SUPPORTING INFORMATION

A MAGNETICALLY RECYCLABLE NANO-Fe₂O₃ CATALYZED CHEMOSELECTIVE SYNTHESIS AND ANTIOXIDANT ACTIVITY OF DIETHYL (3-((5-ARYL-1H-1,2,4-TRIAZOL-3-YL)THIO)PROPYL)PHOSPHONATES

M. S. R. Murty^{1,*}, Mohana Rao Katiki¹, B. Ramalingeswara Rao¹, Jagadeesh Babu Nanubolu², Sudheer Kumar Buddana³, and R. S. Prakasam³.

¹*Medicinal Chemistry & Pharmacology Division, Discovery Laboratory, CSIR-Indian Institute of Chemical Technology, Uppal Road, Hyderabad-500007, India.*

²*Centre for X-ray Crystallography, CSIR-Indian Institute of Chemical Technology, Uppal Road, Hyderabad-500007, India.*

³*Bioengineering & Environmental Sciences, CSIR-Indian Institute of Chemical Technology, Uppal Road, Hyderabad-500007, India.*

E-mail: msrmurty@ymail.com; Tel.: +91-40-27191658

Contents:

1. General information	S2
2. Experimental section for X-ray crystallography	S2–S4
3. General procedure for the synthesis of diethyl (3-((5-aryl-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonates	S4
4. Spectral data of representative compounds 3a–l	S5–S9
5. ¹ H NMR, ¹³ C NMR and HRMS Spectra of representative	

compounds 3a–l	S10–S27
6. Powder X-ray diffraction spectra of nanoFe ₂ O ₃	S28

1. General information:

All chemicals and reagents were obtained from Aldrich (Sigma–Aldrich, Saint Louis, MO, USA) or Spectrochem Pvt. Ltd. (Mumbai, India) and were used without further purification. The reactions were monitored by thin-layer chromatography (TLC) using Merck silica gel glass plate (60 F254, 0.25 mm), and TLC plates were visualized by UV light or I₂ stain. Column chromatography was carried out with Merck 60–120 sized mesh silica gel using ethyl acetate and hexane as eluent. All products were characterized by their NMR, IR and HRMS spectra. The ¹H NMR (500 MHz) spectra and ¹³C NMR (75 MHz) spectra were recorded on Bruker Avance 500 Nuclear Magnetic Resonance spectrometer taking the compounds in CDCl₃ using TMS as an internal standard. The chemical shifts (δ) were reported in parts per million (ppm) downfield from TMS and coupling constants ⁿJ values were expressed in Hz. IR spectra (KBr) were recorded on Thermo Nicolet Nexus 670 FTIR Spectrometer (ν in cm⁻¹). HRMS were recorded on Thermo Scientific Exactive Orbitrap Mass Spectrometer under Electron Spray Ionization conditions preparing sample solution in Methanol. Melting point was measured on Electrothermal 9100 Melting point apparatus. Surface morphology was recorded on Hitachi S-3000N Scanning Electron Microscope. X-Ray diffraction (XRD) pattern was obtained on a Bruker D8 Advance X-Ray Powder Diffractometer.

2. Experimental section for X-ray crystallography

X-ray data for the compound were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated Mo-K α radiation ($\lambda=0.71073\text{\AA}$) with ω -scan method [1]. Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 6741 reflections for AT76 data. Integration and scaling of intensity data was accomplished using SAINT program [1]. The structures were solved by Direct Methods using SHELXS97 [2] and refinement was carried out by full-matrix least-squares technique using SHELXL97 [2]. Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93–0.97 $\text{\AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}$ for methyl atoms. The N bound H atom was located from the difference Fourier map.

Crystal data for compound 3g (AT76): $\text{C}_{19}\text{H}_{30}\text{N}_3\text{O}_4\text{PS}$, $M = 427.49$, colourless block, $0.32 \times 0.18 \times 0.14 \text{ mm}^3$, triclinic, space group $P-1$ (No. 2), $a = 9.2569(6)$, $b = 9.6629(6)$, $c = 14.5141(9) \text{ \AA}$, $\alpha = 82.3560(10)$, $\beta = 83.2900(10)$, $\gamma = 61.5380(10)^\circ$, $V = 1129.08(12) \text{ \AA}^3$, $Z = 2$, $D_c = 1.257 \text{ g/cm}^3$, $F_{000} = 456$, CCD area detector, Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2)\text{K}$, $2\theta_{\text{max}} = 50.0^\circ$, 10844 reflections collected, 3962 unique ($R_{\text{int}} = 0.0157$), Final $GooF = 1.036$, $R1 = 0.0413$, $wR2 = 0.1132$, R indices based on 3553 reflections with $I > 2\sigma(I)$ (refinement on F^2), 260 parameters, $\mu = 0.242 \text{ mm}^{-1}$. CCDC 965121 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the

Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

[1] SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.

[2] Sheldrick, G. M. SHELXS97 and SHELXL97, Programs for crystal structure solution and refinement; University of Gottingen: Germany, 1997.

3. General procedure for the synthesis of diethyl (3-((5-aryl-1*H*-1,2,4-triazol-3-ylthio)propyl)phosphonates:

To a mixture of 5-aryl-1*H*-1,2,4-triazole-3-thiones (1.0 mmol) and diethyl (3-bromopropyl)phosphonate (1.0 mmol) in water (3 mL) was added nano-Fe₂O₃ (10 mol%, 16mg). The reaction mixture was warmed to 80 °C and allowed to stir for 1h. The progress of the reaction was monitored by thin layer chromatography (TLC). After completion of the reaction indicated by TLC, the reaction mixture was cooled to room temperature. The catalyst was separated with the aid of external magnet and the resulting reaction mixture was extracted with ethyl acetate (3×10 mL). The combined organic layer was dried over anhydrous Na₂SO₄. The solvent was evaporated under vacuum to give the crude product, which was purified by column chromatography using ethyl acetate/hexane (8:2) as eluent to get the expected products in excellent yields. Structural assignments of the products are based on their ¹H NMR, ¹³C NMR, FT-IR and Mass analysis.

4. Spectroscopic data for the synthesized compounds 3a–l

Diethyl (3-((5-phenyl-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3a)

Yield 92%. Brown oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 8.08–8.02 (m, 2H); 7.45–7.34 (m, 3H); 4.18–4.05 (m, 4H); 3.26 (t, J = 6.8 Hz, 2H); 2.16–1.93 (m, 4H); 1.30 (t, J = 7.0 Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3): δ (ppm) 158.9, 129.5, 128.5, 126.3, 61.9 (d, J = 6.3 Hz), 32.7 (d, J = 17.2 Hz), 24.5, 23.4, 22.7, 16.3 (d, J = 5.4 Hz). IR (KBr, cm^{-1}): 3421, 2986, 1556, 1264, 1027. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{15}\text{H}_{22}\text{O}_3\text{N}_3\text{NaPS}$: 378.10117, found: 378.10114.

*Diethyl (3-((5-(*o*-tolyl)-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3b)*

Brown oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.76 (d, J = 8.0 Hz, 1H); 7.34–7.22 (m, 3H); 4.17–4.03 (m, 4H); 3.26 (t, J = 7.0 Hz, 2H); 2.56 (s, 3H); 2.14–1.91 (m, 4H); 1.30 (t, J = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 159.4, 137.0, 131.0, 129.4, 129.2, 125.7, 61.9 (d, J = 6.5 Hz), 32.5 (d, J = 16.4 Hz), 25.0, 22.8 (t, J = 16.4 Hz), 21.1, 16.3 (d, J = 6.0 Hz). IR (KBr, cm^{-1}): 3436, 2924, 1550, 1256, 1028. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{16}\text{H}_{24}\text{O}_3\text{N}_3\text{NaPS}$: 392.11682, found: 392.11697.

*Diethyl (3-((5-(*m*-tolyl)-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3c)*

Brown oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.92–7.79 (m, 2H); 7.34–7.16 (m, 3H); 4.19–4.03 (m, 4H); 3.25 (t, J = 6.7 Hz, 2H); 2.36 (s, 3H); 2.19–1.90 (m, 4H); 1.29 (t, J = 7.5 Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 158.9, 156.4, 138.2, 130.4, 128.4, 126.9, 123.3, 61.9 (d, J = 6.5 Hz), 32.7 (d, J = 17.0 Hz), 24.8, 22.9 (d, J = 18.6 Hz), 21.2,

16.3 (d, $J = 5.4$ Hz). IR (KBr, cm^{-1}): 3414, 2983, 1552, 1264, 1027. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. Calcd. for $\text{C}_{16}\text{H}_{24}\text{O}_3\text{N}_3\text{NaPS}$: 392.11682, found: 392.11689.

*Diethyl (3-((5-(*p*-tolyl)-1*H*-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3d)*

Yellow oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.91 (d, $J = 8.0$ Hz, 2H); 7.21 (d, $J = 8.0$ Hz, 2H); 4.18–4.03 (m, 4H); 3.25 (t, $J = 7.0$ Hz, 2H); 2.37 (s, 3H); 2.20–1.92 (m, 4H); 1.30 (t, $J = 7.0$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 159.2, 156.2, 139.7, 129.3, 126.2, 62.0 (d, $J = 6.5$ Hz), 32.6 (d, $J = 16.4$ Hz), 24.8, 22.9 (d, $J = 15.9$ Hz), 21.3, 16.3 (d, $J = 6.0$ Hz). IR (KBr, cm^{-1}): 3422, 2984, 1583, 1264, 1027. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{16}\text{H}_{24}\text{O}_3\text{N}_3\text{NaPS}$: 392.11690, found: 392.11697.

*Diethyl (3-((5-(4-(*tert*-butyl)phenyl)-1*H*-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3e)*

Brown oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.96 (d, $J = 8.3$ Hz, 2H); 7.42 (d, $J = 8.3$ Hz, 2H); 4.19–4.01 (m, 4H); 3.25 (t, $J = 6.7$ Hz, 2H); 2.19–1.90 (m, 4H); 1.40–1.18 (m, 15H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 158.4, 156.8, 152.8, 126.1, 125.4, 61.8 (d, $J = 6.0$ Hz), 34.6, 32.7 (d, $J = 17.5$ Hz), 31.0, 24.9, 22.9 (d, $J = 22.5$ Hz), 16.2 (d, $J = 6.0$ Hz). IR (KBr, cm^{-1}): 2961, 1563, 1263, 1027. ESI-HRMS (m/z): $[\text{M}+\text{H}]^+$. calcd. for $\text{C}_{19}\text{H}_{31}\text{O}_3\text{N}_3\text{PS}$: 412.18183, found: 412.18192.

*Diethyl (3-((5-(4-methoxyphenyl)-1*H*-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3f)*

Yellow oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.97 (d, $J = 8.8$ Hz, 2H); 6.93 (d, $J = 8.8$ Hz, 2H); 4.20–4.03 (m, 4H); 3.84 (s, 3H); 3.25 (t, $J = 7.3$ Hz, 2H); 2.19–1.90 (m, 4H); 1.31 (t, $J = 6.9$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 160.7, 157.6, 127.8,

114.0, 62.0 (d, $J = 6.5$ Hz), 55.2, 32.6 (d, $J = 15.9$ Hz), 24.9, 23.0, 22.9 (d, $J = 11.5$ Hz), 16.3 (d, $J = 6.0$ Hz). IR (KBr, cm^{-1}): 3401, 2926, 1614, 1254, 1026. ESI-HRMS (m/z): $[\text{M}+\text{H}]^+$. calcd. for $\text{C}_{16}\text{H}_{25}\text{O}_4\text{N}_3\text{PS}$: 386.12979, found: 386.13004.

*Diethyl (3-((5-(4-(*n*-butoxy)phenyl)-1*H*-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3g)*

Yellow crystal. Mp: 103-105 °C. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.94 (d, $J = 8.8$ Hz, 2H); 6.91 (d, $J = 8.8$ Hz, 2H); 4.17–4.04 (m, 4H); 3.98 (t, $J = 6.5$ Hz, 2H); 3.24 (t, $J = 7.0$ Hz, 2H); 2.15–1.93 (m, 4H); 1.77 (pentet, $J = 14.3, 7.1$ Hz, 2H); 1.49 (sextet, $J = 14.9, 7.6$ Hz, 2H); 1.3(t, $J = 7.1$ Hz, 6H); 0.98 (t, $J = 7.4$, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 160.3, 127.8, 114.5, 67.6, 61.9 (d, $J = 7.2$ Hz), 32.7 (d, $J = 16.3$ Hz), 31.1, 24.5, 23.4, 22.8 (d, $J = 3.6$ Hz), 19.1, 16.3 (d, $J = 6.3$ Hz), 13.7. IR (KBr, cm^{-1}): 2989, 1582, 1253, 1024. ESI-HRMS (m/z): $[\text{M}+\text{H}]^+$. calcd. for $\text{C}_{19}\text{H}_{31}\text{O}_4\text{N}_3\text{PS}$: 428.17268, found: 428.17635.

*Diethyl (3-((5-(4-fluorophenyl)-1*H*-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3h)*

Yellow oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 8.09–7.99 (m, 2H); 7.08 (d, $J = 8.3$ Hz, 2H); 4.20–4.04 (m, 4H); 3.26 (t, $J = 6.7$ Hz, 2H); 2.19–1.92 (m, 4H); 1.31 (t, $J = 7.5$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 164.4, 162.4, 128.3, 128.2, 125.3, 115.6, 115.4, 62.0 (d, $J = 6.3$ Hz), 32.7 (d, $J = 16.3$ Hz), 24.4, 23.3, 22.8 (d, $J = 3.6$ Hz), 16.3 (d, $J = 6.3$ Hz). IR (KBr, cm^{-1}): 3422, 2985, 1609, 1264, 1027. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{15}\text{H}_{21}\text{O}_3\text{N}_3\text{FNaPS}$: 396.09175, found: 396.09189.

Diethyl (3-((5-(2-chlorophenyl)-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3i)

Yellow oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 8.05–7.99 (m, 1H); 7.48–7.43 (m, 1H); 7.38–7.32 (m, 2H); 4.13–4.04 (m, 4H); 3.26 (t, $J = 7.0$ Hz, 2H); 2.15–1.90 (m, 4H); 1.29 (t, $J = 7.0$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 156.9, 155.9, 131.9, 131.2, 130.5, 130.2, 126.8, 61.7 (d, $J = 6.5$ Hz), 32.4 (d, $J = 17.5$ Hz), 24.9, 23.1, 22.6 (d, $J = 3.8$ Hz), 16.2 (d, $J = 6.0$ Hz). IR (KBr, cm^{-1}): 3423, 2982, 1514, 1264, 1028. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{15}\text{H}_{21}\text{O}_3\text{N}_3\text{ClNaPS}$: 412.06220, found: 412.06230.

Diethyl (3-((5-(3-chlorophenyl)-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3j)

Brown oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 8.12–8.09 (m, 1H); 7.98–7.94 (m, 1H); 7.37–7.33 (m, 2H); 4.20–4.05 (m, 4H); 3.28 (t, $J = 7.1$ Hz, 2H); 2.22–1.76 (m, 4H); 1.37–1.30 (m, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 134.5, 129.8, 129.3, 126.4, 124.4, 62.0 (d, $J = 6.6$ Hz), 32.6 (d, $J = 15.4$ Hz), 24.9, 23.1, 22.9 (d, $J = 3.8$ Hz), 16.3 (d, $J = 6.0$ Hz). IR (KBr, cm^{-1}): 3407, 2983, 1575, 1028. ESI-HRMS (m/z): $[\text{M}+\text{H}]^+$. calcd. for $\text{C}_{15}\text{H}_{21}\text{O}_3\text{N}_3\text{ClPS}$: 390.08025, found: 390.08295.

Diethyl (3-((5-(4-chlorophenyl)-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3k)

Brown oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.99 (d, $J = 8.5$ Hz, 2H); 7.37 (d, $J = 8.5$ Hz, 2H); 4.18–4.06 (m, 4H); 3.27 (t, $J = 7.0$ Hz, 2H); 2.19–1.90 (m, 4H); 1.31 (t, $J = 7.1$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 158.8, 155.5, 135.3, 128.7, 127.6, 62.0 (d, $J = 6.6$ Hz), 32.7 (d, $J = 16.5$ Hz), 24.8, 23.0, 22.8 (d, $J = 4.4$ Hz), 16.3 (d, $J = 6.0$ Hz). IR (KBr, cm^{-1}): 2983, 1606, 1265, 1026. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{15}\text{H}_{21}\text{O}_3\text{N}_3\text{ClNaPS}$: 412.06220, found: 412.06220.

Diethyl (3-((5-(4-bromophenyl)-1H-1,2,4-triazol-3-yl)thio)propyl)phosphonate (3l)

Yellow oil. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.93 (d, $J = 8.6$ Hz, 2H); 7.53 (d, $J = 8.6$ Hz, 2H); 4.20–4.04 (m, 4H); 3.27 (t, $J = 6.9$ Hz, 2H); 2.26–1.84 (m, 4H); 1.42–1.14 (m, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ (ppm): 159.0, 155.3, 131.6, 128.3, 127.8, 123.5, 61.9 (d, $J = 6.0$ Hz), 32.6 (d, $J = 16.4$ Hz), 24.5, 23.1, 22.8 (d, $J = 3.2$ Hz), 16.3 (d, $J = 5.4$ Hz). IR (KBr, cm^{-1}): 3425, 2980, 1263, 1027. ESI-HRMS (m/z): $[\text{M}+\text{Na}]^+$. calcd. for $\text{C}_{15}\text{H}_{21}\text{O}_3\text{N}_3\text{BrNaPS}$: 456.01168, found: 456.01172.

5. ^1H NMR, ^{13}C NMR and HRMS spectra of representative compounds 3(a-l)

MSR-PS8 #40-90 RT: 0.14-0.31 AV: 51 NL: 2.05E8
T: FTMS {1,1} + p ESI Full ms [150.00-1500.00]

K. MONANA RAO
11/9/2011 11:52:32 AM

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

PDCH #17-87 RT: 0.07-0.31 AV: 71 NL: 1.26E8
T: FTMS {1,1} + p ESI Full ms [150.00-1500.00]

MSR-PMCH #20-64 RT: 0.10-0.25 AV: 45 NL: 2.34E8
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

K. MONANA RAO
11/9/2011 11:57:51 AM

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

MSR-PET #13-79 RT: 0.08-0.30 AV: 67 NL: 2.07E8
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

MSQ-PSBT #31-83 RT: 0.11-0.29 AV: 53 NL: 1.51E8
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

K. MONANA RAO
11/9/2011 11:55:17 AM

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

MSR-POME #13-71 RT: 0.08-0.27 AV: 59 NL: 8.66E7
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

MSR-OBT #23-55 RT: 0.10-0.20 AV: 33 SB: 334 0.63-0.93, 1.03-1.85 SM: 15G NL: 2.25E8
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

K. MONANA RAO
11/9/2011 12:11:29 PM

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

MSR-PSF #32-79 RT: 0.11-0.27 AV: 48 NL: 1.66E8
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

396.09189
C₁₅ H₂₁ O₃ N₃ F Na P S = 396.09175
6.5 RDBE
0.35357 ppm

POCL #23-81 RT: 0.08-0.28 AV: 59 NL: 1.97E8
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

K MOHAN RAO
8/13/2012 9:35:31 PM

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

MSR-MCL #16-55 RT: 0.05-0.19 AV: 40 NL: 2.11E8
T: FTMS {1,1} + p ESI Full lock ms [100.00-2000.00]

PSCL #23-69 RT: 0.09-0.25 AV: 47 NL: 9.00E7
T: FTMS {1,1} + p ESI Full ms [150.00-1500.00]

K. MONANA RAO
11/9/2011 12:14:15 PM

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY

PSBR #21-76 RT: 0.09-0.28 AV: 56 NL: 7.27E7
T: FTMS (1,1) + p ESI Full ms [150.00-1500.00]

6. Powder X-ray diffraction spectra of nanoFe₂O₃