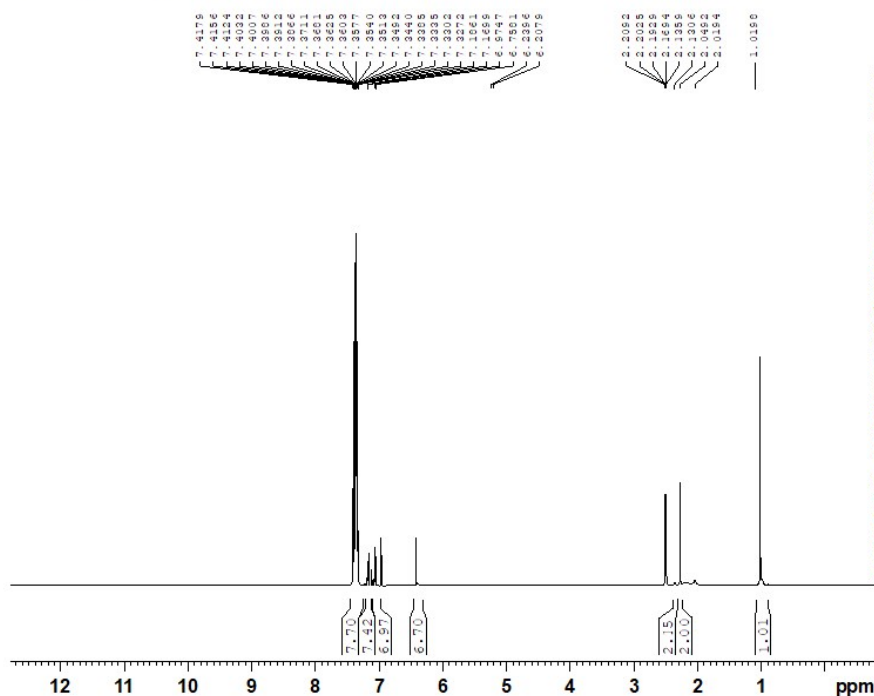
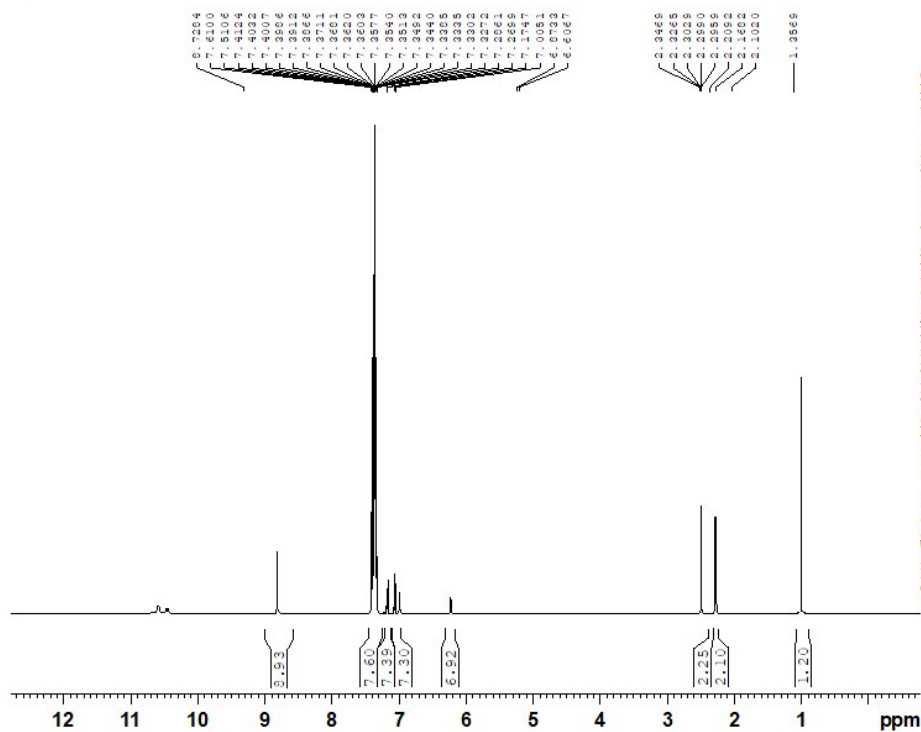


ACR-TOLU
1H_8scan DMSO {D:\Spectra} nmr 28



(4h) 10-(2-chlorophenyl)-3,3,6-tetramethyl-4',4'-diphenyl-3,4,6,7-tetrahydro-1H-spiro[acridine-9,2'-imidazolidine]-1,5',8(2H,5H,10H)-trione

ACR-TOLU
1H_8scan DMSO {D:\Spectra} nmr 28



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME May22-2020
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
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Time 11.14 h
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DE 6.79 usec
TE 298.1 K
D1 1.00000000 sec
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NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700024 MHz
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PC 1.00

(4i) 3,3,6,6-tetramethyl-10-(2-nitrophenyl)-4',4'-diphenyl-3,4,6,7-tetrahydro-1H-spiro[acridine-9,2'-imidazolidine]-1,5',8(2H,5H,10H)-trione

XRD DATA OF Fe₃O₄@TiO₂-PTA:

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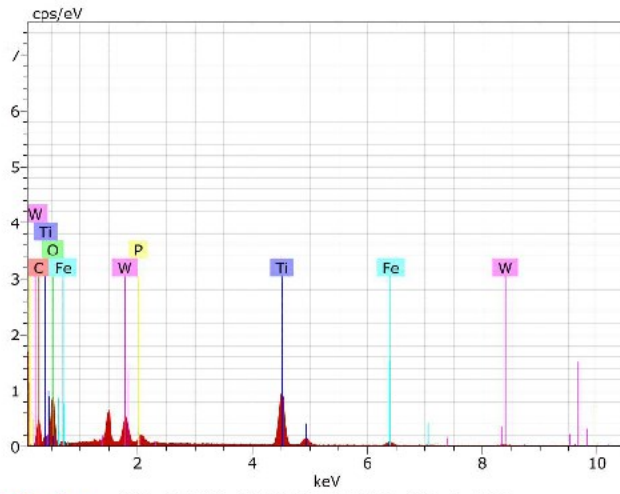
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EDAX SPECTRA:



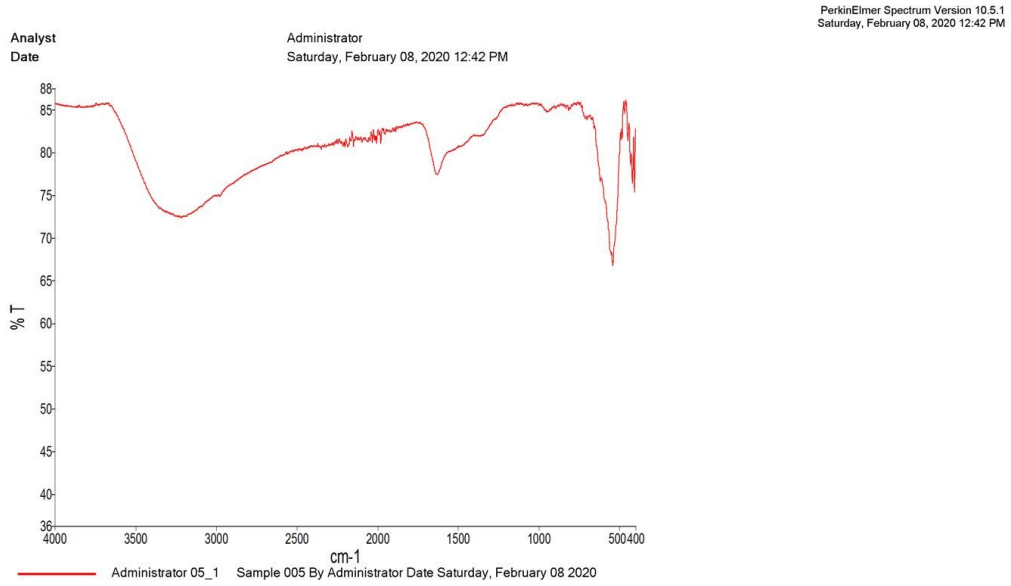
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Spectrum: test 6140

Element	Series	unn. C [wt. %]	norm. C [wt. %]	Atom. C [at. %]	Error (3 Sigma) [wt. %]
Carbon	K-series	16.27	15.53	30.21	7.99
Oxygen	K-series	26.57	24.32	50.34	15.42
Titanium	K-series	30.86	29.47	14.33	2.86
Iron	K-series	4.91	4.69	1.96	0.70
Tungsten	L-series	15.26	14.57	1.85	2.49
Phosphorus	K-series	0.87	0.83	0.62	0.21
Total:		104.73	100.00	100.00	

Fe₃O₄-IR:

Administrator 06 fe3o4 np

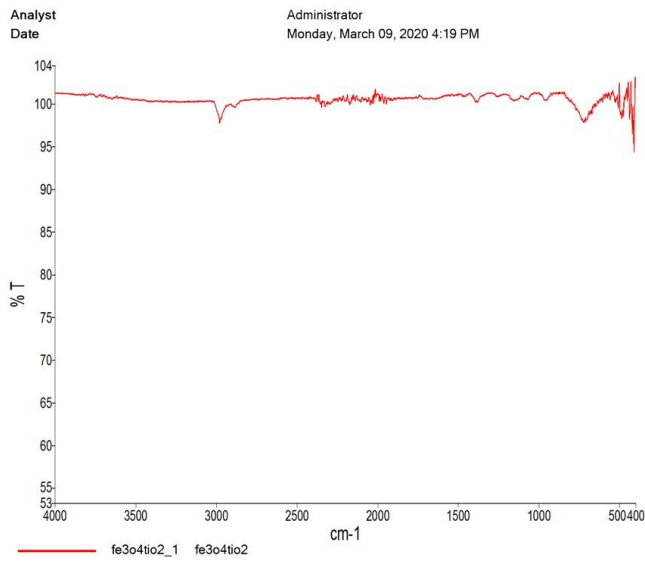


Peak Number X (cm-1) Y (%T)

1	3224.42	72.4
2	2204.43	80.69
3	2187.81	80.75
4	2150.75	80.79
5	2032.92	81.27
6	2006.99	81.16
7	1981.02	81.13
8	1628.21	77.46
9	950.63	84.83
10	540.1	66.74
11	483.02	81.73

12	467.79	84.68
13	447.98	81.47
14	431.89	78.66
15	419.58	76.45
16	406.52	75.4

PerkinElmer Spectrum Version 10.5.1
Monday, March 09, 2020 4:19 PM

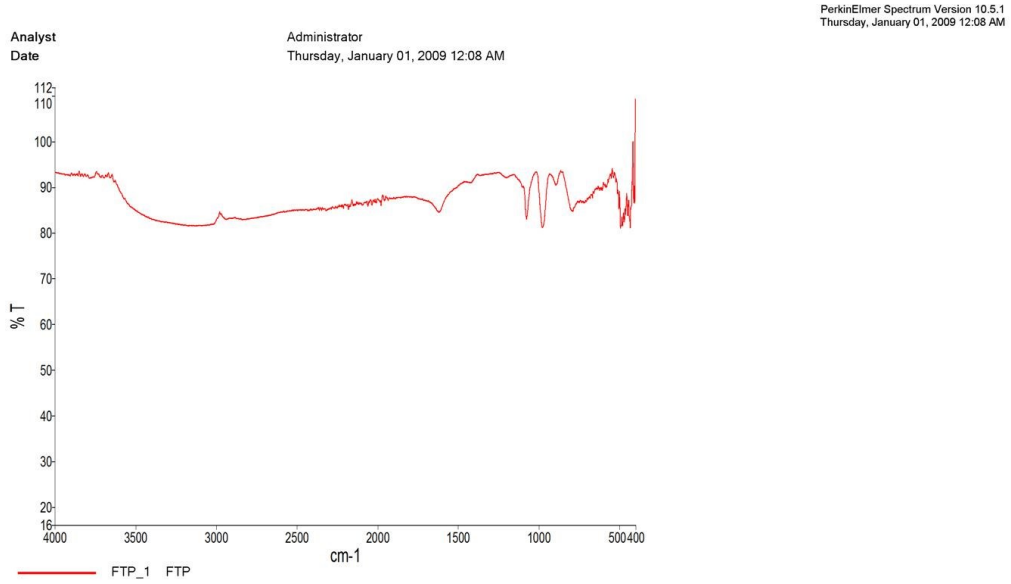


$\text{Fe}_3\text{O}_4\text{-TiO}_2$

Peak Number	X (cm-1)	Y (%T)
1	2981.64	97.78
2	2349.26	99.64
3	2173.06	99.95
4	2048.13	99.94
5	1946.27	100.07
6	1392.15	100.26

7	722.94	97.86
8	507.04	99.53
9	483.38	98.3
10	449.92	100.42
11	435.76	98.24
12	419.33	96.5
13	407.36	94.36

Fe₃O₄@TiO₂-PTA:



Peak Number	X (cm-1)	Y (%T)
1	3791.39	90.68
2	3698.38	90.75
3	3178.95	81.34
4	2842.29	82.57
5	2181.8	84.64
6	2153	85.3
7	2061.7	85.22

8	2036.78	85.44
9	1979.08	85.36
10	1620.77	84.06
11	1076.69	82.71
12	978.78	81.02
13	894.69	89.31
14	788.74	84.21
15	584.06	88.85
16	535.26	90.75
17	502.18	84.73
18	491.76	80.93
19	480.71	81.34
20	469.04	82.12
21	462.99	83.62
22	448.94	83.42
23	433.21	80.99
24	411.02	85.91
25	405.86	85.85

VSM DATA OF Fe₃O₄-TiO₂-PTA:

Temperature (K),Magnetic Field (Oe),Moment (emu)

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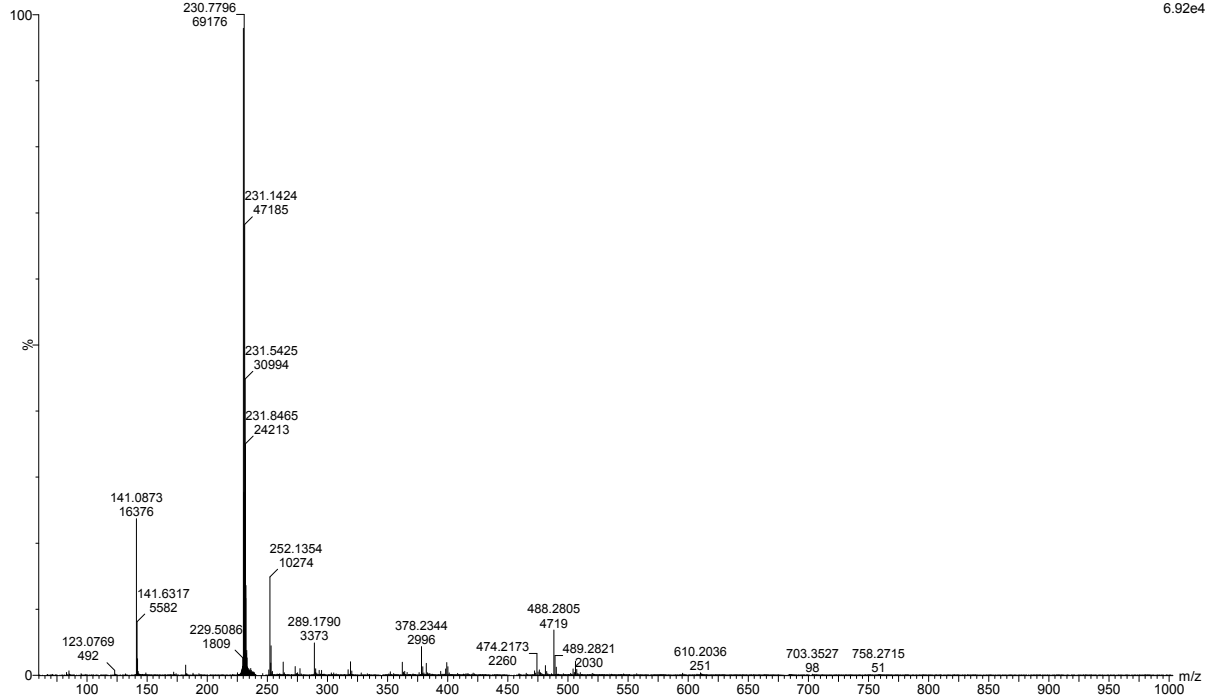
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WATERS,Q-TOF MICROMASS (ESI-MS)

NIKITA SPA 4 (0.134) AM (Top,4, Ar,4000.0,556.28,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (1:9-10:27)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

1: TOF MS ES+
6.92e4

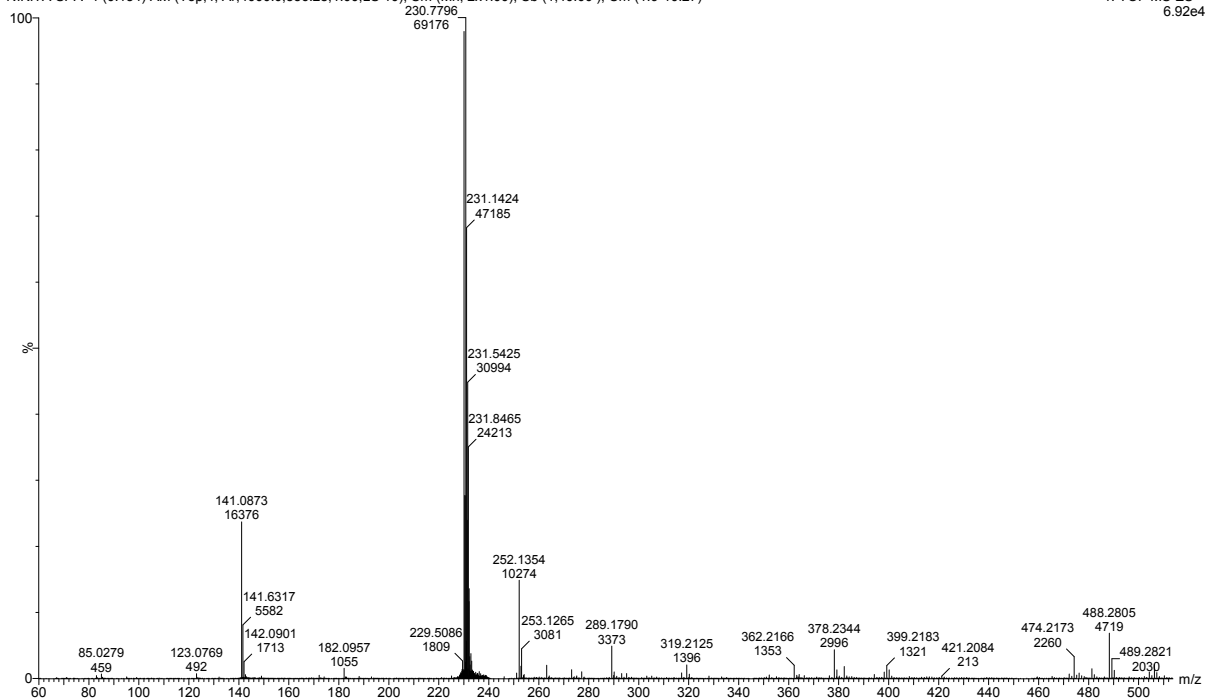


WATERS,Q-TOF MICROMASS (ESI-MS)

NIKITA SPA 4 (0.134) AM (Top,4, Ar,4000.0,556.28,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (1:9-10:27)

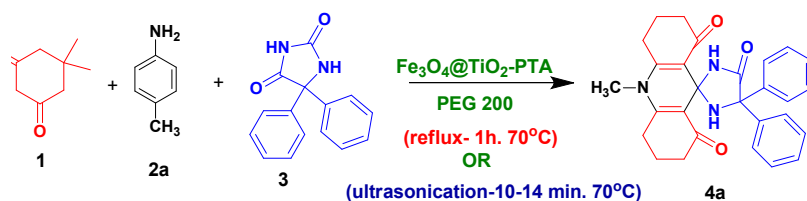
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

1: TOF MS ES+
6.92e4



Mass spectrum of (4a) 3,3,6,6-tetramethyl-4',4'-diphenyl-10-(*p*-tolyl)-3,4,6,7-tetrahydro-1*H*-spiro[acridine-9,2'-imidazolidine]-1,5',8(2*H*,5*H*,10*H*)-trione

Table A: Calculation of E-factor, mass intensity and atom economy for the reaction of 5,5 Dimethyl-1,3-cyclohexanedione, *p*-toluidine, and phenytoin in the presence of PEG 200:



- **Total amount of reactants** = Reactant 1 + Reactant (2a) + Reactant 3
 = 0.2803 gm + 0.1071 gm + 0.2522 gm
 = 0.6396 gm
- **Amount of final product (4a) = 0.6143 gm**
- **Amount of waste** = Total amount of reactants- amount of final product
 = 0.6396 gm-0.6143 gm
 = 0.0253 gm
- E Factor = Amount of waste/Amount of Product = 0.0253/0.6143 = 0.0411
 Thus,

$$\text{E Factor} = 0.0411$$

- **Process Mass Intensity (PMI)**
 Process mass intensity = E Factor + 1 = 0.0411 + 1 = 1.0411
 Thus,

$$\text{PMI} = 1.0411$$

- **Atom Economy (AE)**

$$\text{Atom Economy} = \frac{\text{MW of desired product}}{\sum \text{of molecular weight of stoichiometric reactants}} \times 100$$

$$\text{Atom Economy} = \frac{0.6143}{0.6396} \times 100 = 96.04\%$$

