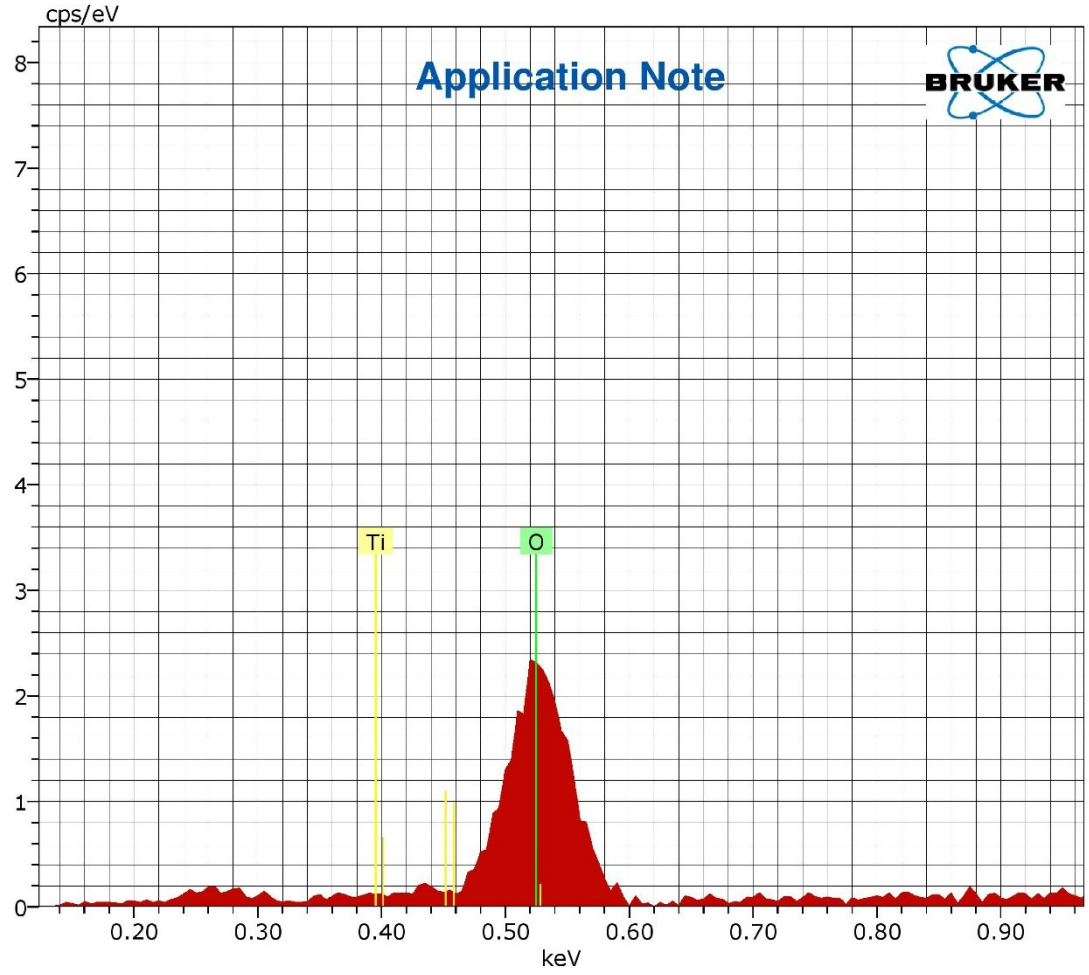


Fig S5.5. FE-SEM image for Compound 2 with Cholic Acid as co-adsorbent coated on TiO_2 film

Supporting information S6

EDAX analysis



1723 Date:12/31/2013 11:26:24 AM HV:15.0kV Puls th.:2.02kcps

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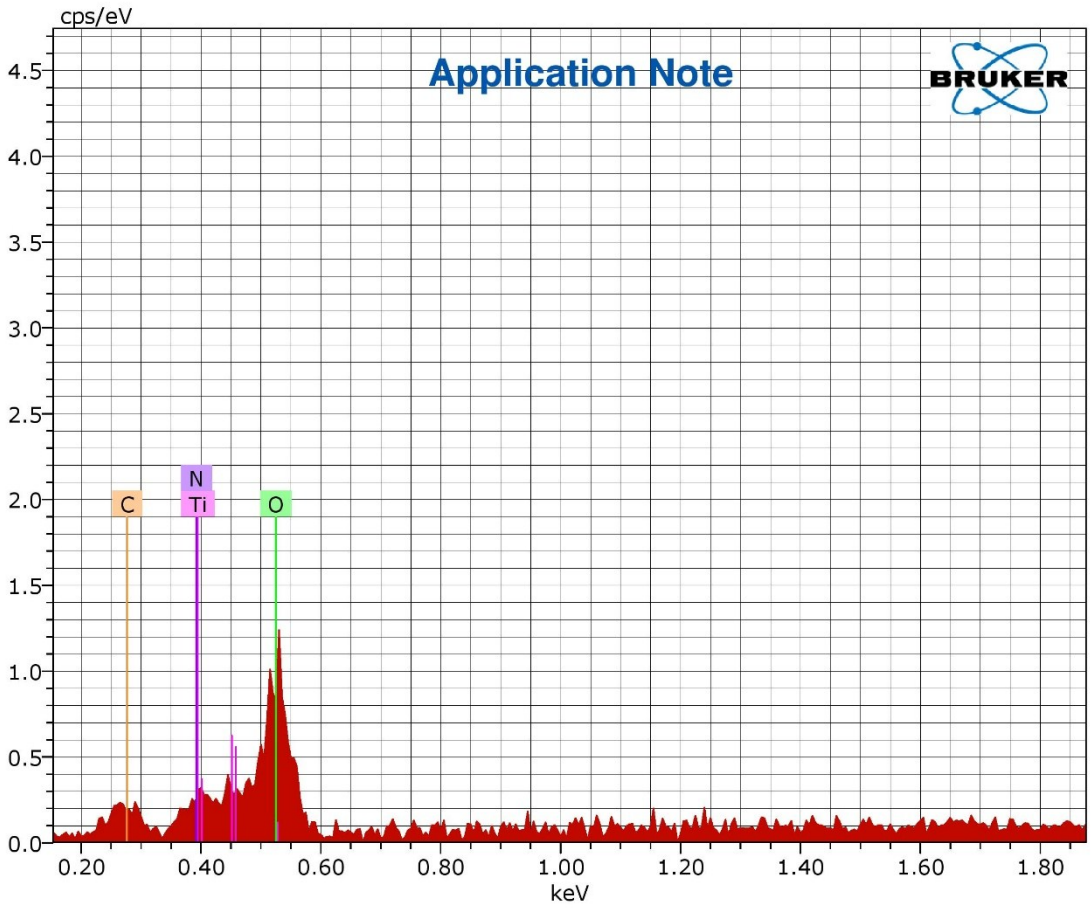
O	8	K-series	6.65	86.33	94.98	1.30
Ti	22	K-series	1.05	13.67	5.02	0.09
		Total:	7.71	100.00	100.00	

Spectrum: 1723

El	AN	Series	unn. C [wt.%]	norm. C [wt.%]	Atom. C [at.%]	Error (1 Sigma) [wt.%]
O	8	K-series	6.65	86.33	94.98	1.30
Ti	22	K-series	1.05	13.67	5.02	0.09
		Total:	7.71	100.00	100.00	

Fig S6.1. EDAX report for TiO_2 thin film



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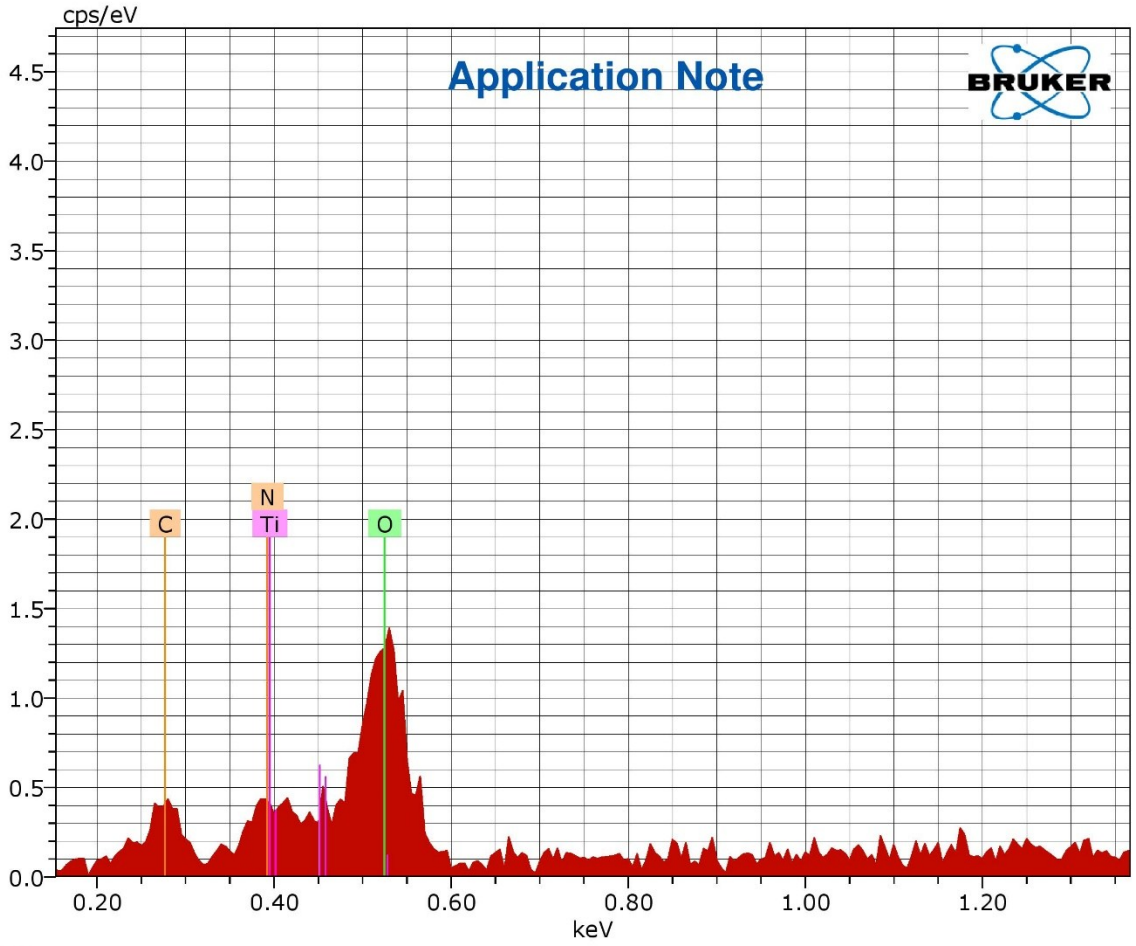
C	6	K-series	3.53	4.09	7.90	1.73
N	7	K-series	0.00	0.00	0.00	0.00
O	8	K-series	40.83	47.33	68.58	10.14
Ti	22	K-series	41.92	48.58	23.52	1.52
		Total:	86.28	100.00	100.00	

Spectrum: 3210

El	AN	Series	unn. C [wt.%]	norm. C [wt.%]	Atom. C [at.%]	Error (1 Sigma) [wt.%]
C	6	K-series	3.53	4.09	7.90	1.73
N	7	K-series	0.00	0.00	0.00	0.00
O	8	K-series	40.83	47.33	68.58	10.14
Ti	22	K-series	41.92	48.58	23.52	1.52
		Total:	86.28	100.00	100.00	

Fig S6.2. EDAX report for Compound 1 without Cholic Acid coated on TiO_2 film



3211 Date:12/9/2014 12:28:16 PM HV:15.0kV Puls th.:1.84kcps

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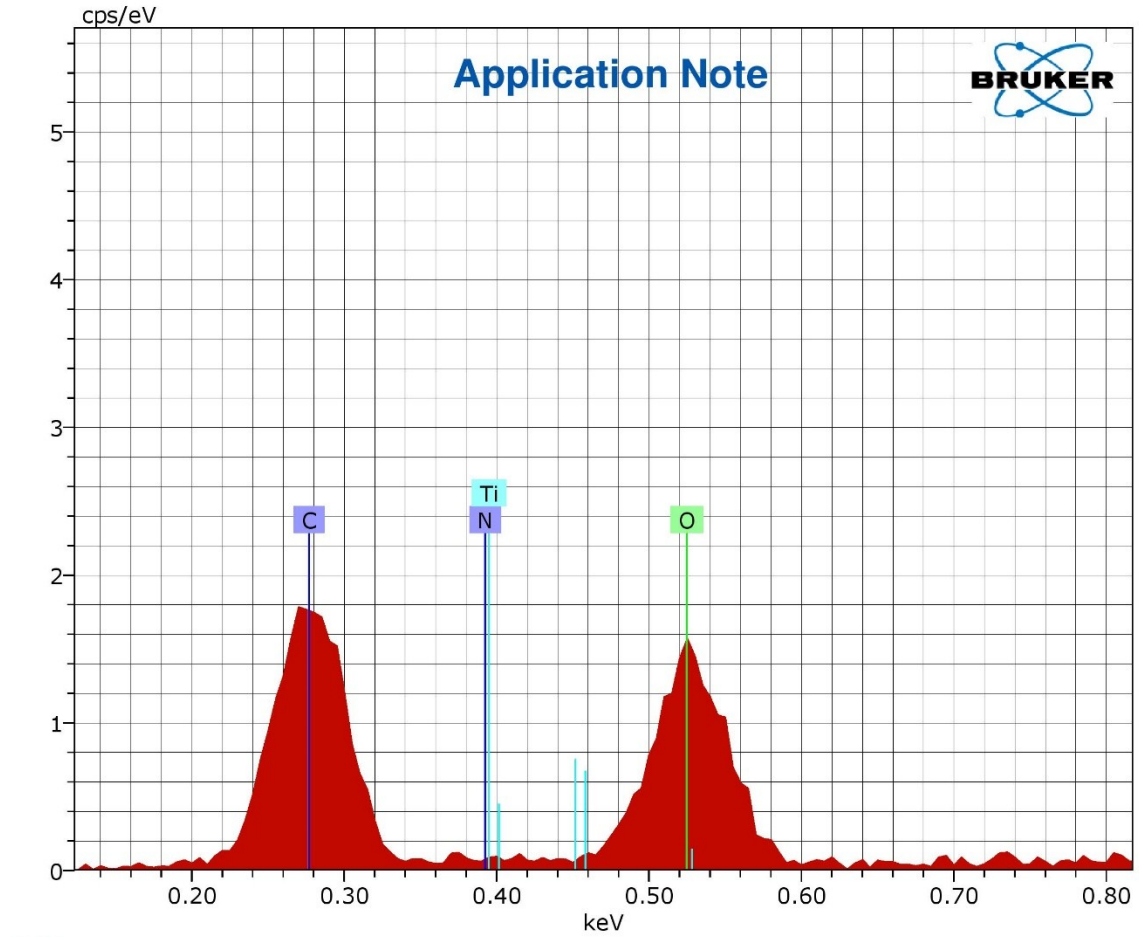
C	6	K-series	7.53	6.14	11.19	3.00
N	7	K-series	0.00	0.00	0.00	0.00
O	8	K-series	61.82	50.36	68.92	14.33
Ti	22	K-series	53.41	43.51	19.90	1.93
		Total:	122.76	100.00	100.00	

Spectrum: 3211

El	AN	Series	unn. C [wt.%]	norm. C [wt.%]	Atom. C [at.%]	Error (1 Sigma) [wt.%]
C	6	K-series	7.53	6.14	11.19	3.00
N	7	K-series	0.00	0.00	0.00	0.00
O	8	K-series	61.82	50.36	68.92	14.33
Ti	22	K-series	53.41	43.51	19.90	1.93
		Total:	122.76	100.00	100.00	

Fig S6.3. EDAX report for Compound 2 without Cholic Acid coated on TiO_2 film



1726 Date:12/31/2013 11:30:34 AM HV:15.0kV Puls th.:1.72kcps

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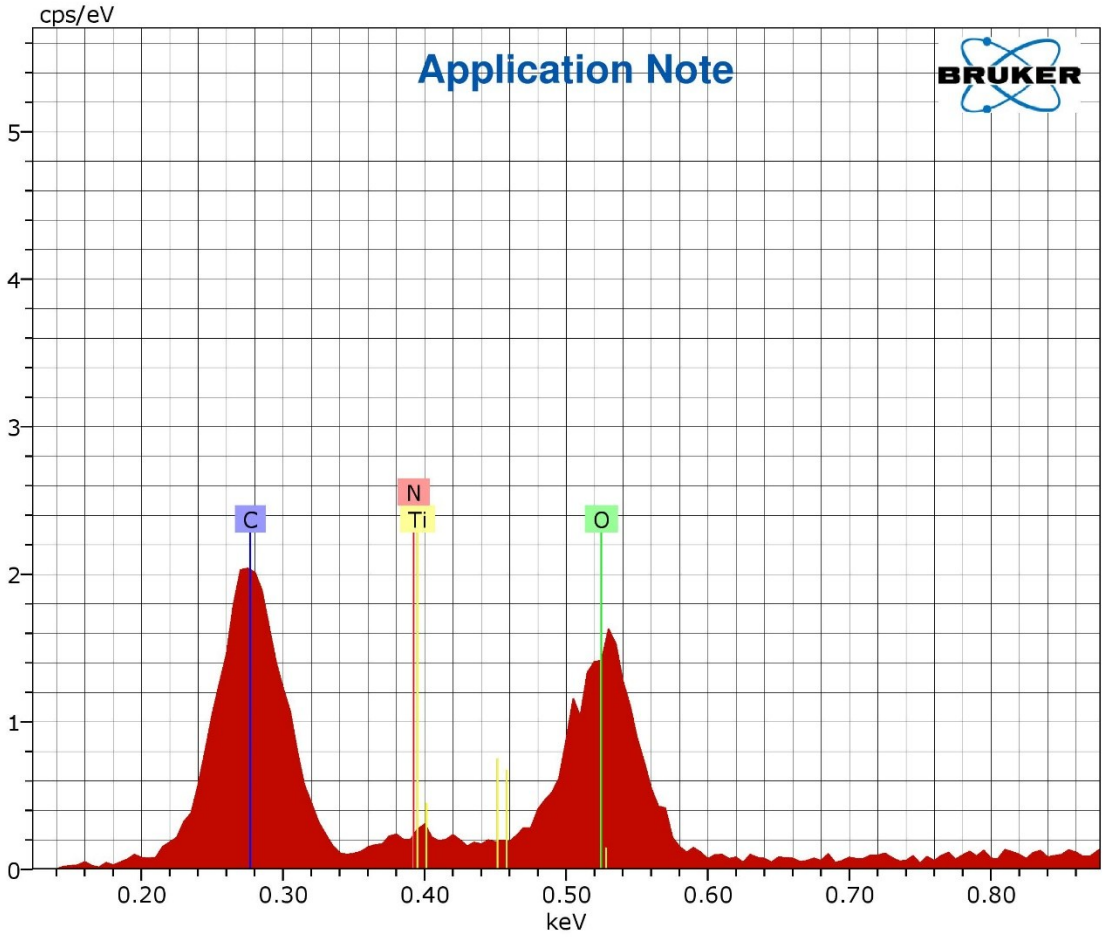
C	6	K-series	41.72	41.72	48.45	8.16
N	7	K-series	5.91	5.91	5.88	3.55
O	8	K-series	52.38	52.38	45.67	10.61
Ti	22	K-series	0.00	0.00	0.00	0.00
Total:			100.00	100.00	100.00	

Spectrum: 1726

El	AN	Series	unn. C [wt.%]	norm. C [wt.%]	Atom. C [at.%]	Error (1 Sigma) [wt.%]
C	6	K-series	41.72	41.72	48.45	8.16
N	7	K-series	5.91	5.91	5.88	3.55
O	8	K-series	52.38	52.38	45.67	10.61
Ti	22	K-series	0.00	0.00	0.00	0.00
Total:			100.00	100.00	100.00	

Fig S6.4. EDAX report for Compound 1 with Cholic Acid as co-adsorbent coated on TiO_2 film



1727 Date:12/31/2013 11:33:03 AM HV:15.0kV Puls th.:1.83kcps

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C	6	K-series	6.19	33.14	43.73	1.05
N	7	K-series	0.77	4.15	4.69	0.35
O	8	K-series	8.73	46.74	46.30	1.53
Ti	22	K-series	2.98	15.96	5.28	0.13
		Total:	18.67	100.00	100.00	

Spectrum: 1727

El	AN	Series	unn. C [wt.%]	norm. C [wt.%]	Atom. C [at.%]	Error (1 Sigma) [wt.%]
C	6	K-series	6.19	33.14	43.73	1.05
N	7	K-series	0.77	4.15	4.69	0.35
O	8	K-series	8.73	46.74	46.30	1.53
Ti	22	K-series	2.98	15.96	5.28	0.13
		Total:	18.67	100.00	100.00	

Fig S6.5. EDAX report for Compound 2 with Cholic Acid as co-adsorbent coated on TiO_2 film

Supporting information S7

Thickness Study of TiO_2

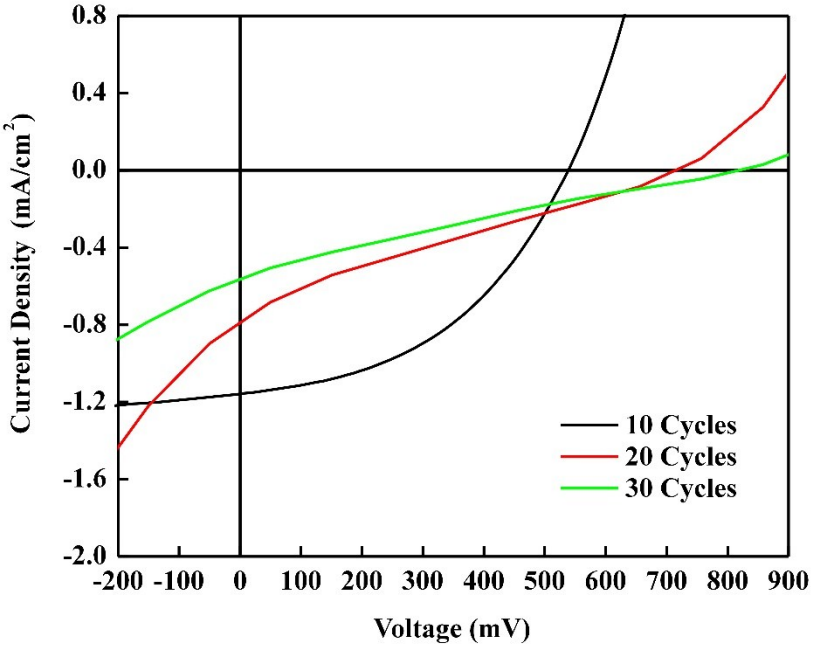

Fig S7. J-V Curve for TiO_2 thickness study