

Supporting Information

Organic Reactions in Water: A Distinct Novel Approach for an Efficient Synthesis of α - Amino Phosphonates Starting Directly from Nitro Compounds

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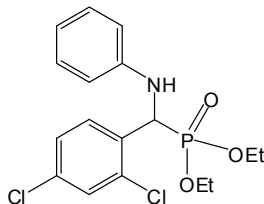
Experimental Details

General Information: The spectra were recorded with the following instruments; IR: FT-IR spectrophotometer, NMR: 200 MHz (^1H) and 50 MHz (^{13}C) spectrometers; ESIMS: Ion trap mass spectrometer and ESIHRMS: Hybrid MS system. Column chromatography was performed with silica gel (100-200 mesh) and TLC with silica gel precoated plates. Visualization was accomplished with UV lamp or stains. Organic extracts were dried over anhydrous Na_2SO_4 . All chemicals used were commercially available.

General Experimental Procedure: To mixture of a nitro compound (1.0 mmol), indium powder (325 mesh, 2 mmol) and 1 *N* aqueous HCl (1 ml) an aldehyde (1.0 mmol), an alkyl phosphite (1.3 mmol) and water (5 ml) were added. The mixture was stirred at room temperature and the reaction was monitored by TLC. After completion, the reaction mixture was washed with saturated NaHCO_3 solution (3x5 ml) and water (3x5 ml) and extracted with EtOAc (3x5 ml). The extract was concentrated and the residue was subjected to column chromatography (silica gel, hexane-EtOAc) to obtain pure α -amino phosphonate.

Spectral Data

Diethyl (2,4-dichlorophenyl)(phenylamino)methylphosphonate (Table 2, Entry 3)



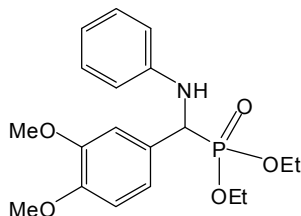
IR: ν_{max} 3309, 1607, 1508, 1247 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.51 (1H, d, $J = 8.0$ Hz), 7.40 (1H, d, $J = 2.0$ Hz), 7.22 (1H, dd, $J = 8.0, 2.0$ Hz), 7.06 (2H, t, $J = 8.0$ Hz), 6.64 (1H, t, $J = 8.0$ Hz), 6.48 (2H, d, $J = 8.0$ Hz), 5.23 (1H, dd, $J = 24.0, 10.0$ Hz), 4.82 (1H, t, $J = 10.0$ Hz), 4.25-4.12 (2H, m), 3.91 (1H, m), 3.67 (1H, m), 1.35 (3H, t, $J = 7.0$ Hz).

Hz), 1.11 (3H, t, $J = 2.0$ Hz); ^{13}C NMR (50 MHz, CDCl_3): δ 146.2 (d, $J = 14.0$ Hz), 130.2, 129.8, 128.2, 119.1, 113.5, 96.2, 63.4 (d, $J = 6.5$ Hz), 63.2 (d, $J = 6.5$ Hz), 51.6 (d,

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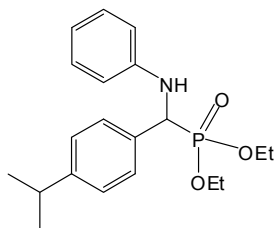
$J = 155.2$ Hz), 16.6 (d, $J = 6.5$ Hz), 16.2 (d, $J = 6.5$ Hz); ESIMS: m/z 387 $[\text{M}]^+$, 388, 390, 392 $[\text{M}+\text{H}]^+$; HRMS (ESI): m/z 410.0459 $[\text{M}+\text{Na}]^+$ (calculated for $\text{C}_{17}\text{H}_{20}\text{Cl}_2\text{NO}_3\text{PNa}$: m/z 410.0455).

Diethyl (3,4-dimethoxyphenyl)(phenylamino)methylphosphonate (Table 2, Entry 4)



IR: ν_{max} 3302, 1604, 1501, 1460, 1234 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.05 (2H, t, $J = 8.0$ Hz), 6.99 (1H, d, $J = 2.0$ Hz), 6.81 (1H, d, $J = 8.0$ Hz), 6.72 (1H, dd, $J = 8.0, 2.0$ Hz), 6.63 (1H, t, $J = 8.0$ Hz), 6.54 (2H, d, $J = 8.0$ Hz), 5.28 (1H, dd, $J = 24.0, 10.0$ Hz), 4.72 (1H, t, $J = 10.0$ Hz), 4.22-4.08 (2H, m), 3.91 (3H, s), 3.82 (1H, m), 3.77 (3H, s), 3.55 (1H, m), 1.32 (3H, t, $J = 7.0$ Hz), 1.05 (3H, t, $J = 7.0$ Hz); ^{13}C NMR (50 MHz, CDCl_3): δ 154.2, 151.6, 146.3 (d, $J = 14.0$ Hz), 129.5, 125.9, 118.0, 113.9, 113.2, 111.1, 63.1 (d, $J = 6.5$ Hz), 62.9 (d, $J = 6.5$ Hz), 56.1, 55.3, 48.2 (d, $J = 155.5$ Hz), 16.2 (d, $J = 6.5$ Hz), 16.0 (d, $J = 6.5$ Hz); ESIMS: m/z 380 $[\text{M}+\text{H}]^+$ HRMS (ESI): m/z 402.1444 $[\text{M}+\text{Na}]^+$ (Calcd. for $\text{C}_{19}\text{H}_{26}\text{NO}_5\text{PNa}$: m/z 402.1446).

Diethyl (4-isopropylphenyl)(phenylamino)methylphosphonate (Table 2, Entry 5)



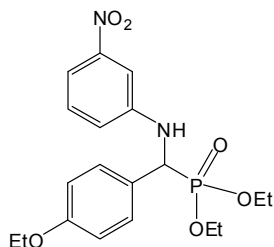
IR: ν_{max} 3314, 1602, 1500, 1235 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.49 (2H, d, $J = 8.0$ Hz), 7.16 (2H, d, $J = 8.0$ Hz), 7.08 (2H, t, $J = 8.0$ Hz), 6.67 (1H, t, $J = 8.0$ Hz), 6.60 (2H, d, $J = 8.0$ Hz), 4.85 (1H, brs), 4.76 (1H, d, $J = 24.0$ Hz), 4.18-4.01 (2H, m), 3.90 (1H, m), 3.63 (1H, m), 2.83 (1H, m), 1.25 (3H, t, $J = 7.0$ Hz), 1.18 (6H, d, $J = 7.0$ Hz), 1.05 (3H, t, $J = 7.0$ Hz); ^{13}C NMR (50 MHz, CDCl_3): δ 146.2 (d, $J = 14.0$ Hz), 133.0, 129.1, 128.0,

126.0, 118.2, 113.9, 62.9 (d, $J = 6.5$ Hz), 55.1 (d, $J = 153.5$ Hz), 33.5, 23.9, 16.8 (d, $J = 6.5$ Hz), 16.2 (d, $J = 6.5$ Hz); ESIMS: m/z 384 $[M+Na]^+$; HRMS (ESI): m/z 362.1875

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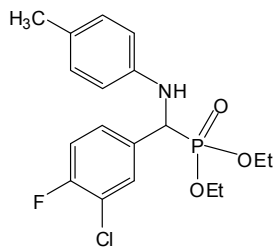
$[M+Na]^+$ (Calcd. for $C_{20}H_{29}NO_3P$: m/z 362.1885).

Diethyl (4-ethoxyphenyl)(3-nitrophenylamino)methylphosphonate (Table2, Entry 6)



IR: $\nu_{\max}$ 3289, 1615, 1529, 1349, 1238 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.50 (1H, dd, $J = 8.0, 2.0$ Hz), 7.46 (1H, d, $J = 2.0$ Hz), 7.37 (2H, d, $J = 8.0$ Hz), 7.19 (1H, t, $J = 8.0$ Hz), 6.84 (1H, dd, $J = 8.0, 2.0$ Hz), 6.81 (2H, d, $J = 8.0$ Hz), 5.68 (1H, t, $J = 10.0$ Hz), 4.68 (1H, dd, $J = 24.0, 10.0$ Hz), 4.22-4.04 (2H, m), 4.02-3.96 (2H, m), 3.84 (1H, m), 3.60 (1H, m), 1.44 (3H, t, $J = 7.0$ Hz), 1.37 (3H, t, $J = 7.0$ Hz), 1.24 (3H, t, $J = 7.0$ Hz), 1.10 (3H, t, $J = 7.0$ Hz); ^{13}C NMR (50 MHz, CDCl_3): δ 159.0, 149.1, 147.2 (d, $J = 14.0$ Hz), 129.9, 129.1, 126.2, 119.6, 115.0, 113.1, 107.9, 63.3 (d, $J = 6.5$ Hz), 63.2, 63.1 (d, $J = 6.5$ Hz), 55.0 (d, $J = 154.8$ Hz), 16.8 (d, $J = 6.0$ Hz), 16.3 (d, $J = 6.0$ Hz), 14.5; ESIMS: m/z 431 $[M+Na]^+$; HRMS (ESI): m/z 431.1362 $[M+Na]^+$ (Calcd. for $C_{19}H_{25}N_2O_6PNa$: m/z 431.1347).

Diethyl (3-chloro-4-fluorophenyl)(p-tolylamino)methylphosphonate (Table 2, Entry 7)



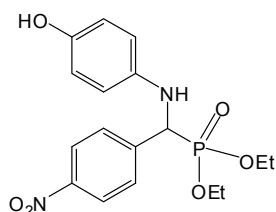
IR: $\nu_{\max}$ 3303, 1616, 1519, 1239 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.50 (1H, d, $J = 8.0$ Hz), 7.32 (1H, brs), 7.04 (1H, t, $J = 8.0$ Hz), 6.85 (2H, d, $J = 8.0$ Hz), 6.42 (2H, d, $J = 8.0$), 4.77 (1H, brs), 4.62 (1H, d, $J = 24.0$ Hz), 4.28-4.05 (2H, m), 3.99 (1H, m), 3.82 (1H, m), 2.19 (3H, s), 1.28 (3H, t, $J = 7.0$ Hz), 1.19 (3H, t, $J = 7.0$ Hz); ^{13}C NMR (50 MHz,

CDCl₃): δ 159.3, 143.5 (d, J = 14.0 Hz), 133.2, 130.0, 129.6, 127.9, 127.2 (d, J = 4.0 Hz), 121.1 (d, J = 16.0 Hz), 116.8 (d, J = 16.0 Hz), 113.5, 63.6 (d, J = 6.5 Hz), 63.0 (d, J = 6.5

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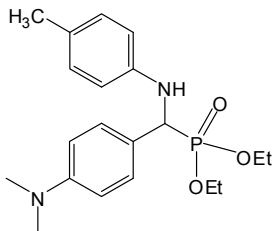
Hz), 55.2 (d, J = 152.5 Hz), 20.2, 16.2 (d, J = 6.0 Hz), 16.0 (d, J = 6.0 Hz); ESIMS: m/z 386, 388 [M+H]⁺; HRMS (ESI): m/z 408.09.4 [M+Na]⁺ (Calcd. for C₁₈H₂₂ClFNO₃PNa: m/z 408.0907).

Diethyl (4-hydroxyphenylamino)(4-nitrophenyl)methylphosphonate (Table 2, Entry 8)



IR: $\nu_{\max}$ 3299, 1666, 1518, 1347, 1231 cm⁻¹; ¹H NMR (200 MHz, CDCl₃): δ 8.18 (2H, d, J = 8.0 Hz), 7.61 (2H, d, J = 8.0 Hz), 6.60 (2H, d, J = 8.0 Hz), 6.35 (2H, d, J = 8.0 Hz), 4.72 (1H, d, J = 24.0 Hz), 4.50 (1H, brs), 4.20-4.05 (2H, m), 4.02 (1H, m), 3.89 (1H, m), 1.30 (3H, t, J = 7.0 Hz), 1.21 (3H, t, J = 7.0 Hz); ¹³C NMR (50 MHz, CDCl₃): δ 150.5, 147.3, 138.8 (d, J = 14.0 Hz), 128.6, 123.3, 116.0, 115.1, 64.0 (d, J = 6.5 Hz), 63.2 (d, J = 6.5 Hz), 57.1 (d, J = 152.0 Hz), 16.1 (d, J = 6.0 Hz), 16.0 (d, J = 6.0 Hz); ESIMS: m/z 403 [M+Na]⁺; HRMS (ESI): m/z 403.1052 [M+Na]⁺ (Calcd. for C₁₇H₂₁N₂O₆PNa: m/z 403.1034).

Diethyl (4-(dimethylamino)phenyl)(p-tolylamino)methylphosphonate (Table 2, Entry 9)



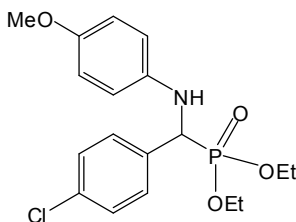
IR: $\nu_{\max}$ 3276, 1616, 1522, 1447, 1232 cm⁻¹; ¹H NMR (200 MHz, CDCl₃): δ 7.25 (2H, d, J = 8.0 Hz), 6.83 (2H, d, J = 8.0 Hz), 6.62 (2H, d, J = 8.0 Hz), 6.46 (2H, d, J = 8.0 Hz), 4.55 (1H, d, J = 24.0 Hz), 4.14-4.02 (2H, m), 3.90 (1H, m), 3.62 (1H, m), 2.90 (6H, s), 2.15 (3H, s), 1.26 (3H, t, J = 7.0 Hz), 1.11 (3H, t, J = 7.0 Hz); ¹³C NMR (50 MHz,

CDCl₃): δ 150.1, 144.1(d, J = 14.0 Hz), 129.2, 128.3, 127.2, 122.9, 113.9, 112.1, 62.8 (d, J = 6.5 Hz), 55.2 (d, J = 155.0 Hz), 40.2, 20.1, 16.2 (d, J = 6.2 Hz), 16.0 (d, J = 6.2 Hz);

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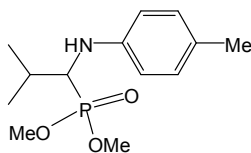
ESIMS: m/z 399 [M+Na]⁺; HRMS (ESI): m/z 399.1852 [M+Na]⁺ (Calcd. for C₂₀H₂₉N₂O₃PNa: m/z 399.1837).

Diethyl (4-chlorophenyl)(4-methoxyphenylamino)methylphosphonate (Table 2, Entry 10)



IR: ν_{max} 3334, 1616, 1511, 1459, 1388, 1220 cm⁻¹; ¹H NMR (200 MHz, CDCl₃): δ 7.39 (2H, d, J = 8.0 Hz), 7.28 (2H, d, J = 8.0 Hz), 6.63 (2H, d, J = 8.0 Hz), 6.47 (2H, d, J = 8.0 Hz), 4.60 (1H, d, J = 24.0 Hz), 4.19-4.02 (2H, m), 3.95 (1H, m), 3.76 (1H, m), 3.65 (3H, s), 1.32 (3H, t, J = 7.0 Hz), 1.13 (3H, t, J = 7.0 Hz); ¹³C NMR (50 MHz, CDCl₃): δ 152.9, 140.0 (d, J = 14.0 Hz), 135.0, 133.8, 129.2, 129.0, 115.1, 114.5, 63.6 (d, J = 6.5 Hz), 63.1 (d, J = 6.5 Hz), 56.3 (d, J = 152.5 Hz), 55.3, 16.1(d, J = 6.2 Hz), 16.0 (d, J = 6.0 Hz); ESIMS: m/z 384 [M+H]⁺; HRMS (ESI): m/z 406.0940 [M+Na]⁺ (Calcd. for C₁₈H₂₃ClNO₄PNa: m/z 406.0950).

Dimethyl 2-methyl-1-(p-tolylamino)propylphosphonate (Table 2, Entry 21)

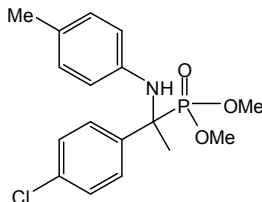


IR: ν_{max} 3429, 2958, 1618, 1521, 1233, 1033 cm⁻¹; ¹H NMR (200 MHz, CDCl₃): δ 6.99 (2H, d, J = 8.0 Hz), 6.59 (2H, d, J = 8.0 Hz), 3.72 (3H, d, J = 10.0 Hz), 3.70 (3H, d, J = 10.0 Hz), 3.65 (1H, dd, J = 24.0, 4.0 Hz), 2.25 (1H, m), 2.22 (3H, s), 1.08 (3H, d, J = 7.0 Hz), 1.02 (3H, d, J = 7.0 Hz); ¹³C NMR (50 MHz, CDCl₃): δ 145.2, 129.9, 127.2, 113.4, 56.6, 53.2 (d, J = 6.0 Hz), 52.1 (d, J = 6.0 Hz), 29.7 (d, J = 6.0 Hz), 20.8 (d, J = 6.0

Hz), 20.2 (d, $J = 6.0$ Hz), 18.1; ESIMS: m/z 272 $[M+H]^+$; HRMS (ESI): m/z 294.1227 $[M+Na]^+$ (Calcd. for $C_{13}H_{22}NO_3PNa$: m/z 294.1235).

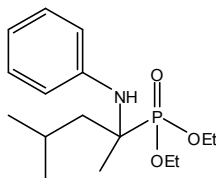
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Dimethyl 1-(4-chlorophenyl)-1-(p-tolylamino)ethylphosphonate (Table 2, Entry 22)



IR: $\nu_{\max}$ 3289, 1616, 1518, 1234 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.51 (2H, d, $J = 8.0$ Hz), 7.32 (2H, d, $J = 8.0$ Hz), 6.79 (2H, d, $J = 8.0$ Hz), 6.24 (2H, d, $J = 8.0$ Hz), 4.50 (1H, brs), 3.70 (3H, d, $J = 10.0$ Hz), 3.56 (3H, d, $J = 10.0$ Hz), 2.17 (3H, s), 1.91 (3H, d, $J = 15.0$ Hz); ^{13}C NMR (50 MHz, CDCl_3): δ 142.0 (d, $J = 14.0$ Hz), 137.2, 133.1, 129.7, 129.2, 128.3, 128.0, 117.0, 59.3 (d, $J = 154.6$ Hz), 54.2 (d, $J = 6.0$ Hz), 54.0 (d, $J = 6.0$ Hz), 20.4, 20.2 (d, $J = 6.0$ Hz); ESIMS: m/z 354, 356 $[M+H]^+$; HRMS (ESI): m/z 376.0835 $[M+Na]^+$ (Calcd. for $C_{17}H_{21}ClNO_3PNa$: m/z 376.0845).

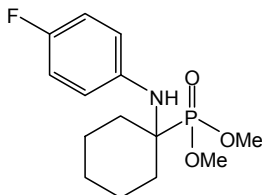
Diethyl 4-methyl-2-(phenylamino)pentan-2-ylphosphonate (Table 2, Entry 23)



IR: $\nu_{\max}$ 3319, 1602, 1500, 1322, 1225 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.11 (2H, t, $J = 8.0$ Hz), 6.90 (2H, d, $J = 8.0$ Hz), 6.75 (1H, t, $J = 8.0$ Hz), 4.12-3.90 (4H, m), 3.52 (1H, brs), 2.01-3.82 (2H, m), 1.69 (1H, m), 1.50 (3H, d, $J = 15.0$ Hz), 1.24 (3H, t, $J = 7.0$ Hz), 1.20 (3H, t, $J = 7.0$ Hz), 0.98 (3H, d, $J = 7.0$ Hz), 0.91 (3H, d, $J = 7.0$ Hz); ^{13}C NMR (50 MHz, CDCl_3): δ 146.2, 128.9, 119.5, 118.8, 62.5 (d, $J = 6.2$ Hz), 62.2 (d, $J = 6.5$ Hz), 57.9 (d, $J = 155.0$ Hz), 43.4, 25.0, 23.4 (d, $J = 6.5$ Hz), 21.2, 16.1 (d, $J = 6.0$ Hz); ESIMS: m/z 314 $[M+H]^+$; HRMS (ESI): m/z 336.1711 $[M+Na]^+$ (Calcd. for $C_{16}H_{28}NO_3PNa$: m/z 336.1704).

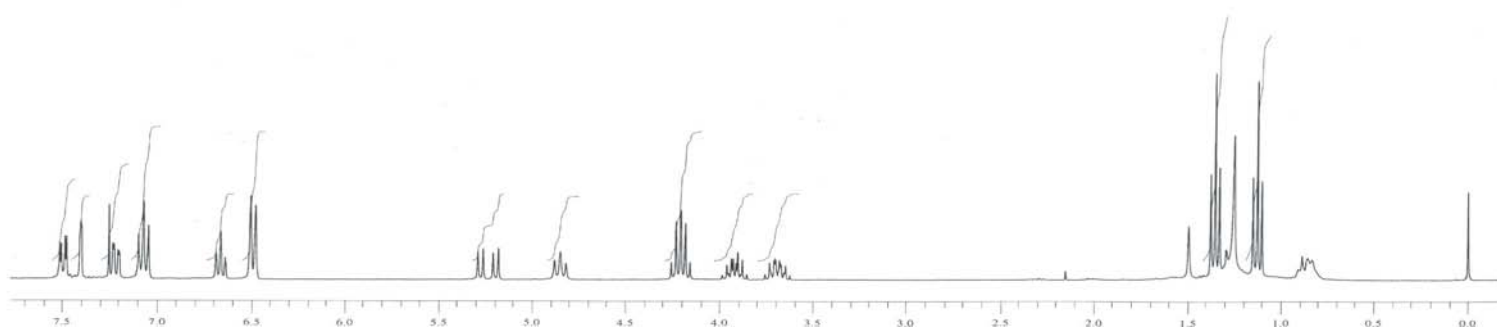
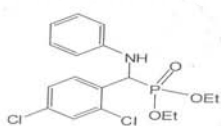
Dimethyl 1-(4-fluorophenylamino)cyclohexylphosphonate (Table 2, Entry 24)

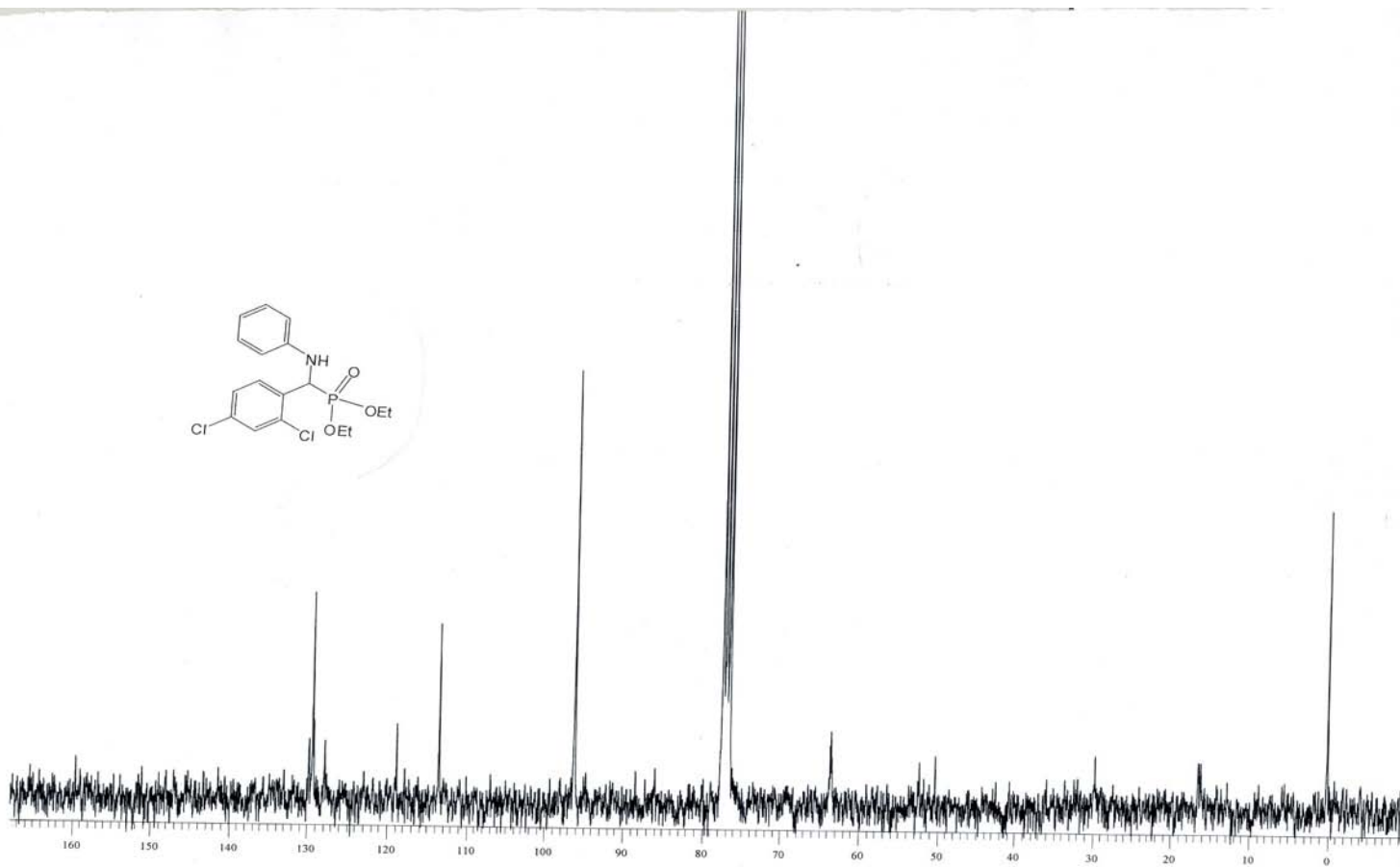
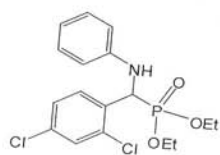
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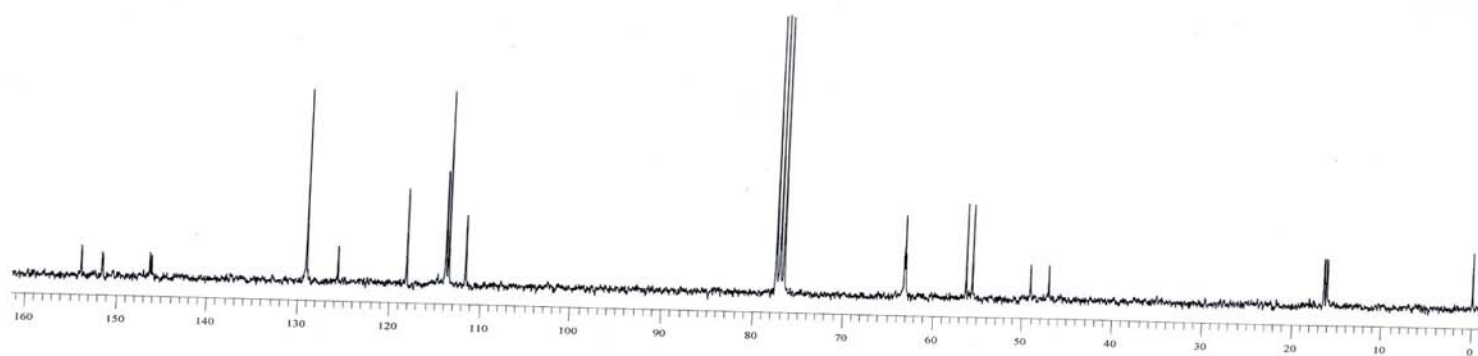
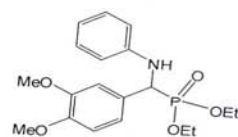
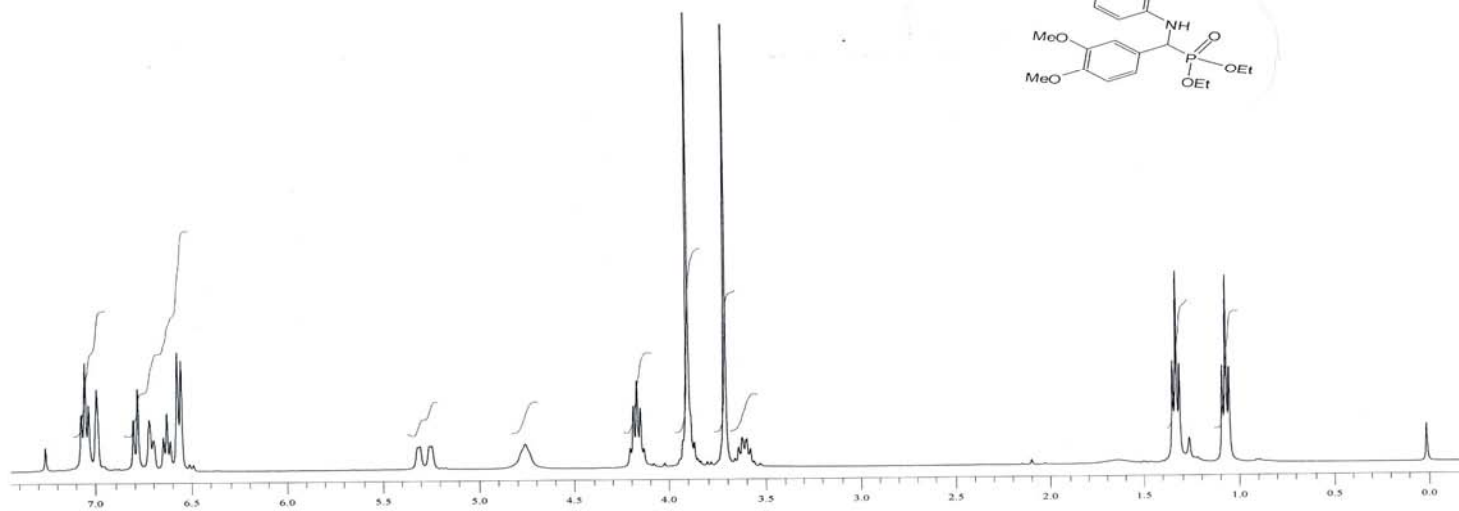
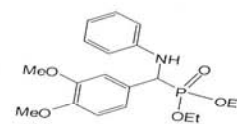


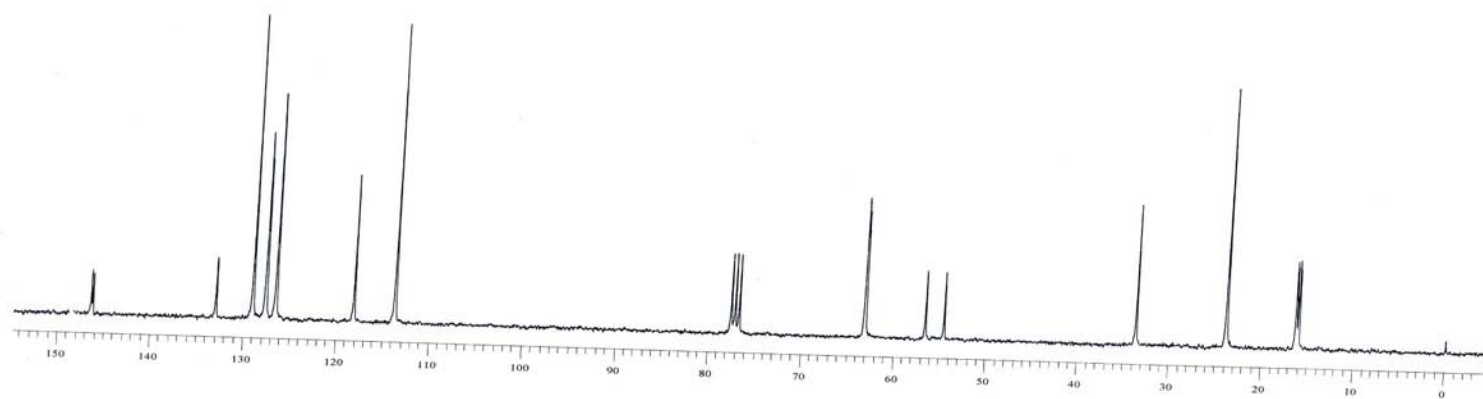
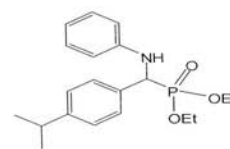
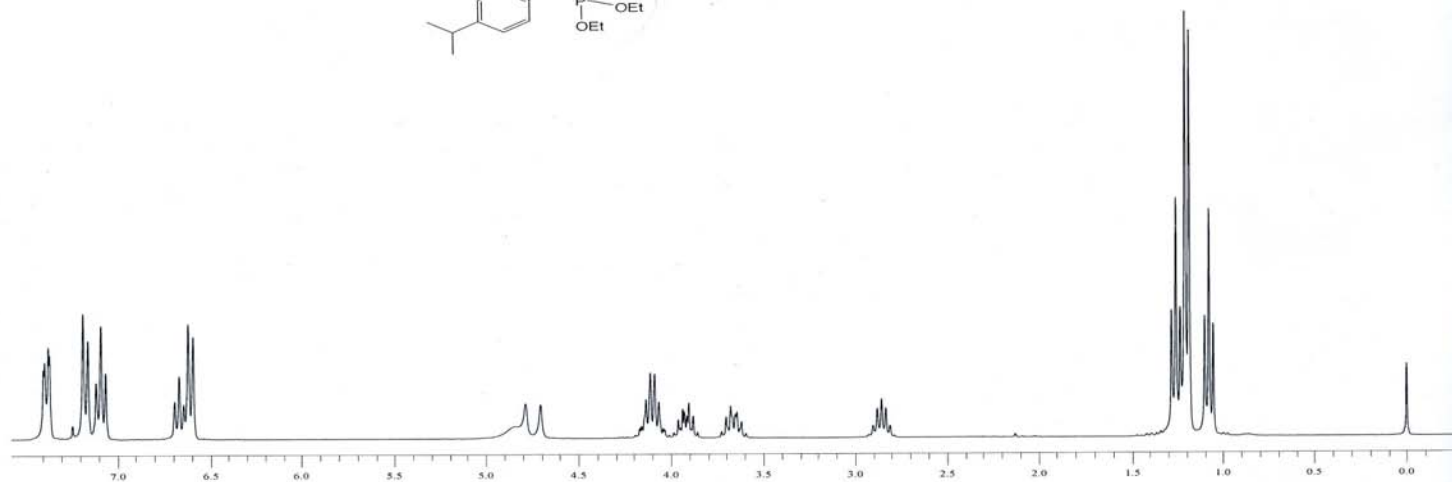
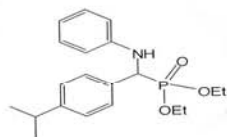
IR: ν_{max} 3314, 1509, 1452, 1321, 1223 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 7.05-6.96 (2H, m), 6.88 (2H, d, $J = 8.0$ Hz), 3.64 (6H, d, $J = 10.0$ Hz), 2.17-2.03 (2H, m), 1.84-1.62 (3H, m), 1.60- 1.49 (4H, m) 1.30 (1H, m); ^{13}C NMR: δ 159.1, 141.8, 120.4, 115.0 (d, $J = 10.0$ Hz), 57.9 (d, $J = 154.8$ Hz), 52.3 (d, $J = 6.0\text{Hz}$), 30.1, 24.6, 20.0 (d, $J = 6.0\text{Hz}$); ESIMS: m/z 302 $[\text{M}+\text{H}]^+$; HRMS (ESI): m/z 324.1136 $[\text{M}+\text{Na}]^+$ (Calcd. for $\text{C}_{14}\text{H}_{21}\text{FNO}_3\text{PNa}$: m/z 324.1140).

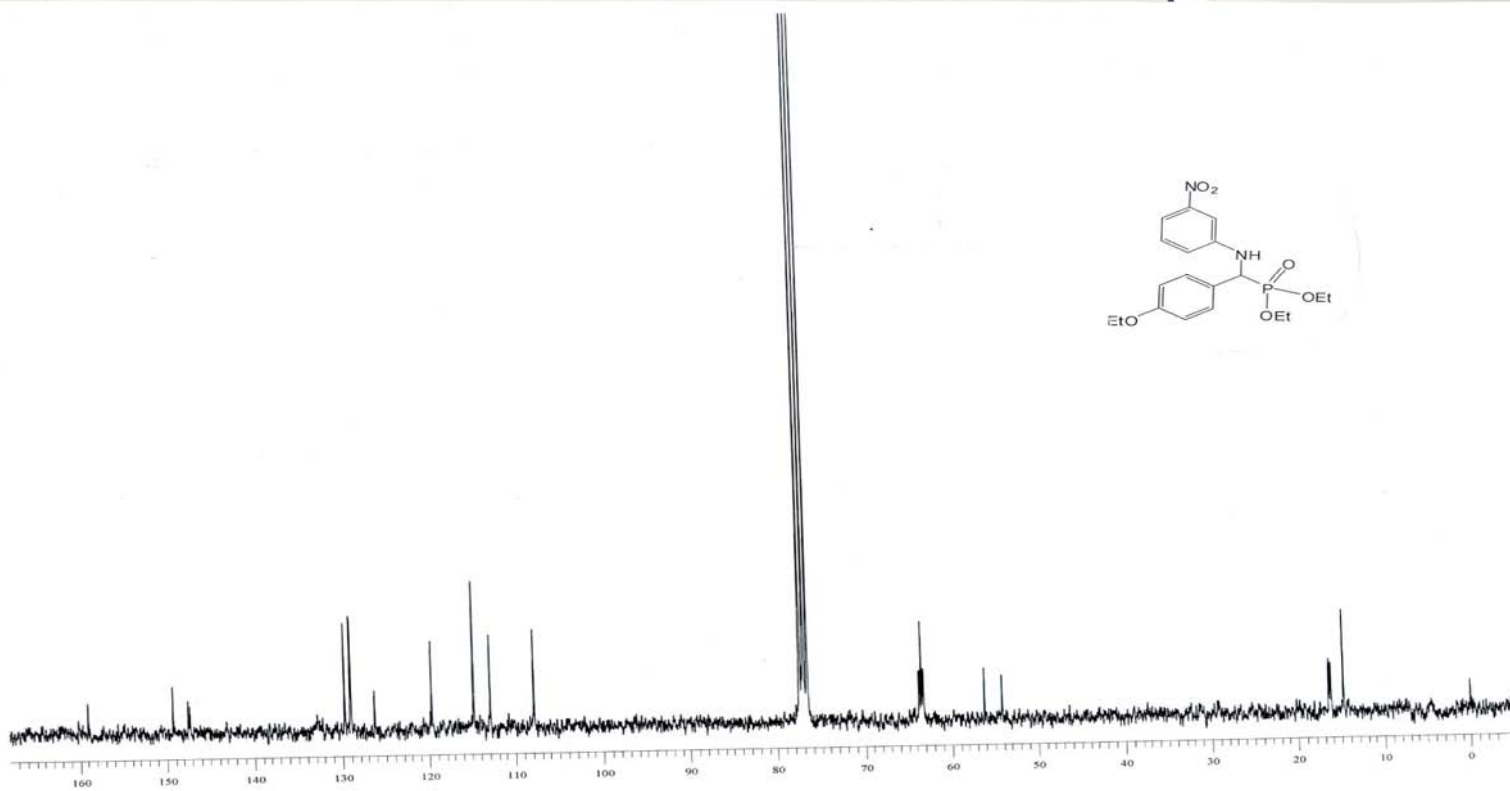
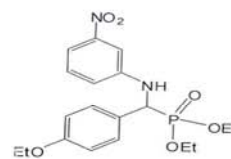
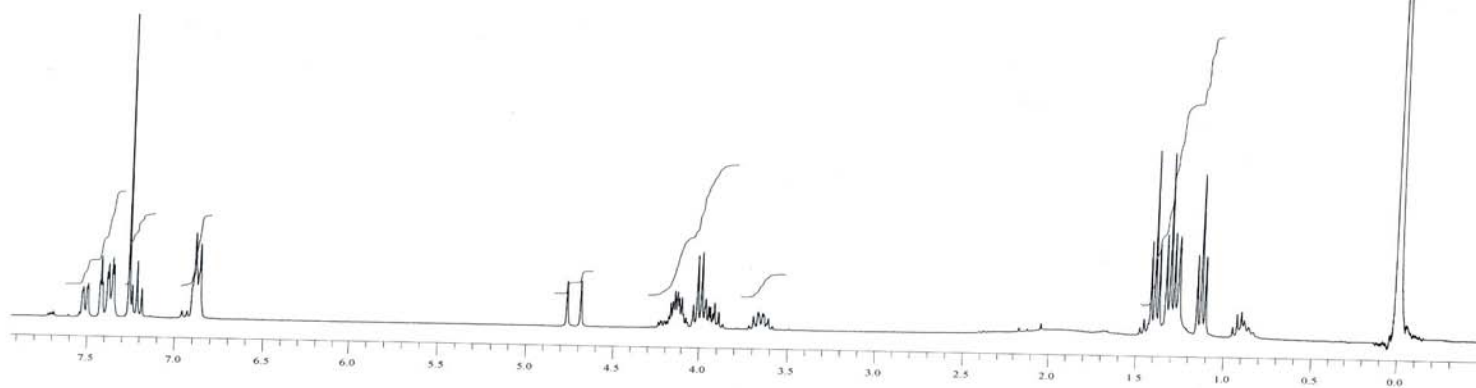
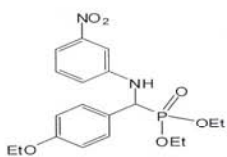
-S8-

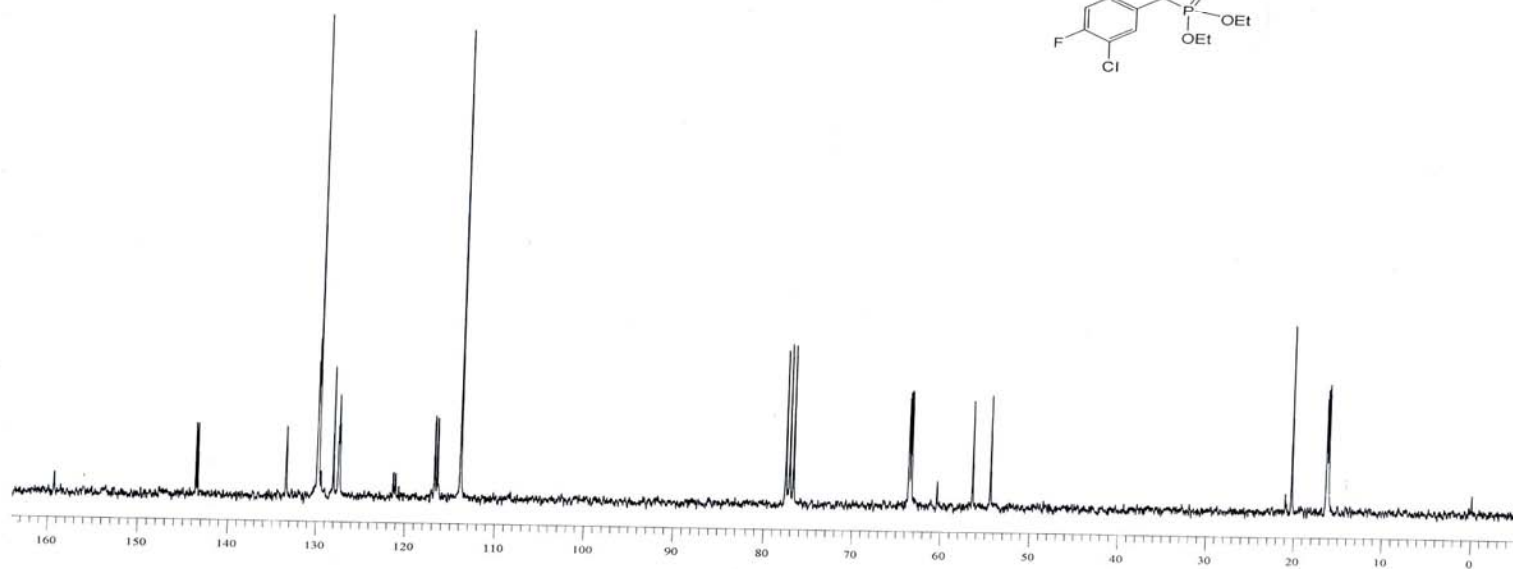
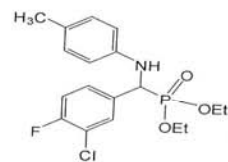
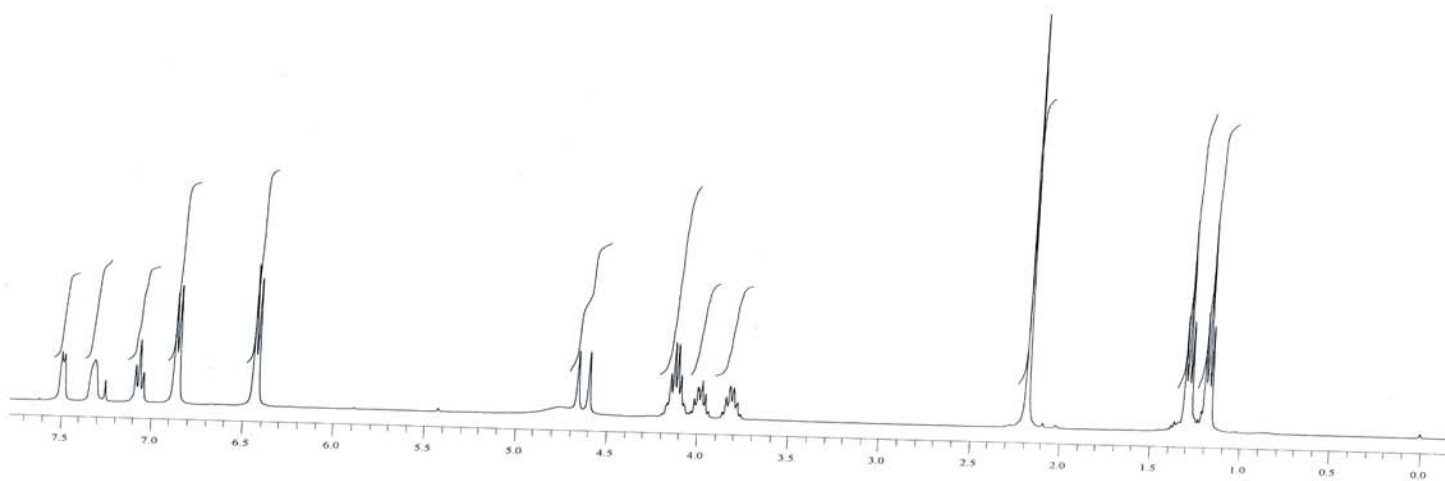
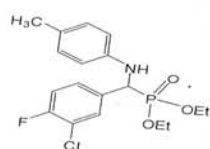


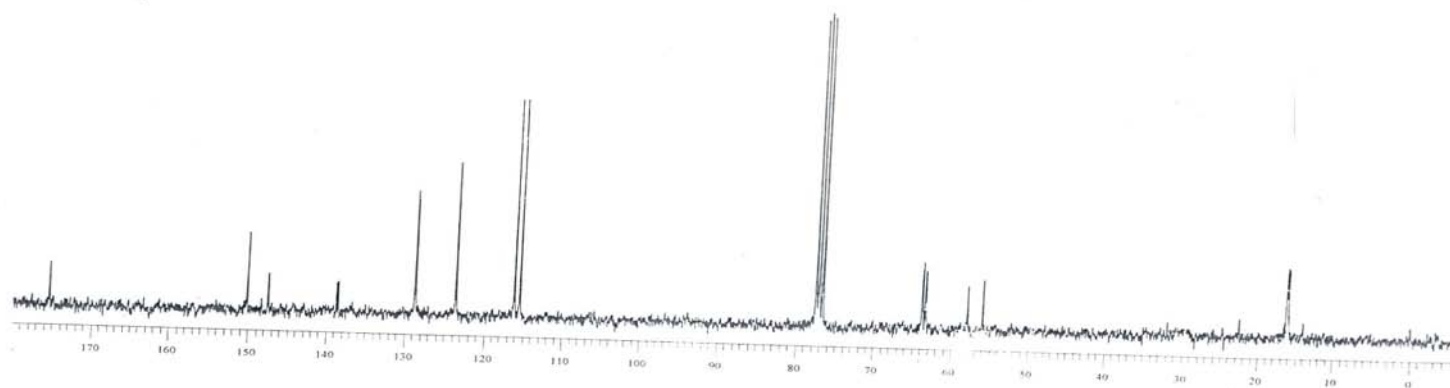
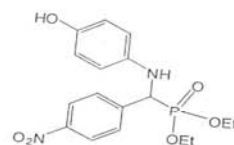
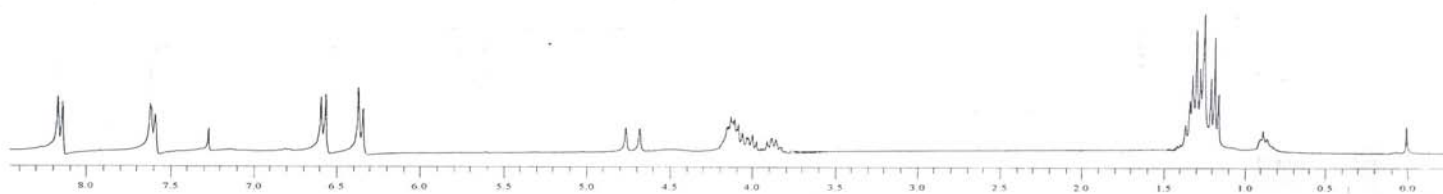
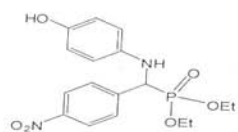


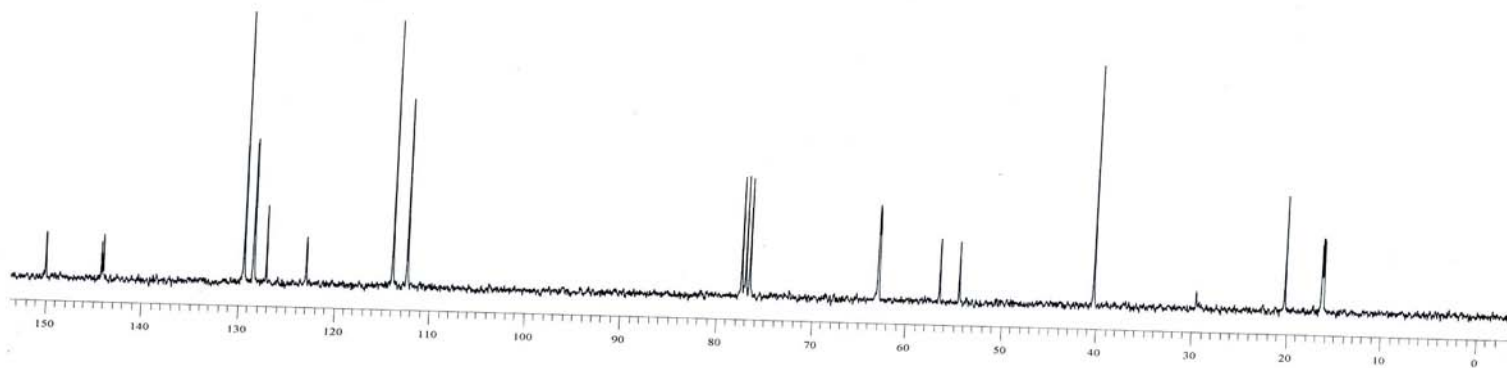
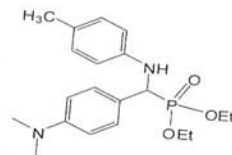
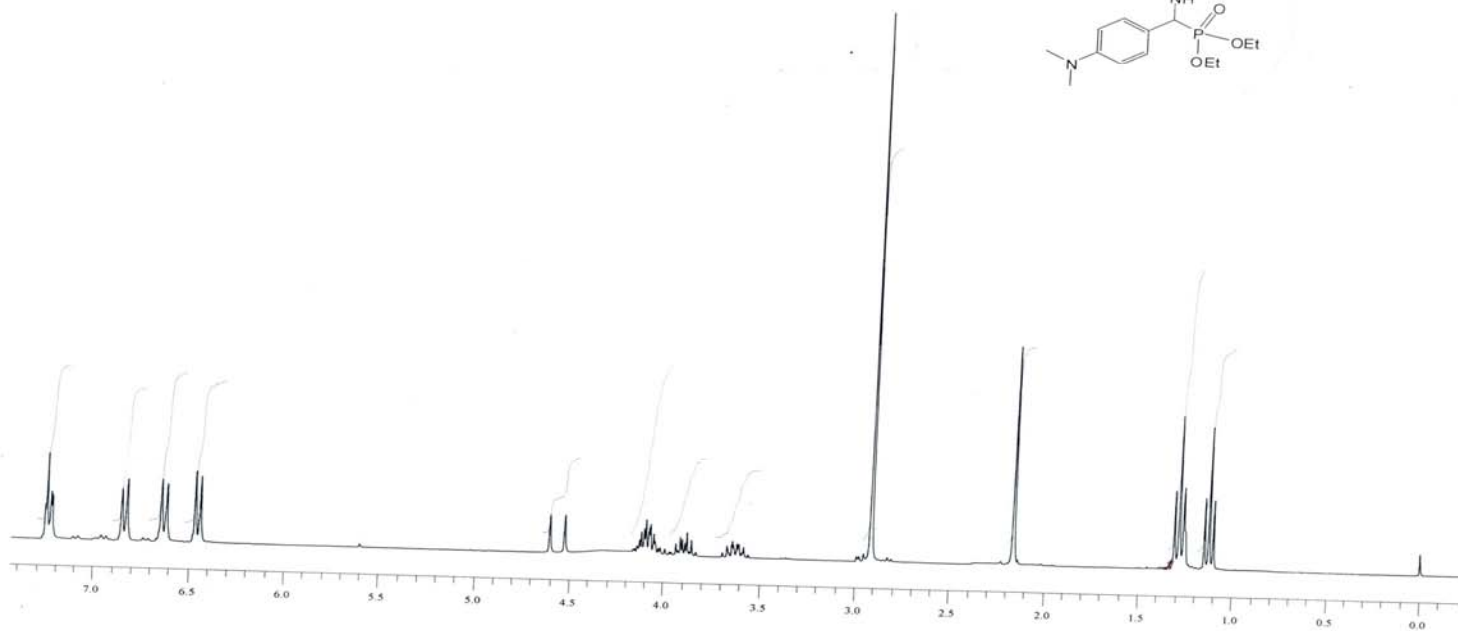
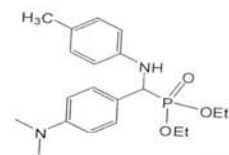


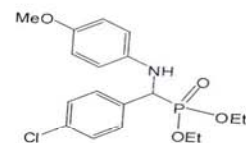
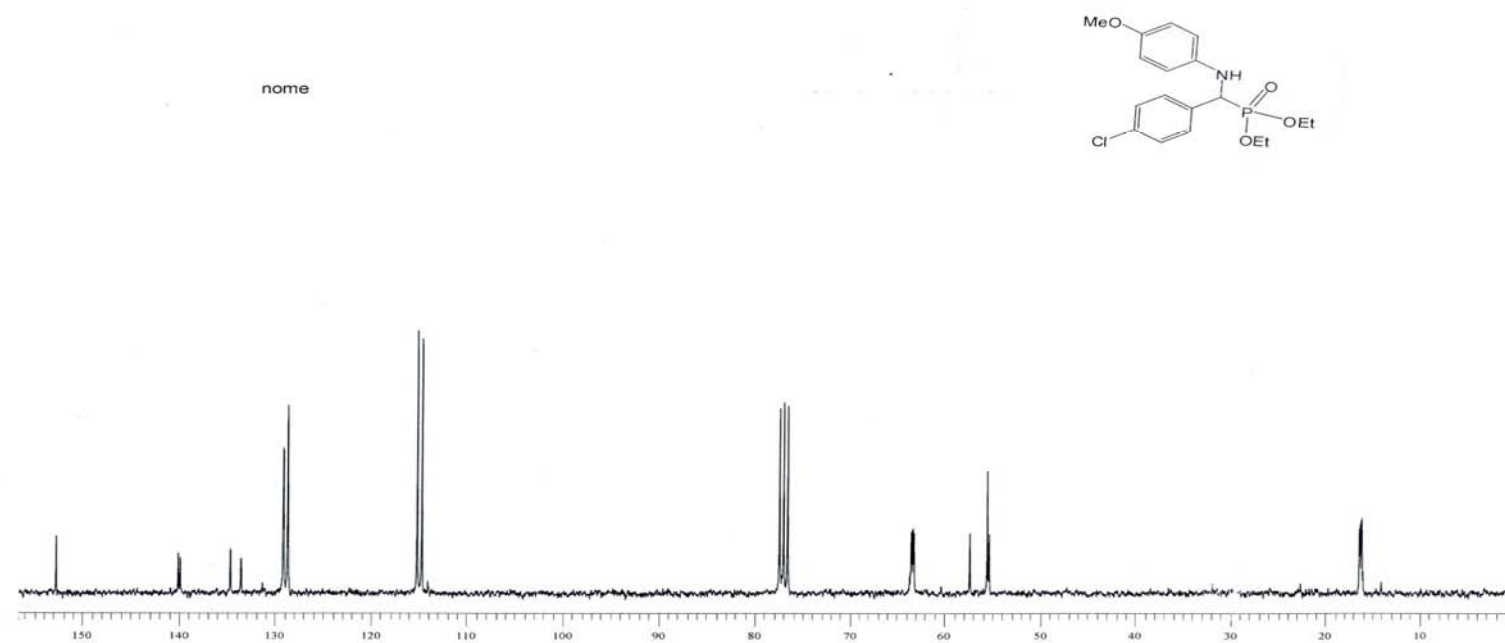
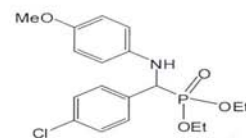
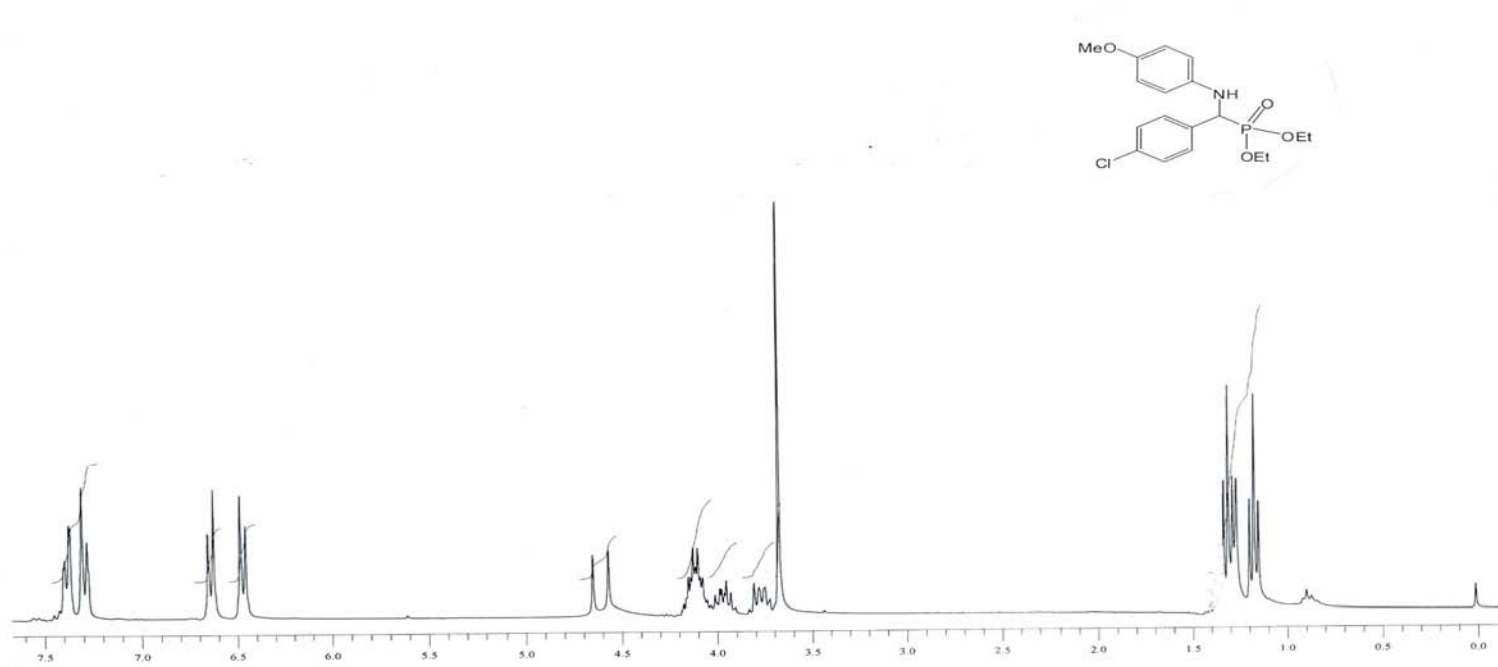


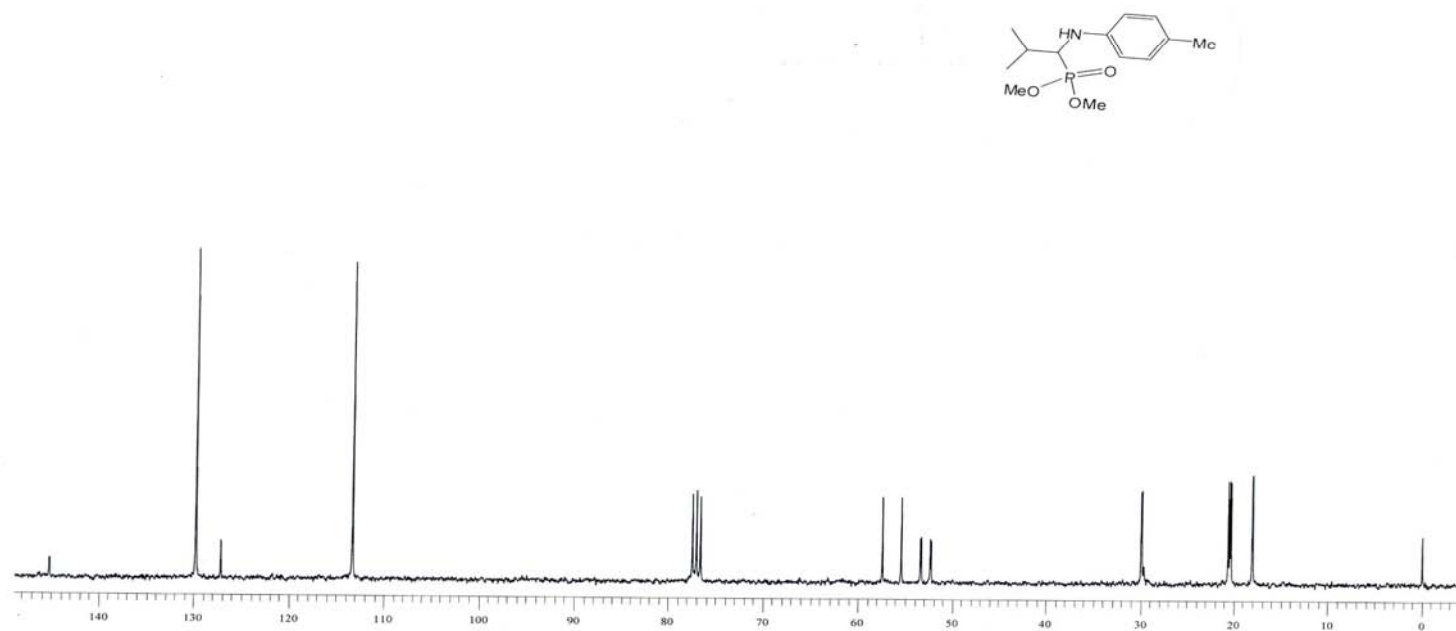
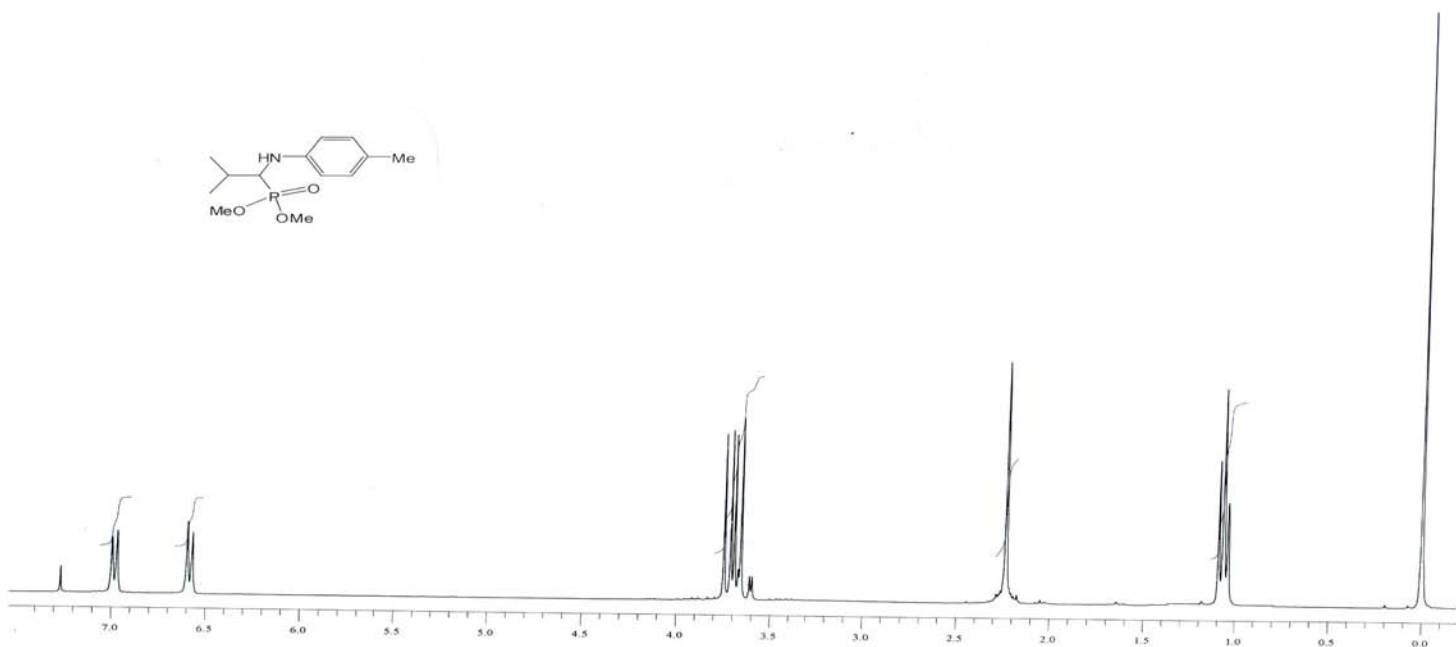


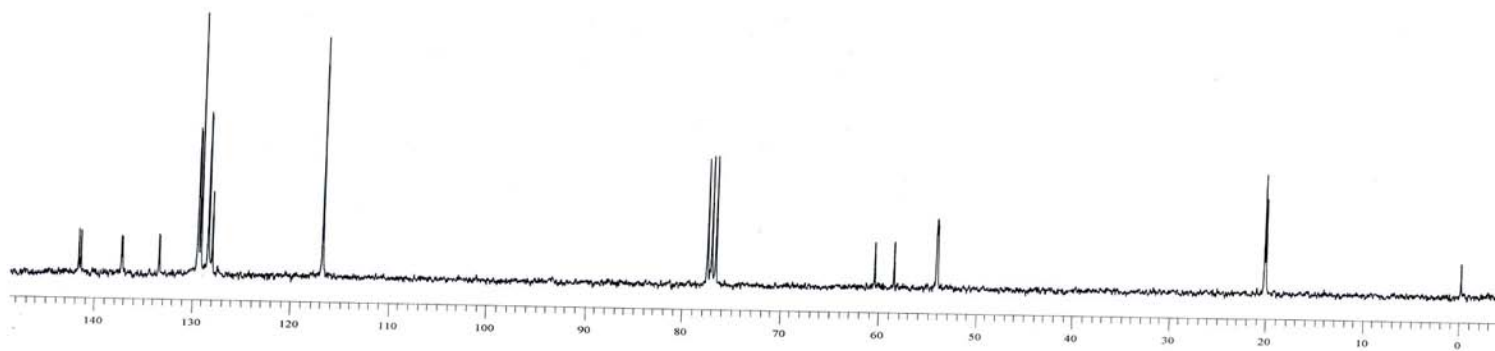
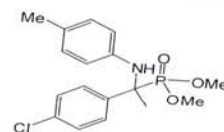
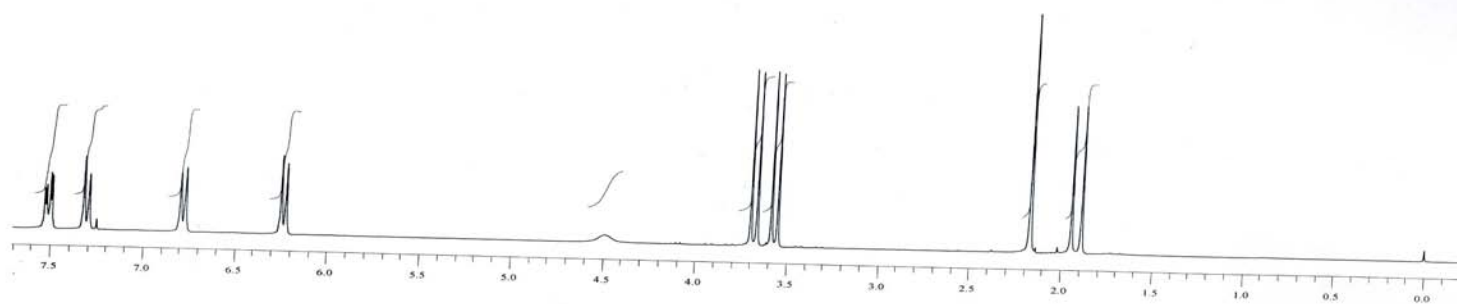
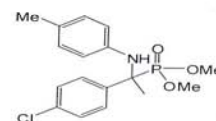


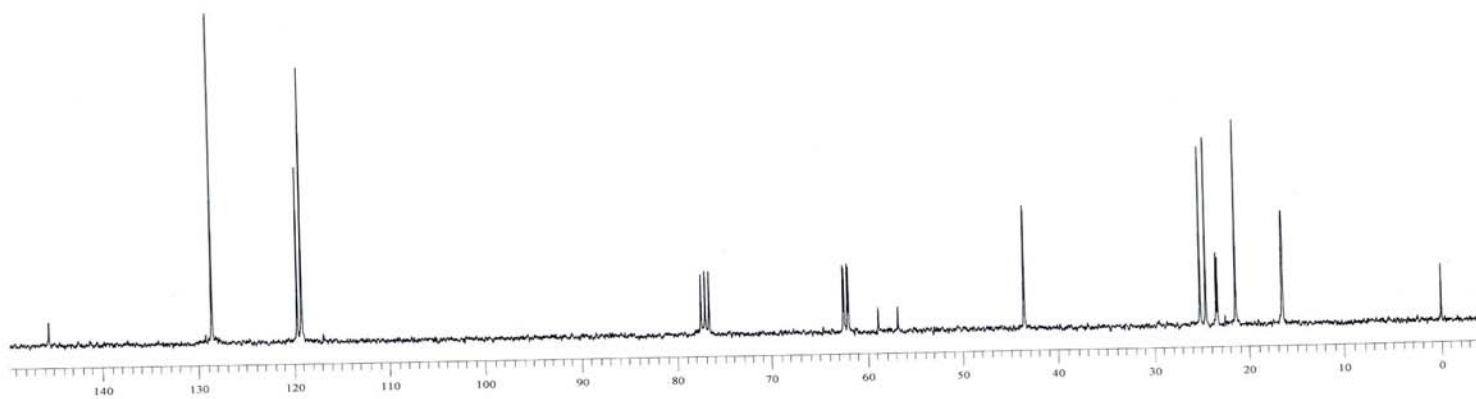
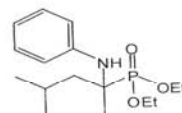
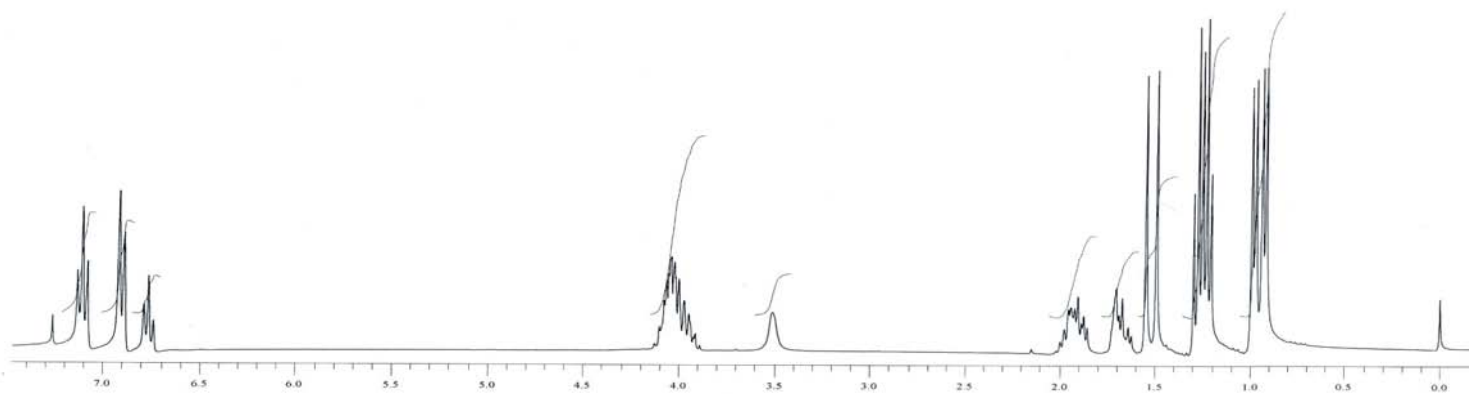
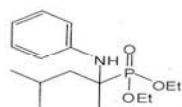


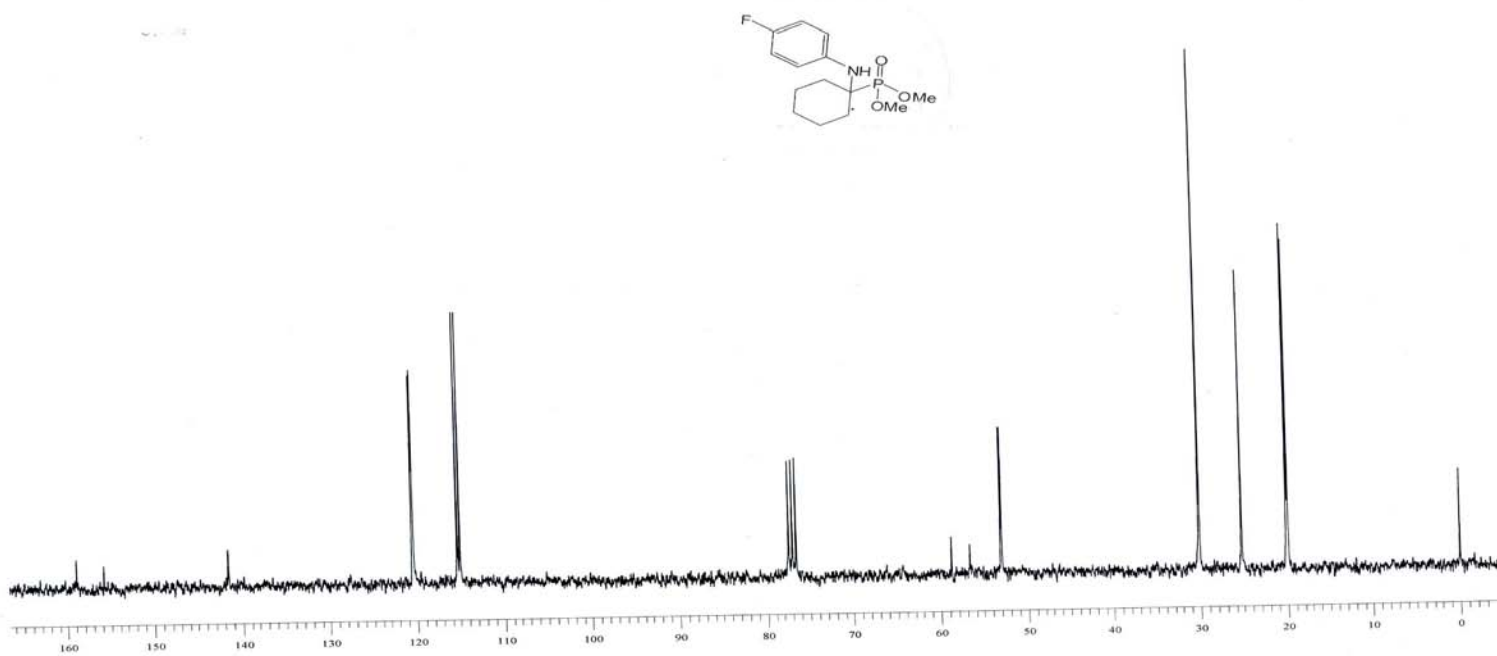
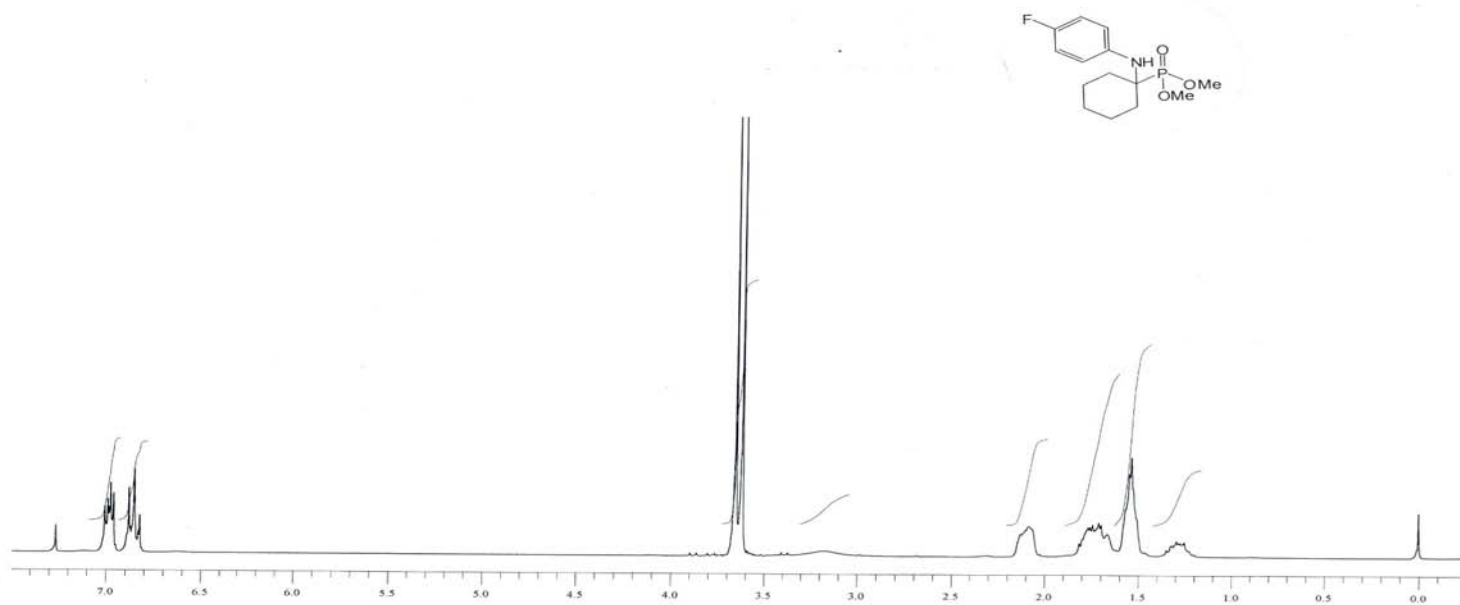












Acq. File: 20JUL09.wiff

Sample Name: BDS-24C

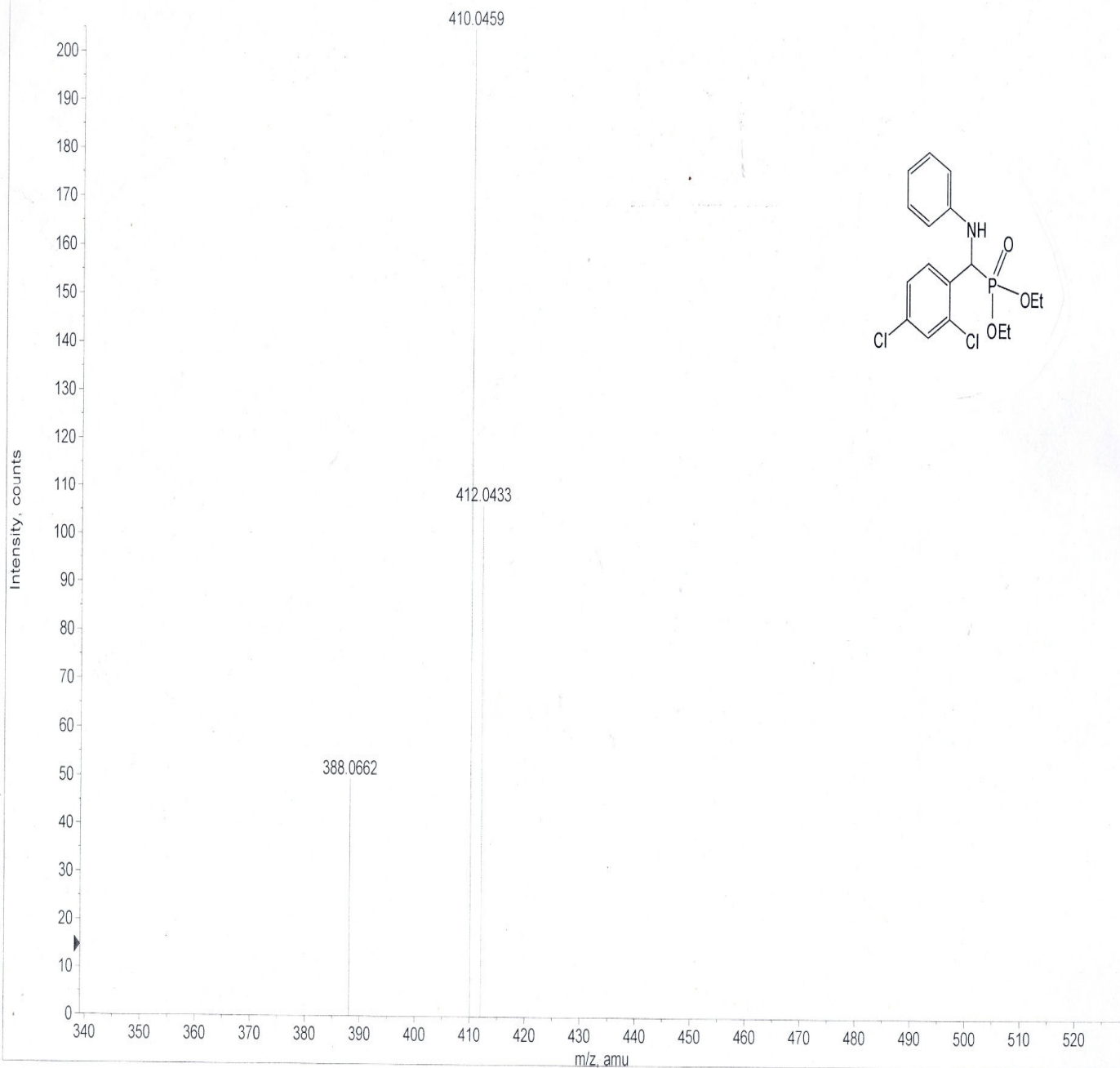
Acq. Date: Monday, July 20, 2009

Sample Comment: M.SRILATHA,BDS-24C,ESI,HRMS,+Ve

Acq. Time: 14:54

+TOF MS: 0.734 to 0.751 min from 20JUL09.wiff
a=3.54816873134171990e-004, t0=-1.47517705134887360e+001, Centroided

Max. 424.0 counts



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

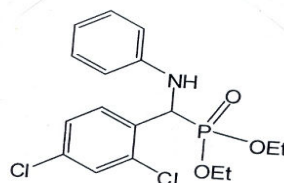
Acq. Time: n/a

Elemental composition calculator

Target m/z: +410.0459 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 20JUL09.wiff

	Elements	Min Number	Max Number
1	C	0	17
2	H	0	21
3	N	0	1
4	Cl	0	2
5	P	0	1
6	Na	0	1
7	O	0	3

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C17 H20 N O3 Na P Cl2	410.0455	0.3427	0.8357	7.5



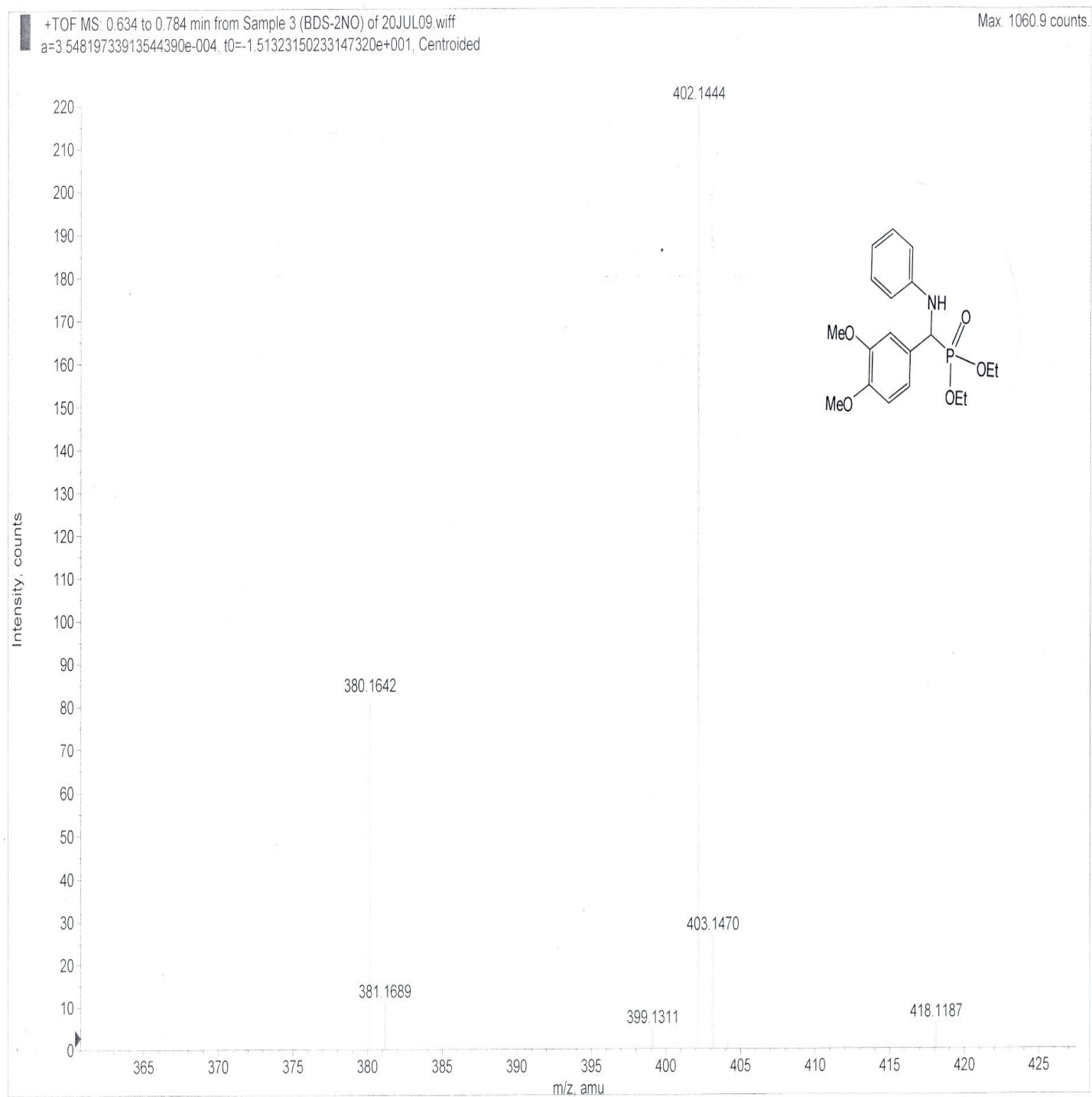
Acq. File: 20JUL09.wiff

Sample Name: BDS-2NO

Acq. Date: Monday, July 20, 2009

Sample Comment: G SATYALAKSHMI , BDS-2NO, ES1, HRMS, +Ve

Acq. Time: 16:39



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

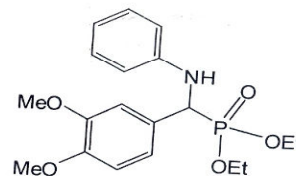
Acq. Time: n/a

Elemental composition calculator

Target m/z: +402.1444 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 20JUL09.wiff

	Elements	Min Number	Max Number
1	C	0	19
2	H	0	26
3	N	0	2
4	Na	0	1
5	O	0	6
6	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C19 H26 N O5 Na P	402.1446	-0.2313	-0.5752	7.5



Acq. File: 11MAY09.wiff

Sample Name: BDS-41SP

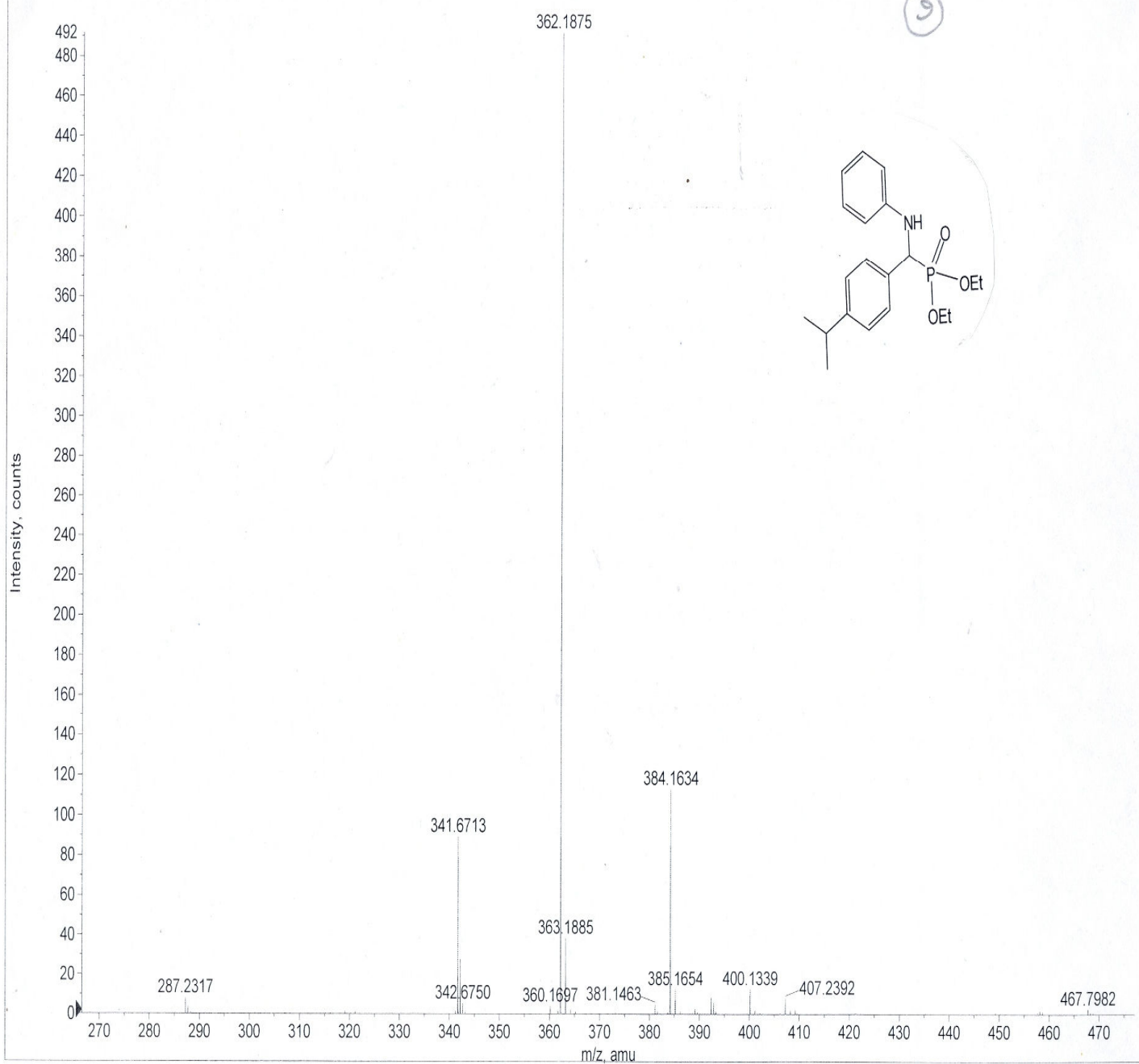
Acq. Date: Monday, May 11, 2009

Sample Comment: M.SRILATHA, BDS-41SP, ESI-TOFHRMS

Acq. Time: 15:03

+TOF MS: 0.950 to 1.017 min from Sample 7 (BDS-41SP) of 11MAY09.wiff
a=3.54753417689455850e-004, t0=-1.97003089585487030e+001

Max. 1359.8 counts.



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

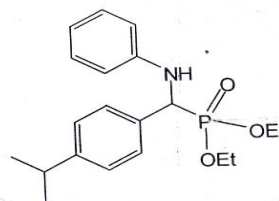
Acq. Time: n/a

Elemental composition calculator

Target m/z: +362.1875 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 11MAY09.wiff

	Elements	Min Number	Max Number
1	C	0	20
2	H	0	30
3	N	0	1
4	O	0	4
5	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C20 H29 N O3 P	362.1885	-1.0074	-2.7816	7.5



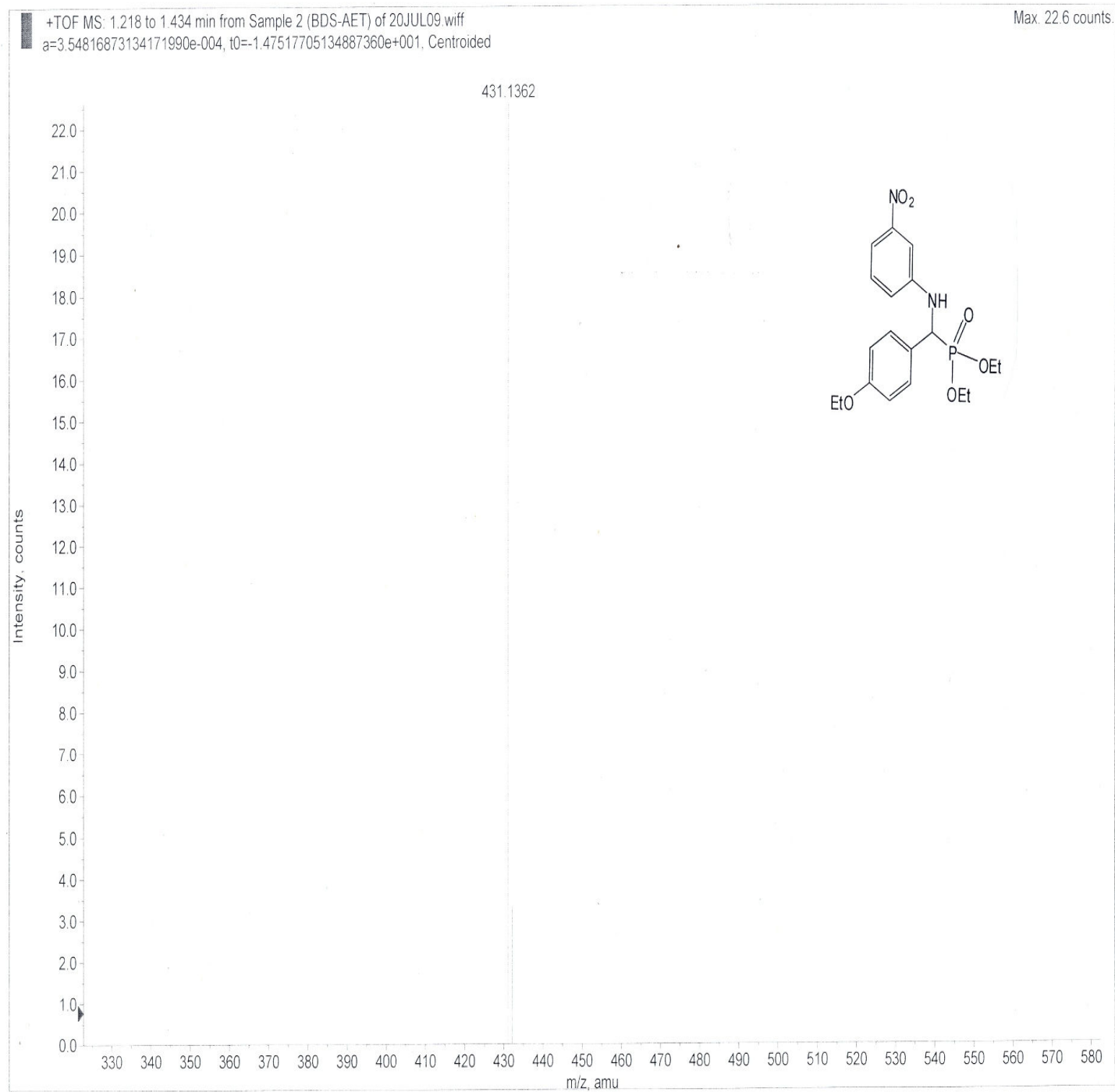
Acq. File: 20JUL09.wiff

Sample Name: BDS-AET

Acq. Date: Monday, July 20, 2009

Sample Comment: M.SRILATHA,BDS-AET,ESI,HRMS,-Ve

Acq. Time: 15:00



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

Acq. Time: n/a

Elemental composition calculator

Target m/z: +431.1362 amu

Tolerance: +10.0000 ppm

Result type: Elemental

Max num of results: 10

Min DBE: +0.0000 Max DBE: +50.0000

Electron state: OddAndEven

Num of charges: 0

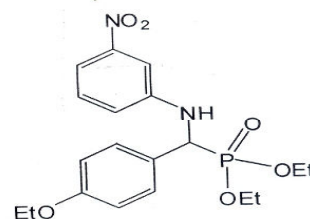
Add water: N/A

Add proton: N/A

File Name: 20JUL09.wiff

	Elements	Min Number	Max Number
1	C	0	19
2	H	0	26
3	N	0	2
4	Na	0	1
5	O	0	6
6	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C19 H25 N2 O6 Na P	431.1347	1.4050	3.2589	8.5



Acq. File: 05JUN09.wiff

Sample Name: BDS4NME

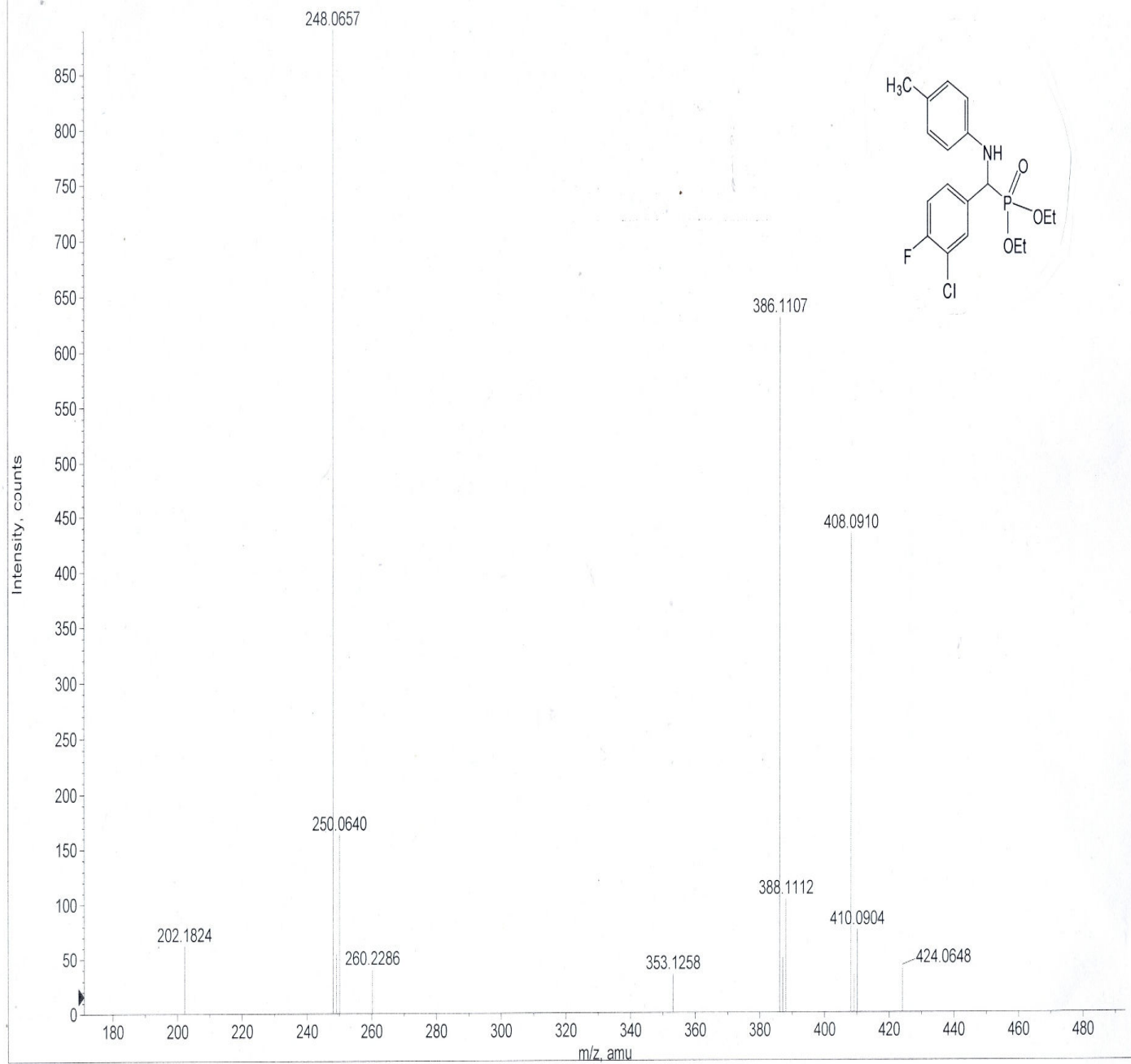
Acq. Date: Friday, June 05, 2009

Sample Comment: ~~NR1TH-3~~, BDS-4NME, ESIHRMS, +VE

Acq. Time: 12:11

+TOF MS: 0.701 to 0.734 min from Sample 7 (BDS4NME) of 05JUN09.wiff
a=3.54814466646532890e-004, t0=-1.43522914553686860e+001, Centroided

Max. 1261.1 counts.



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

Acq. Time: n/a

Elemental composition calculator

Target m/z: +408.0910 amu

Tolerance: +5.0000 ppm

Result type: Elemental

Max num of results: 10

Min DBE: +0.0000 Max DBE: +50.0000

Electron state: OddAndEven

Num of charges: 0

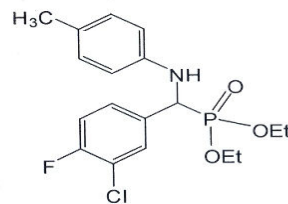
Add water: N/A

Add proton: N/A

File Name: 05JUN09.wiff

	Elements	Min Number	Max Number
1	C	0	18
2	H	0	40
3	N	0	2
4	Na	0	1
5	O	0	4
6	P	0	1
7	Cl	0	1
8	F	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C18 H22 N O3 F Na P Cl	408.0907	0.2421	0.5932	7.5



Acq. File: 05JUN09.wiff

Sample Name: BDS4NOH

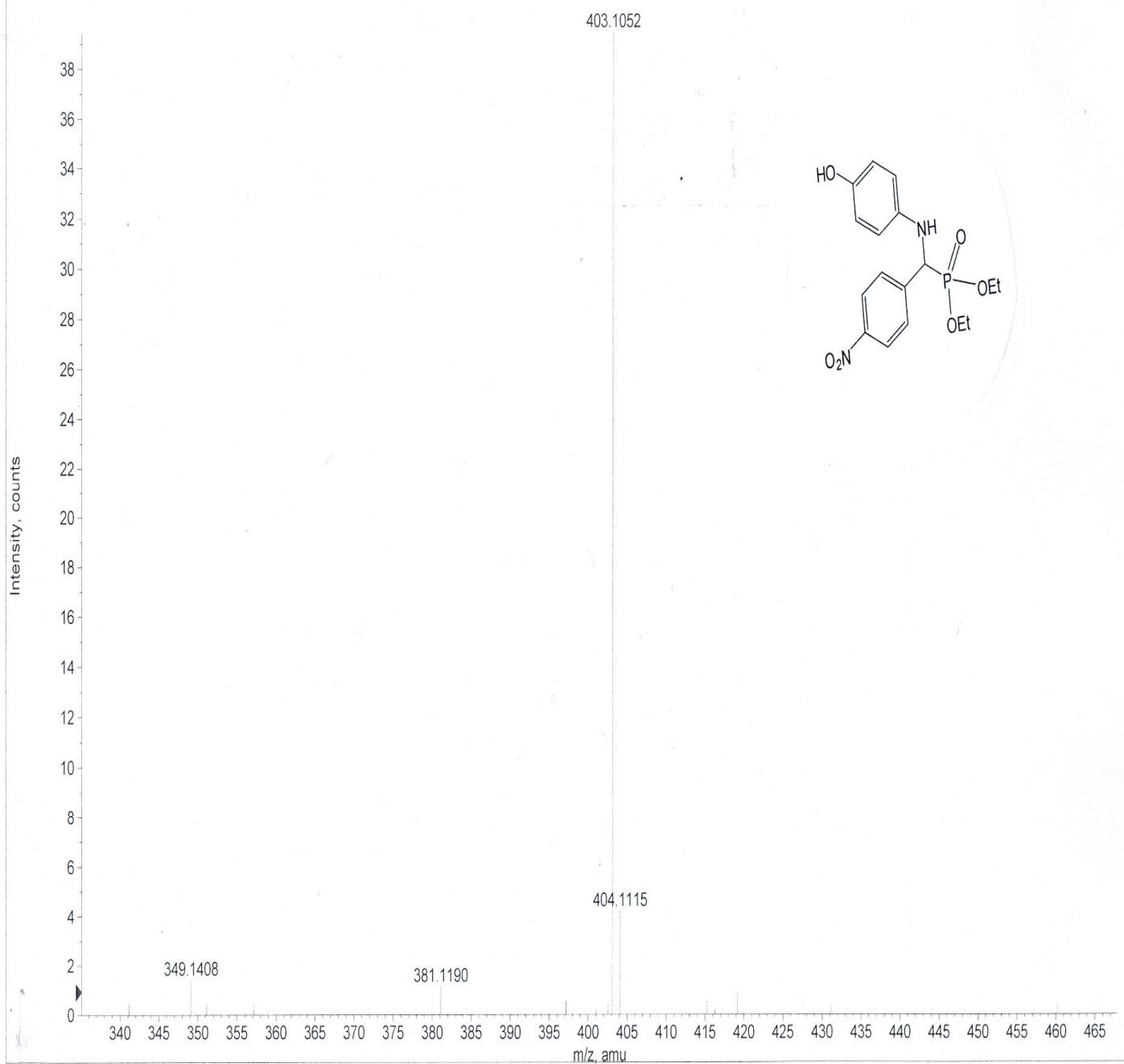
Acq. Date: Friday, June 05, 2009

Sample Comment: NIRITH B, BDS-4NOH, ESIHRMS, +VE

Acq. Time: 11:57

+TOF MS: 0.934 to 0.968 min from Sample 5 (BDS4NOH) of 05JUN09.wiff
a=3.54814466646532890e-004, t0=-1.43522914553686860e+001, Centroided

Max. 39.4 counts



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

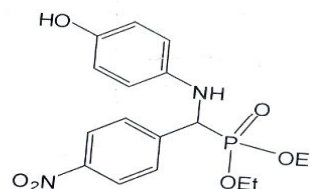
Acq. Time: n/a

Elemental composition calculator

Target m/z: +403.1052 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 05JUN09.wiff

	Elements	Min Number	Max Number
1	P	0	1
2	C	0	17
3	H	0	25
4	N	0	2
5	Na	0	1
6	O	0	7

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C17 H21 N2 O6 Na P	403.1034	1.7052	4.2301	8.5



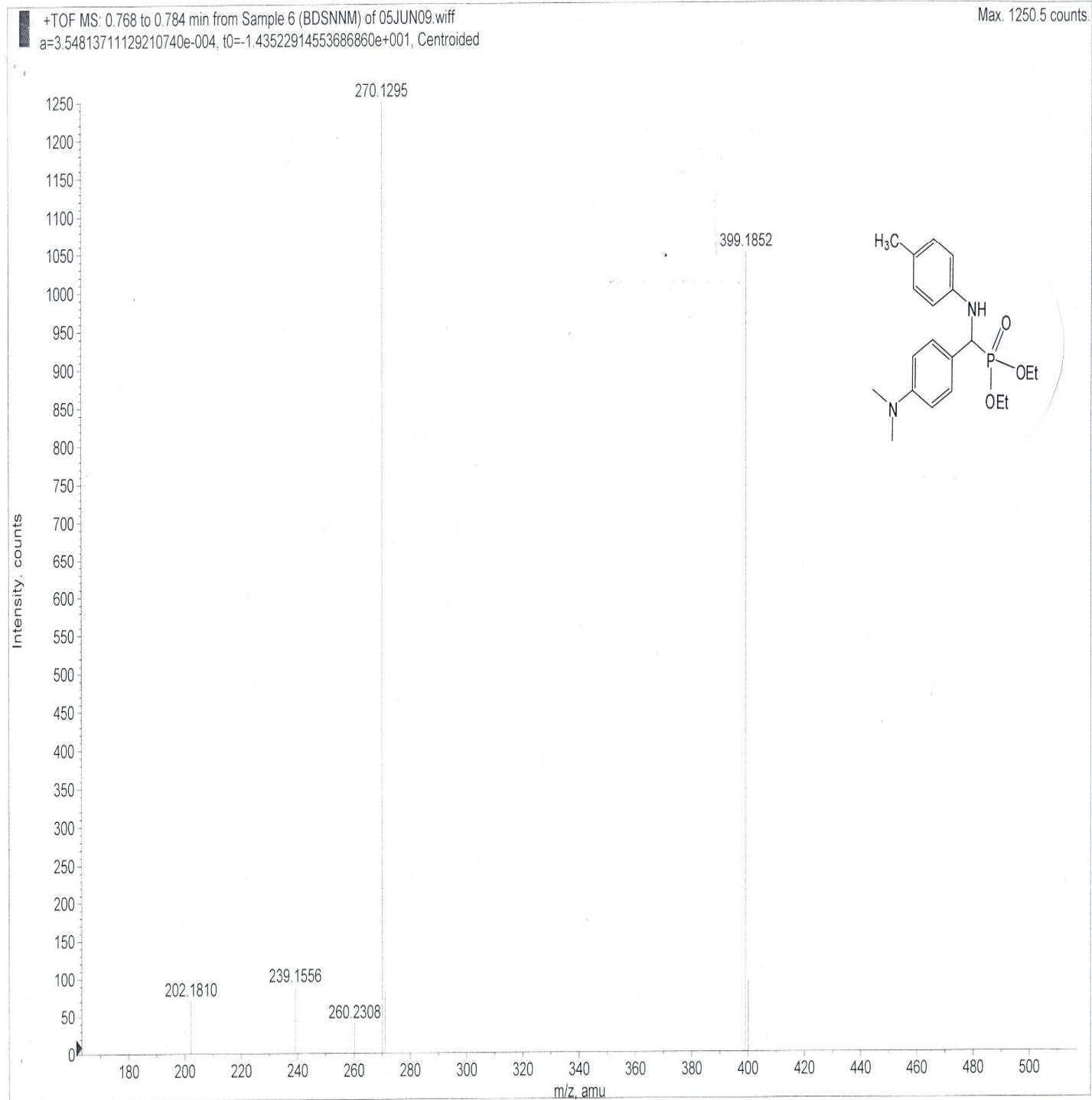
Acq. File: 05JUN09.wiff

Sample Name: BDSNNM

Acq. Date: Friday, June 05, 2009

Sample Comment: NIRITH B , BDS-NNM , ESIHRMS , +VE

Acq. Time: 12:02



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

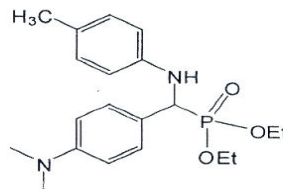
Acq. Time: n/a

Elemental composition calculator

Target m/z: +399.1852 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 05JUN09.wiff

	Elements	Min Number	Max Number
1	C	0	20
2	H	0	40
3	N	0	4
4	Na	0	1
5	O	0	7
6	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C15 H28 N4 O7 Na	399.1855	-0.3693	-0.9252	3.5
2	C20 H29 N2 O3 Na P	399.1837	1.4435	3.6162	10.5



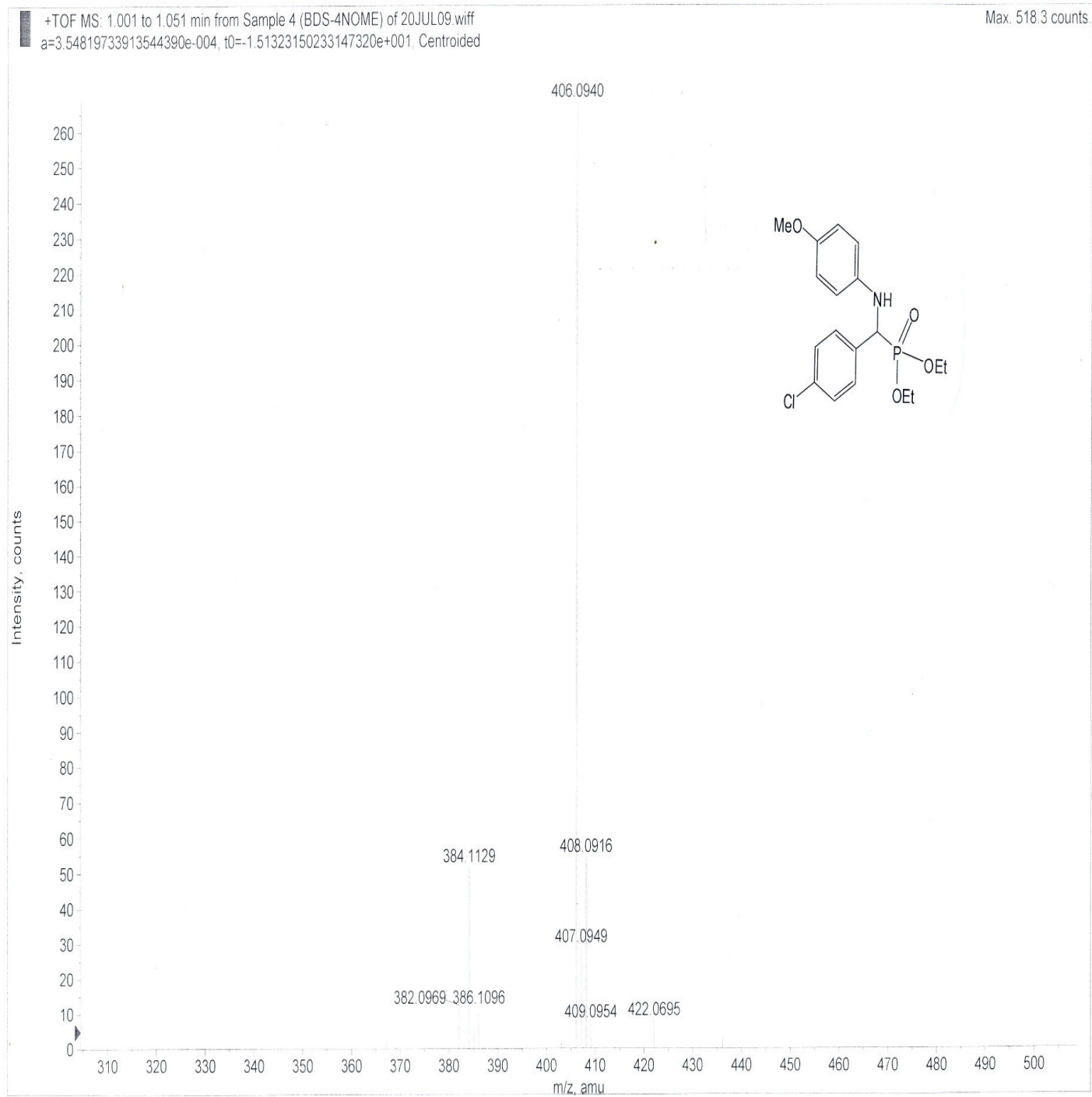
Acq. File: 20JUL09.wiff

Sample Name: BDS-4NOME

Acq. Date: Monday, July 20, 2009

Sample Comment: G SATYALAKSHMI, BDS-4NOME, ESI, HRMS, +Ve

Acq. Time: 16:46



Acq. File: n/a
Sample Comment: n/a

Sample Name: n/a

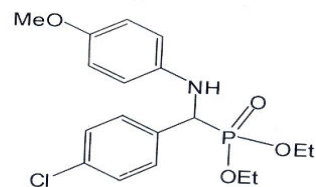
Acq. Date: n/a
Acq. Time: n/a

Elemental composition calculator

Target m/z: +406.0940 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 20JUL09.wiff

	Elements	Min Number	Max Number
1	C	0	19
2	H	0	26
3	N	0	1
4	Na	0	1
5	O	0	6
6	P	0	1
7	Cl	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C18 H23 N O4 Na P Cl	406.0950	-1.0943	-2.6947	7.5



Acq. File: 29July2009.wiff

Sample Name: ISB

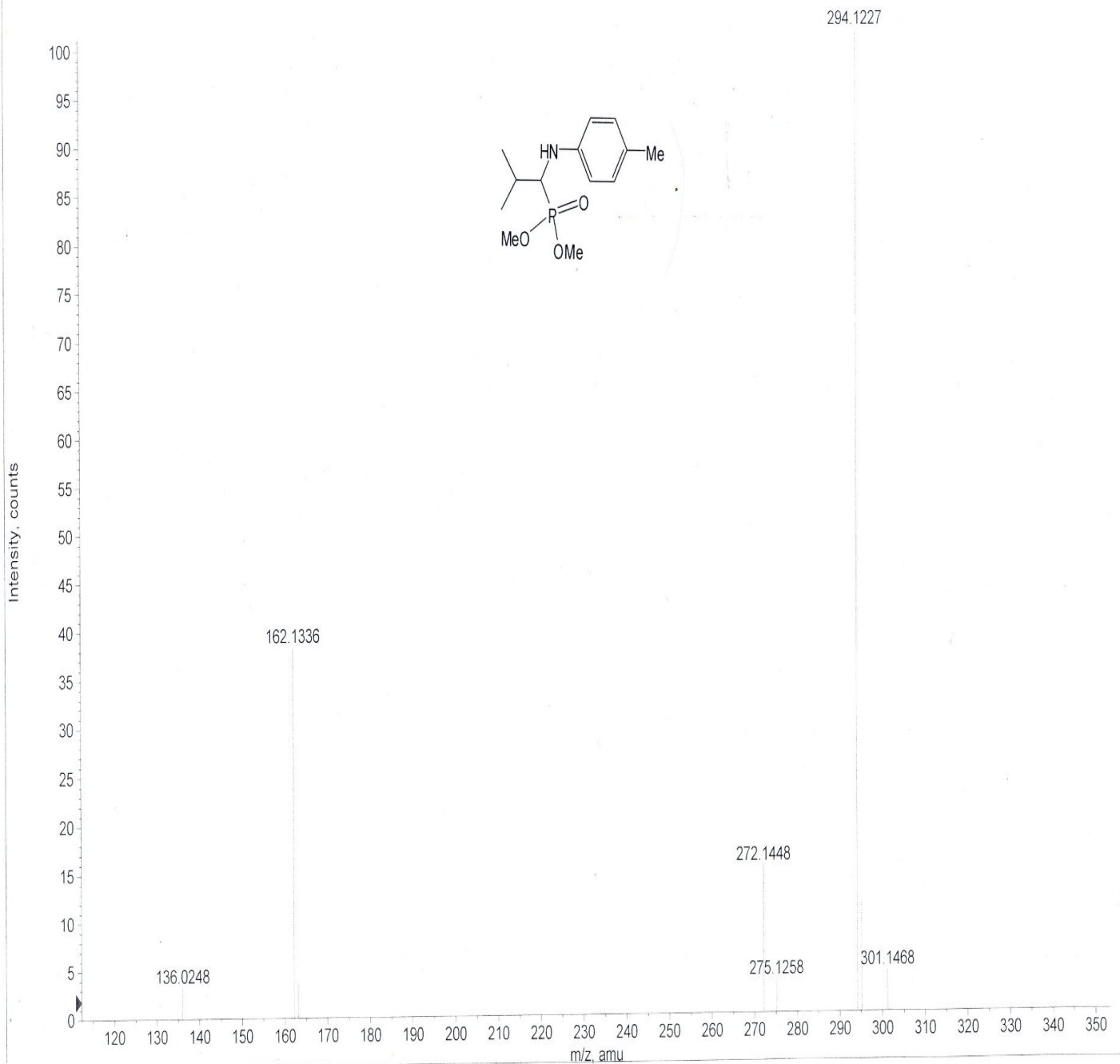
Acq. Date: Wednesday, July 29, 2009

Sample Comment: M SRILATHA , ISB, ESI-TOFHRMS

Acq. Time: 17:09

Max. 101.3 counts

+TOF MS: 1.017 min from Sample 5 (ISB) of 29July2009.wiff
a=3.54847135288408230e-004, t0=-1.61071351847713230e+001, Centroided



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

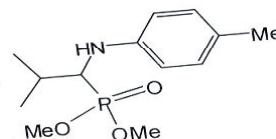
Acq. Time: n/a

Elemental composition calculator

Target m/z: +294.1227 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 29July2009.wiff

	Elements	Min Number	Max Number
1	C	0	13
2	F	0	2
3	H	0	29
4	N	0	1
5	Na	0	1
6	O	0	3
7	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C13 H22 N O3 Na P	294.1235	-0.8019	-2.7264	3.5



Acq. File: 29July2009.wiff

Sample Name: KETO

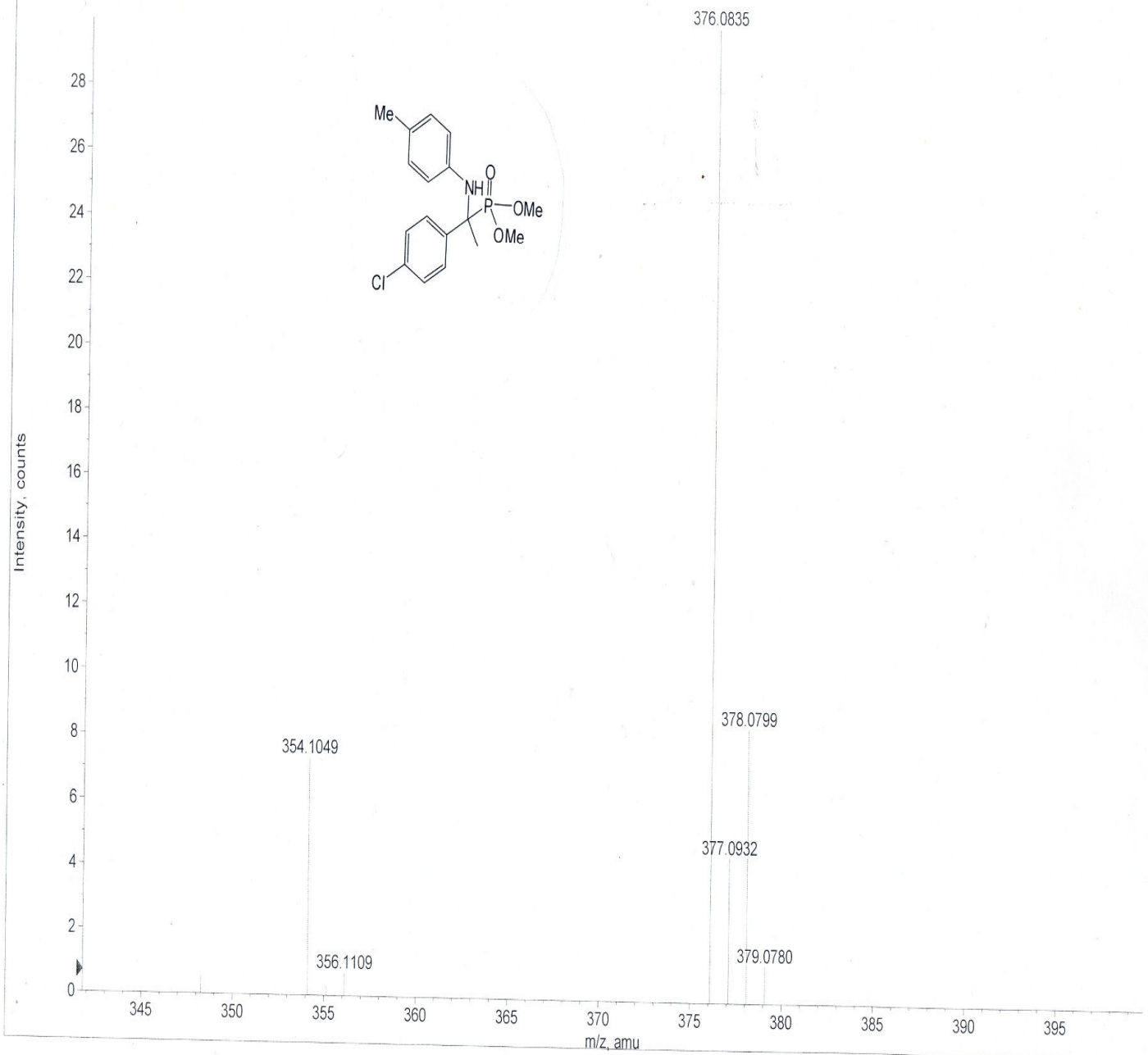
Acq. Date: Wednesday, July 29, 2009

Sample Comment: G SATYALAKSHMI , KETO, ESI-TOFHRMS

Acq. Time: 16:48

+TOF MS: 0.900 to 0.933 min from Sample 2 (KETO) of 29July2009.wiff
a=3.54853568164836660e-004, t0=-1.52436629057556270e+001, Centroided

Max. 33.8 counts.



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

* Sample Comment: n/a

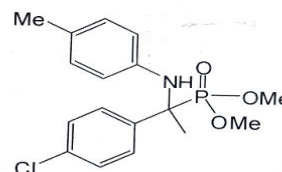
Acq. Time: n/a

Elemental composition calculator

Target m/z: +376.0835 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 29July2009.wiff

	Elements	Min Number	Max Number
1	C	0	17
2	H	0	22
3	N	0	1
4	Na	0	1
5	O	0	3
6	Cl	0	2
7	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C17 H21 N O3 Na P Cl	376.0845	-1.0295	-2.7376	7.5



Acq. File: 29July2009.wiff

Sample Name: ISBT

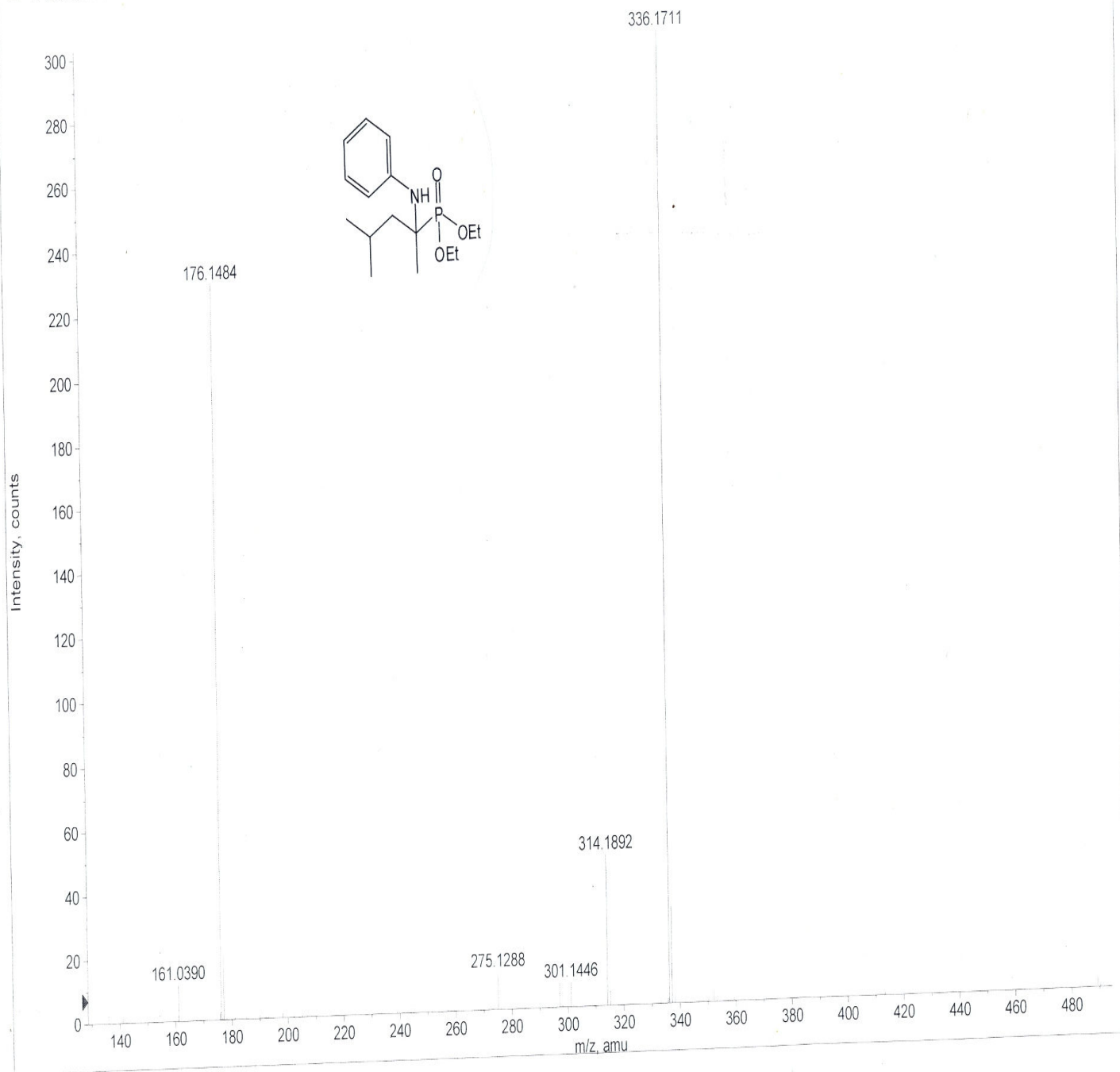
Acq. Date: Wednesday, July 29, 2009

Sample Comment: G SATYALAKSHMI, ISBT, ESI-TOFMS

Acq. Time: 17:03

Max. 303.0 counts

+TOF MS: 0.867 to 0.933 min from Sample 4 (ISBT) of 29July2009.wiff
a=3.54847135288408230e-004, t0=-1.61071351847713230e+001, Centroided



Acq. File: n/a
Sample Comment: n/a

Sample Name: n/a

Acq. Date: n/a

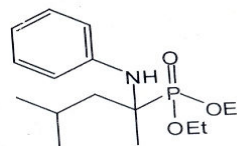
Acq. Time: n/a

Elemental composition calculator

Target m/z: +336.1711 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 29July2009.wiff

	Elements	Min Number	Max Number
1	C	0	16
2	F	0	2
3	H	0	29
4	N	0	1
5	Na	0	1
6	O	0	3
7	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C16 H28 N O3 Na P	336.1704	0.6478	1.9271	3.5



Acq. File: 29July2009.wiff

Sample Name: CY-ME

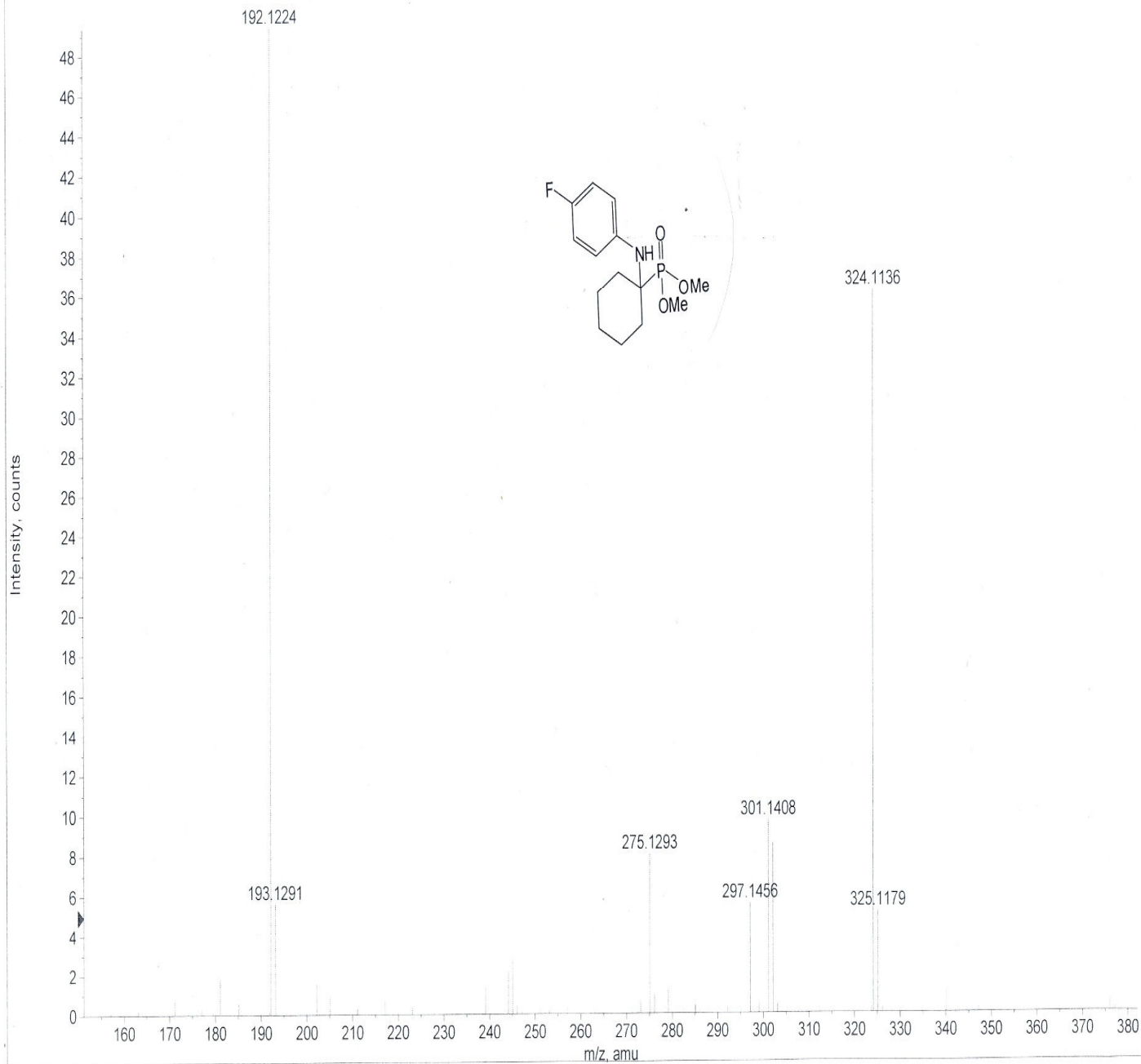
Acq. Date: Wednesday, July 29, 2009

Sample Comment: G SATYALAKSHMI, CY-ME, ESI-TOFHRMS

Acq. Time: 16:57

+TOF MS: 0.933 to 1.033 min from Sample 3 (CY-ME) of 29July2009.wiff,
a=3.54847135288408230e-004, t0=-1.61071351847713230e+001, Centroided

Max. 49.4 counts.



Acq. File: n/a

Sample Name: n/a

Acq. Date: n/a

Sample Comment: n/a

Acq. Time: n/a

Elemental composition calculator

Target m/z: +324.1136 amu
Tolerance: +5.0000 ppm
Result type: Elemental
Max num of results: 10
Min DBE: +0.0000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 29July2009.wiff

	Elements	Min Number	Max Number
1	C	0	14
2	F	0	2
3	H	0	22
4	N	0	1
5	Na	0	1
6	O	0	3
7	P	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C14 H21 N O3 F Na P	324.1140	-0.4801	-1.4813	4.5

