Electronic Supplementary Material (ESI) for RSC Medicinal Chemistry.

Supplementary data for phenoxyphenyl triazolyl derivatives

-NMR spectra

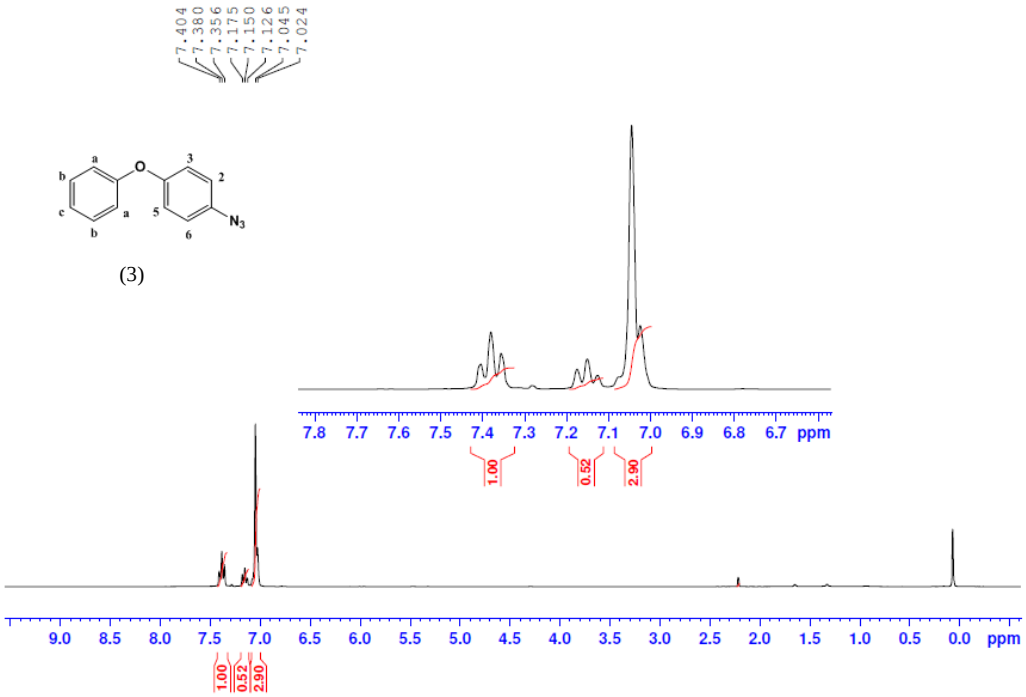
-IR spectra

-HRMS spectra

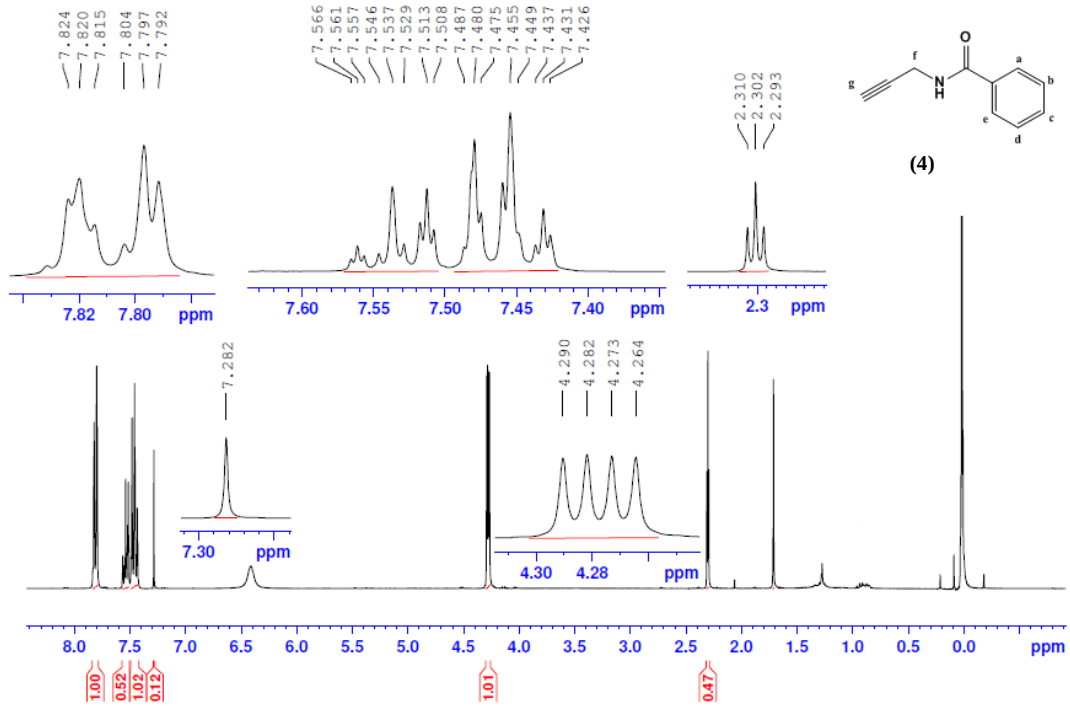
-HPLC Chromatograms

^{1}H-NMR and ^{13}C-NMR spectra

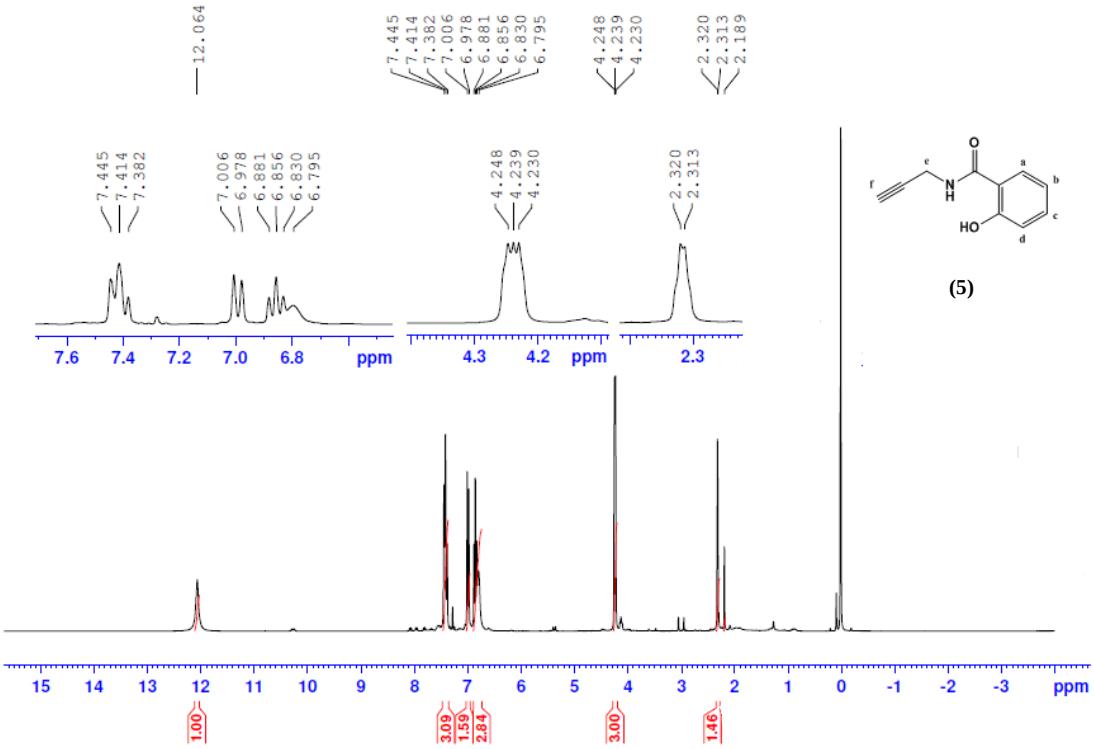
1. ^{1}H-NMR of 4-Phenoxyphenylazide (3)



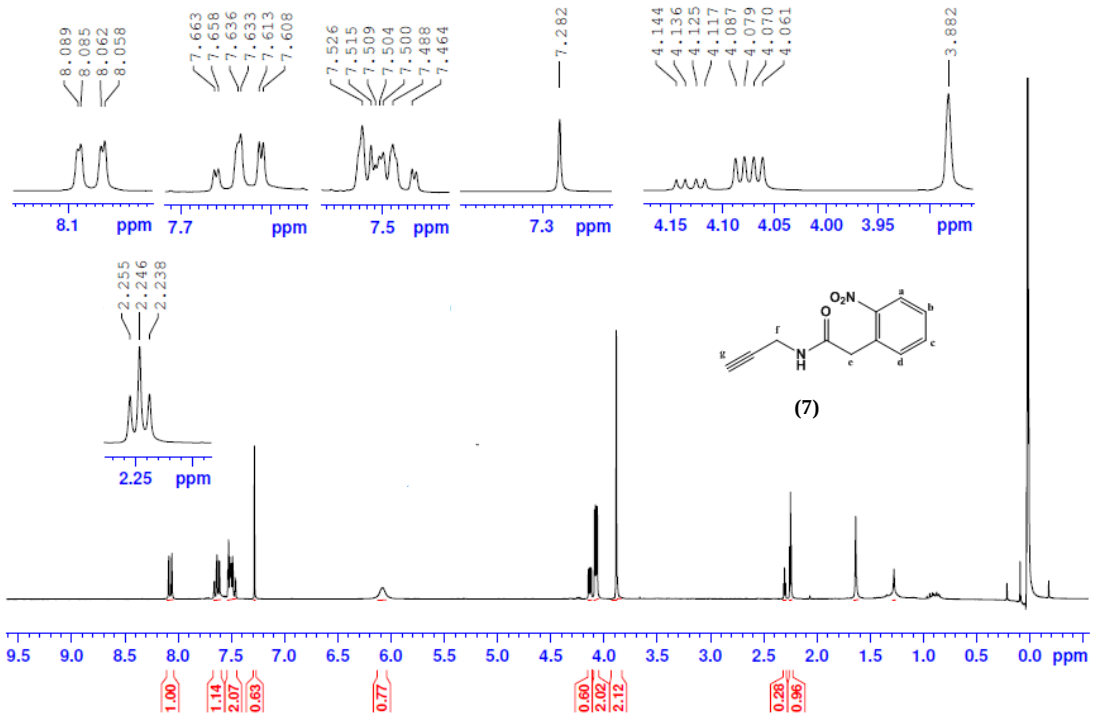
2. ^{1}H-NMR of Propargyl benzamide (4)



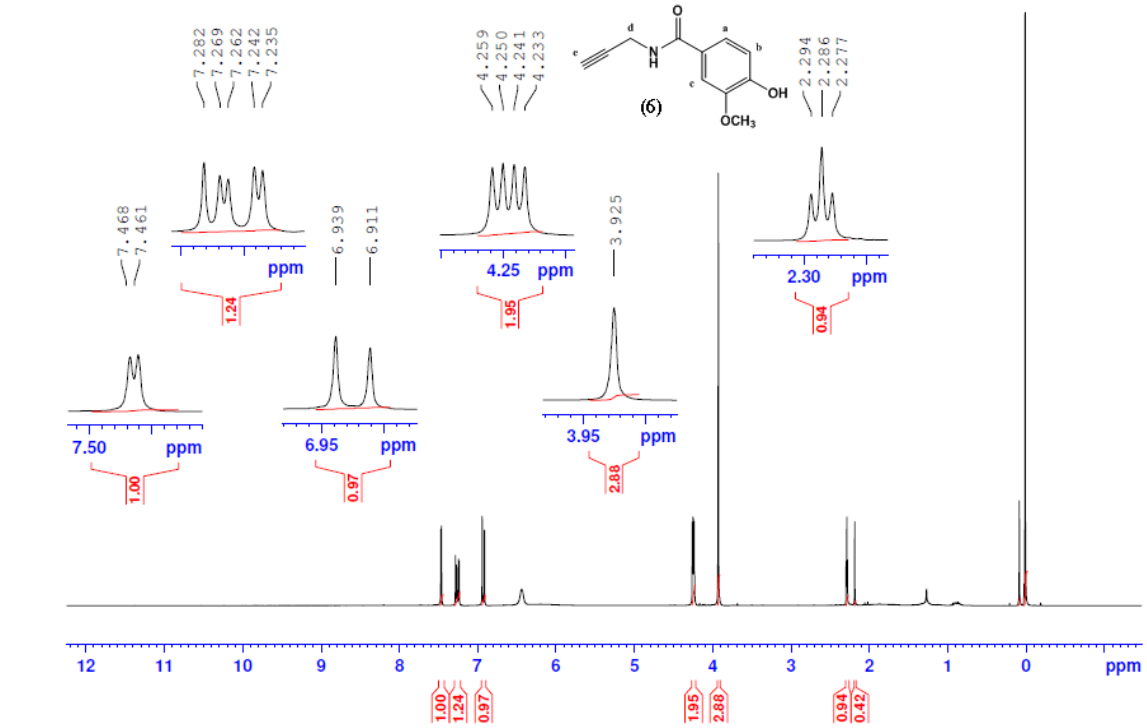
3. ^{1}H-NMR of Propargyl 2-hydroxybenzamide (5)



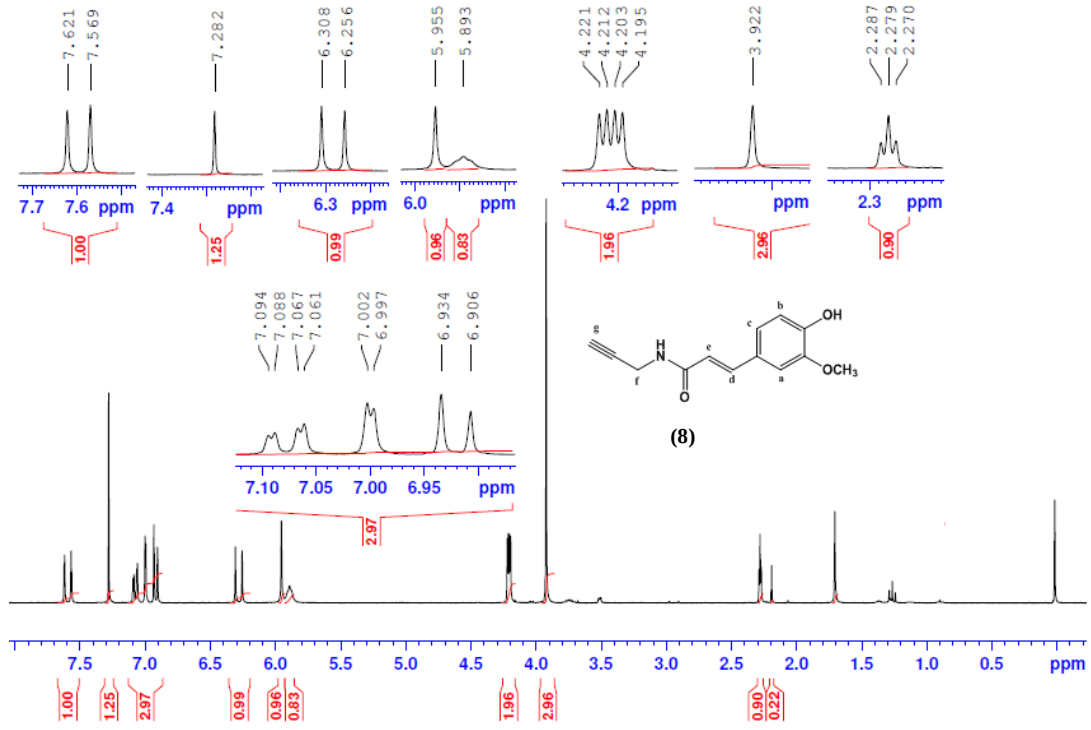
4. ^{1}H-NMR of Propargyl 2-(2-nitrophenyl)acetamide (7)



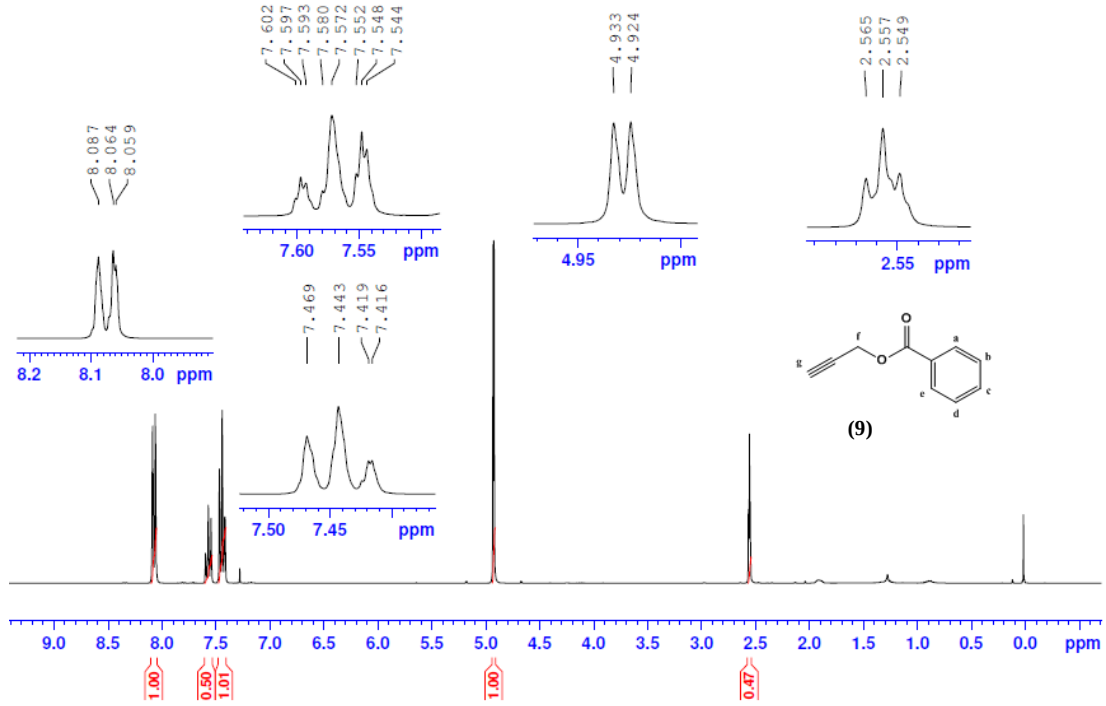
5. ^{1}H-NMR of Propargyl 4-hydroxy-3-methoxybenzamide (6)



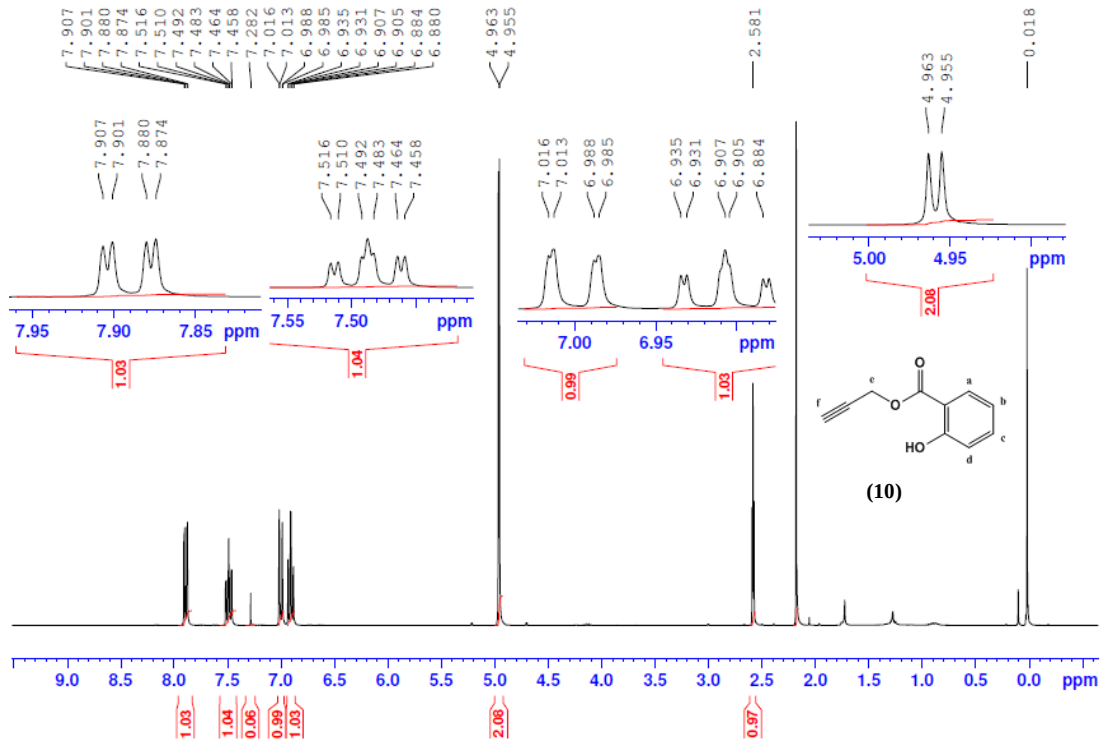
6. ^{1}H-NMR of Propargyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylamide (8)



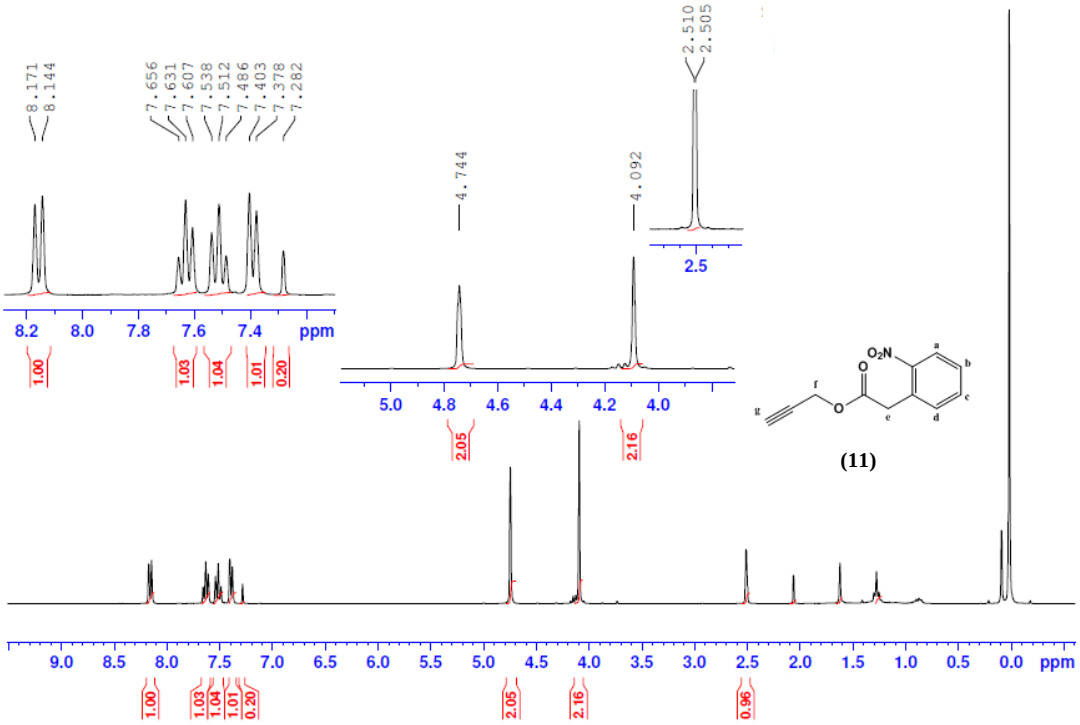
7. ^{1}H-NMR of Propargyl benzoate (9)



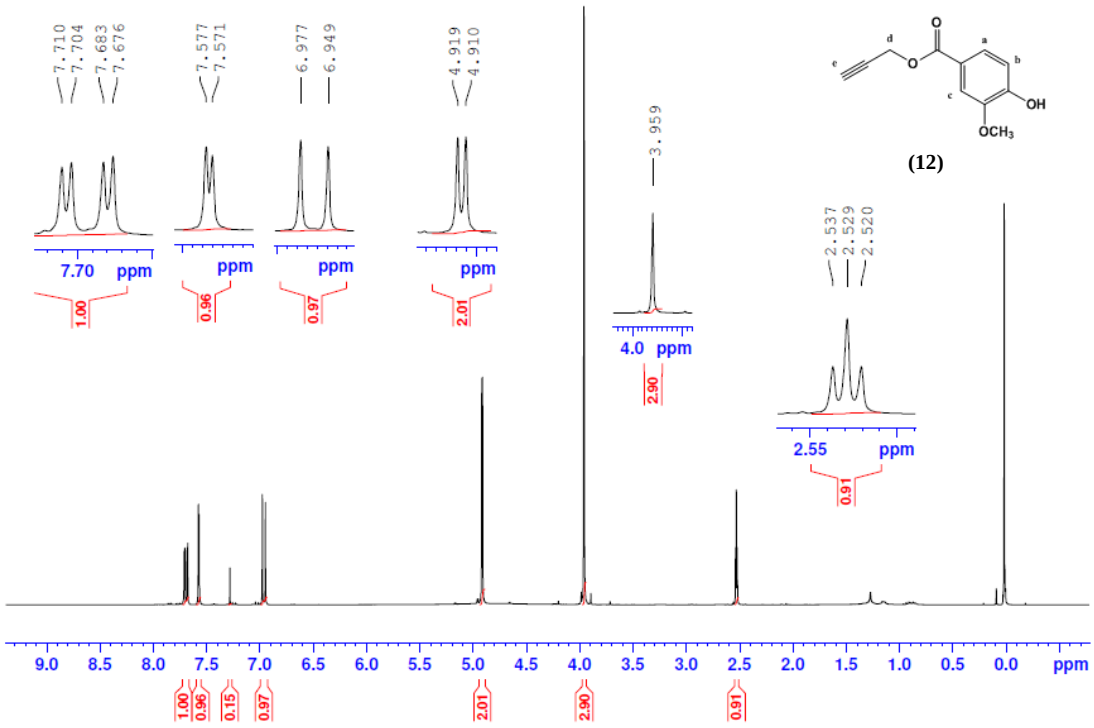
8. ^{1}H-NMR of Propargyl 2-hydroxybenzoate (10)



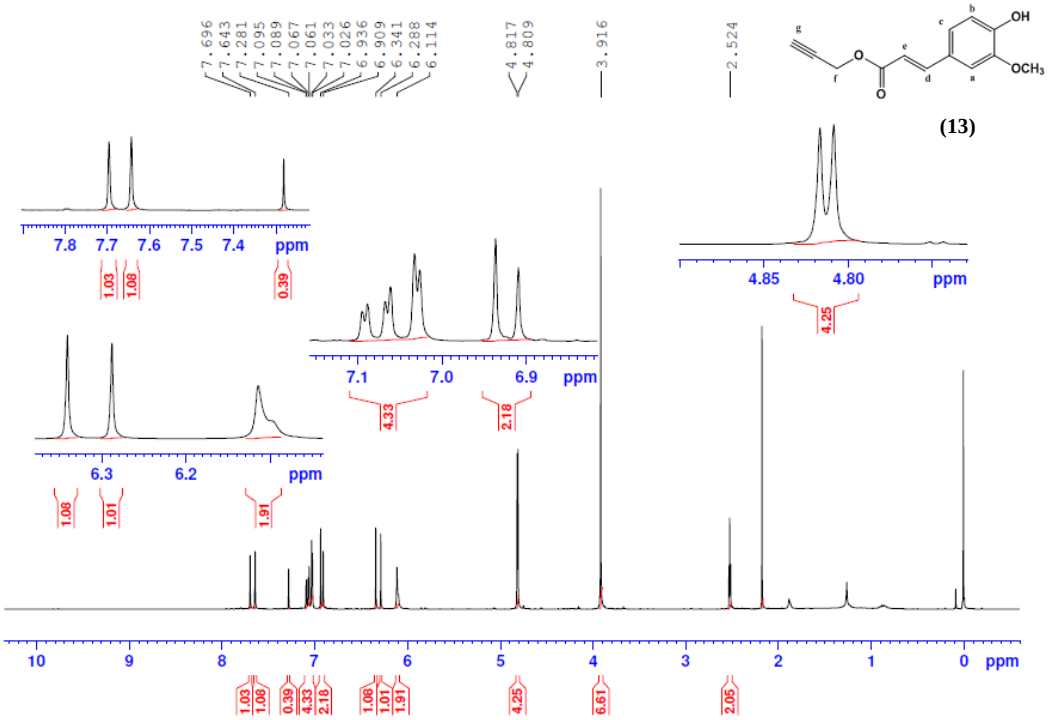
9. ^{1}H-NMR of Propargyl (2-nitrophenyl)acetate (12)



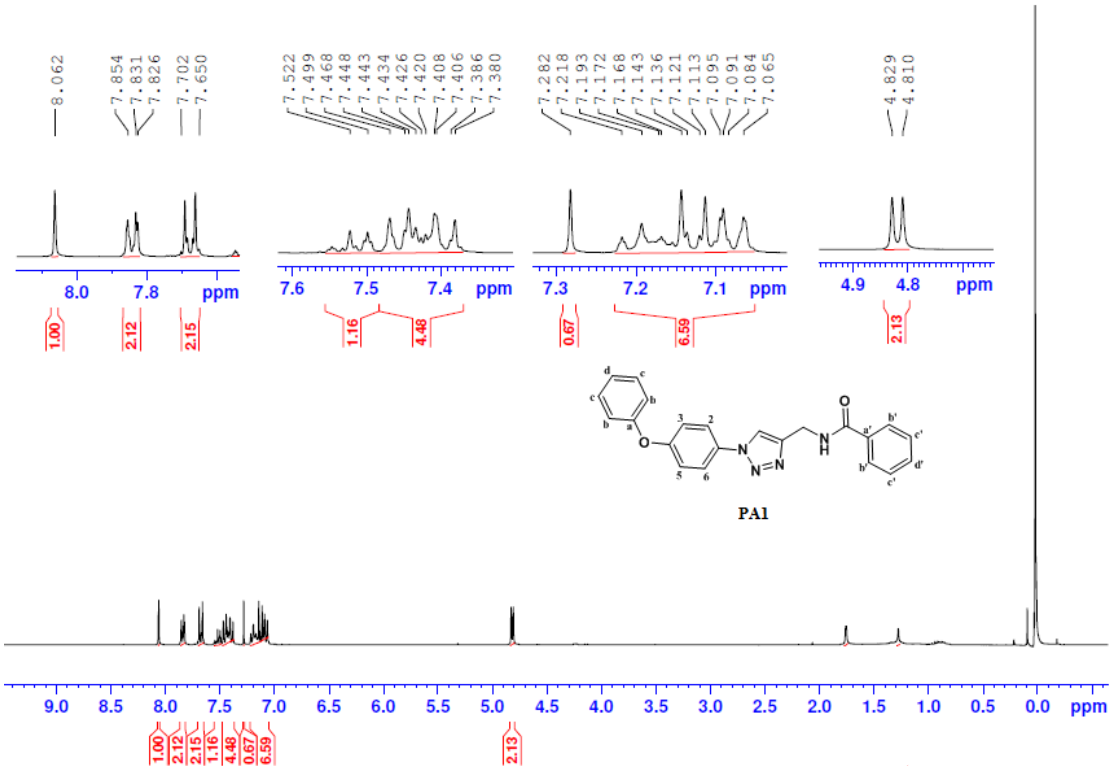
10. ^{1}H-NMR of Propargyl 4-hydroxy-3-methoxybenzoate (11)



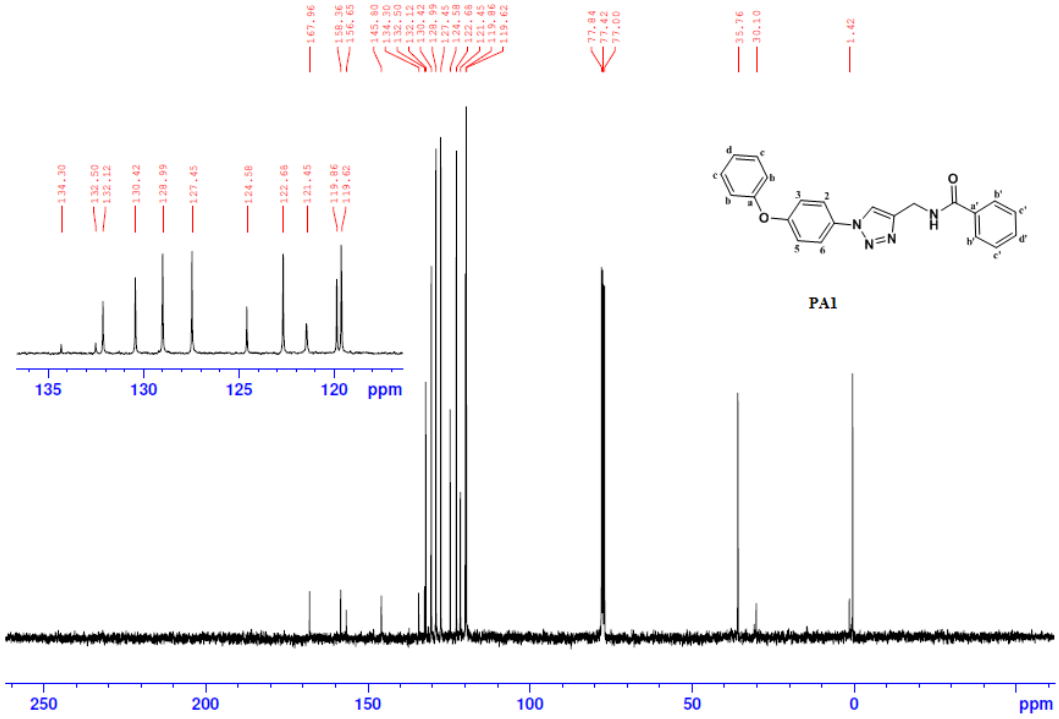
11. ^{1}H-NMR of Propargyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (13)



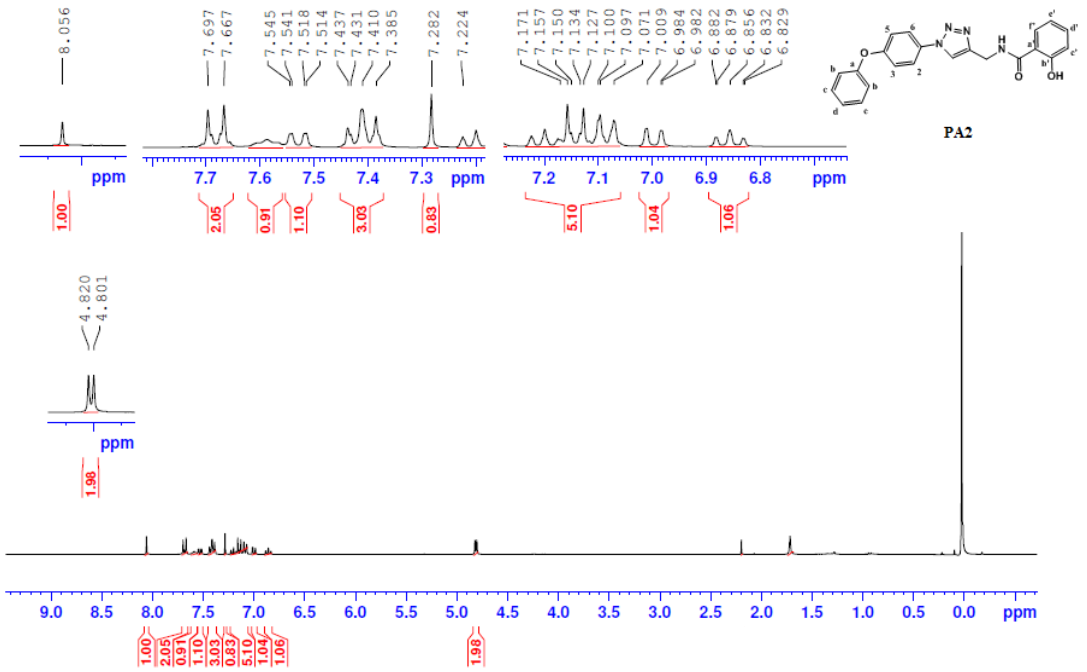
12. ^{1}H-NMR of *N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA1)



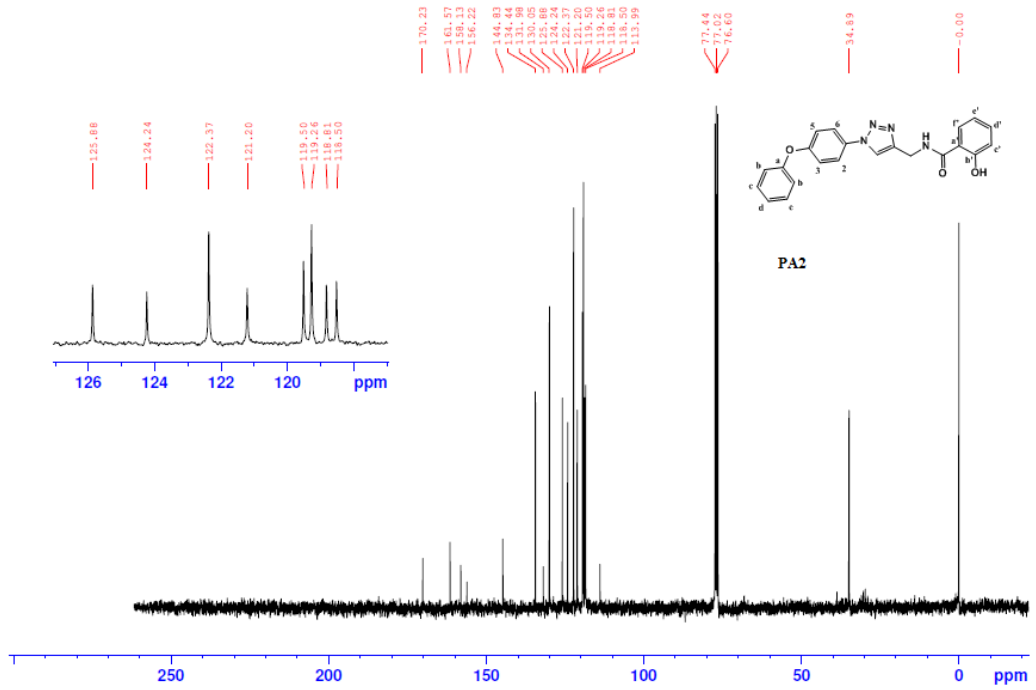
13. ^{13}C-NMR of *N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA1)



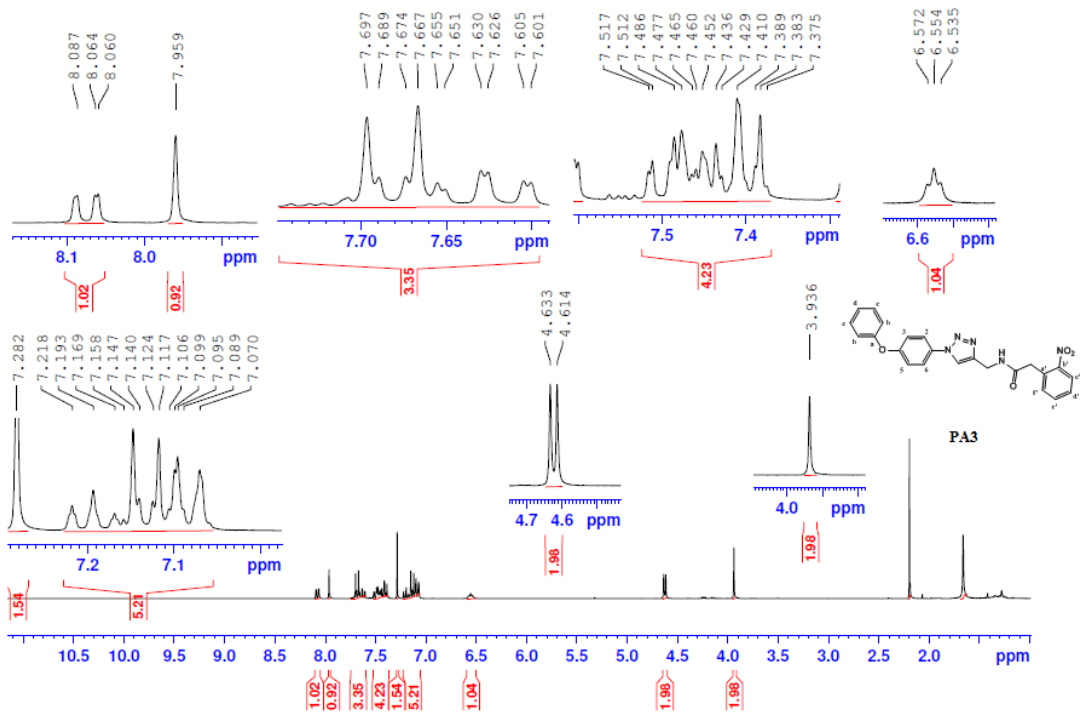
14. ^{1}H-NMR of 2-hydroxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA2)



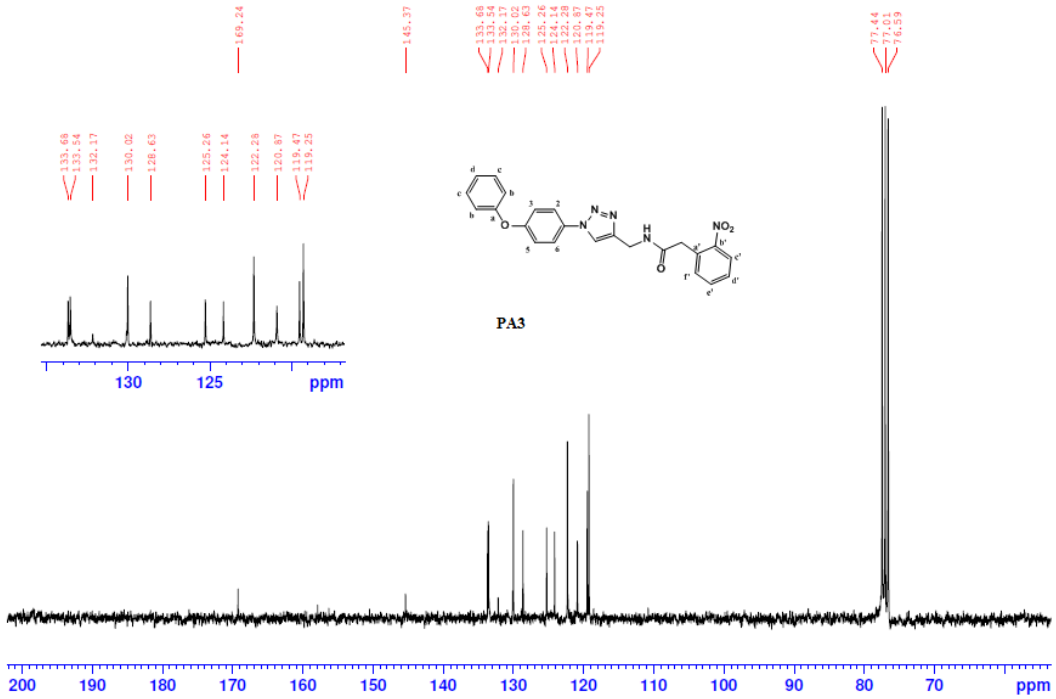
15. ^{13}C-NMR of 2-hydroxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA2)



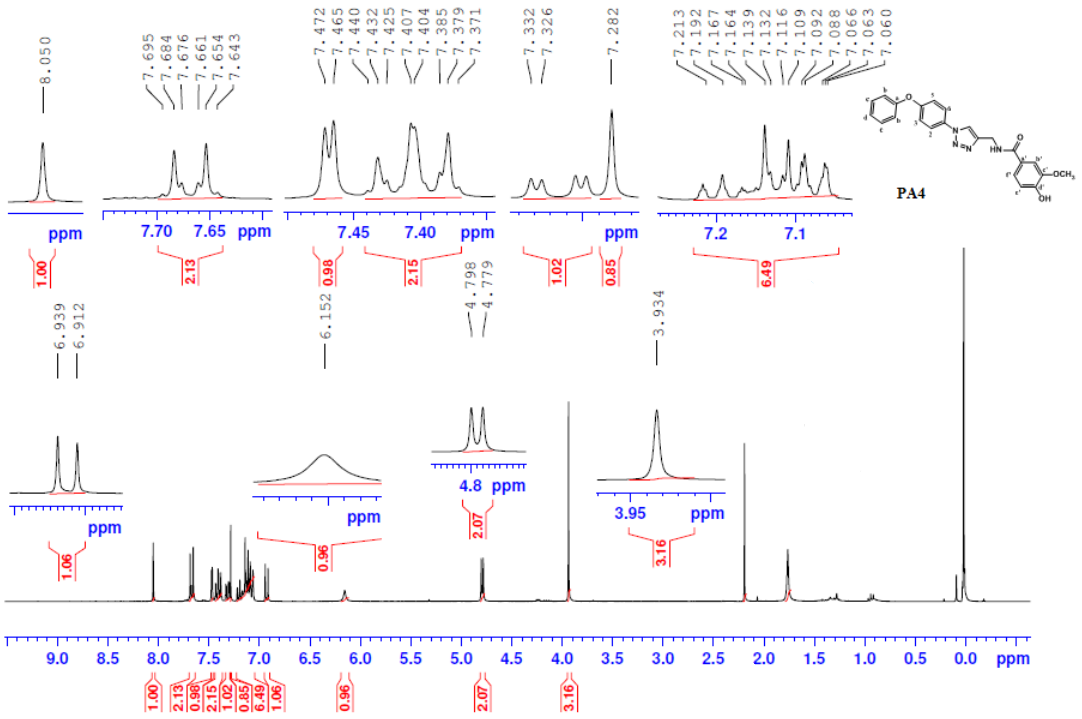
16. ^{1}H-NMR of 2-(2-nitrophenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide (PA3)



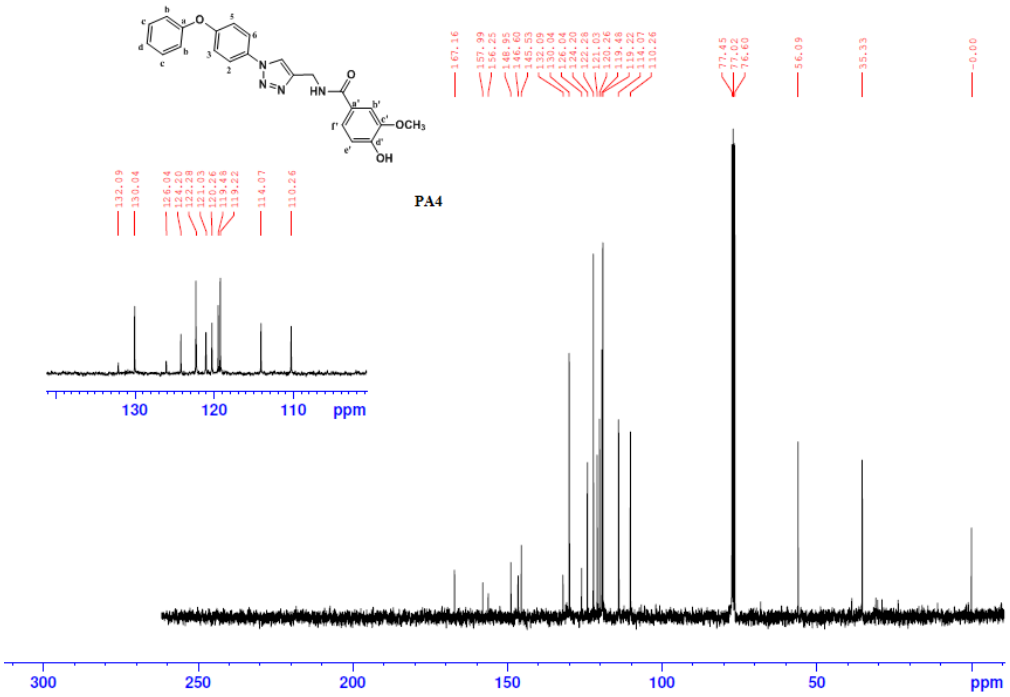
17. ^{13}C-NMR of 2-(2-nitrophenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide (PA3)



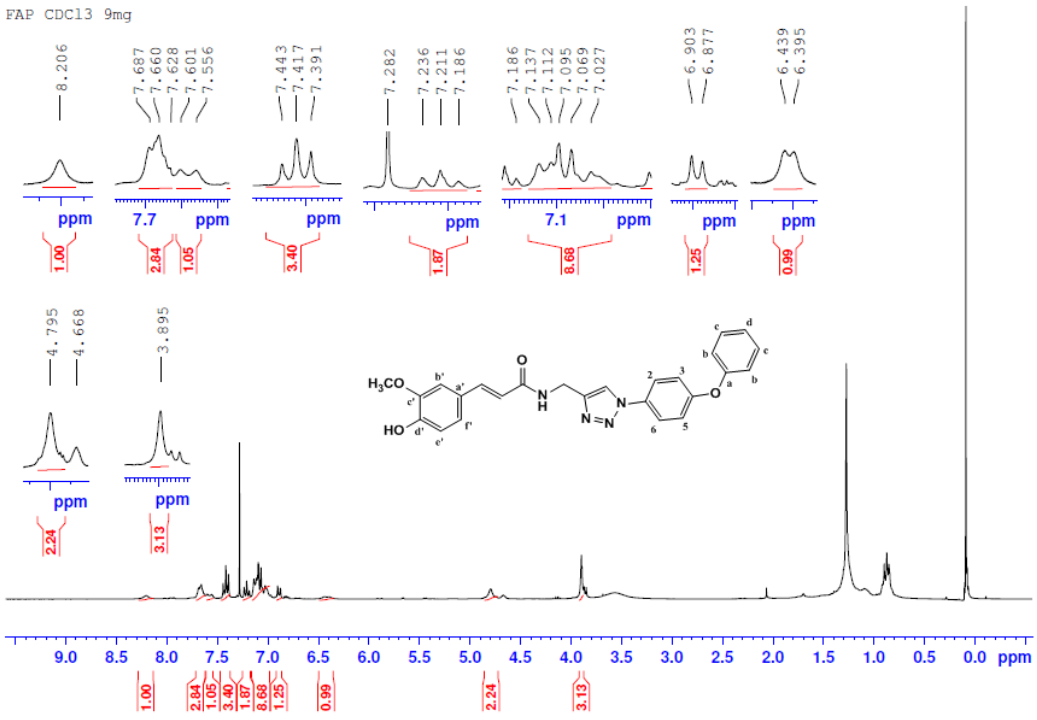
18. ^{1}H-NMR of 4-hydroxy-3-methoxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA4)



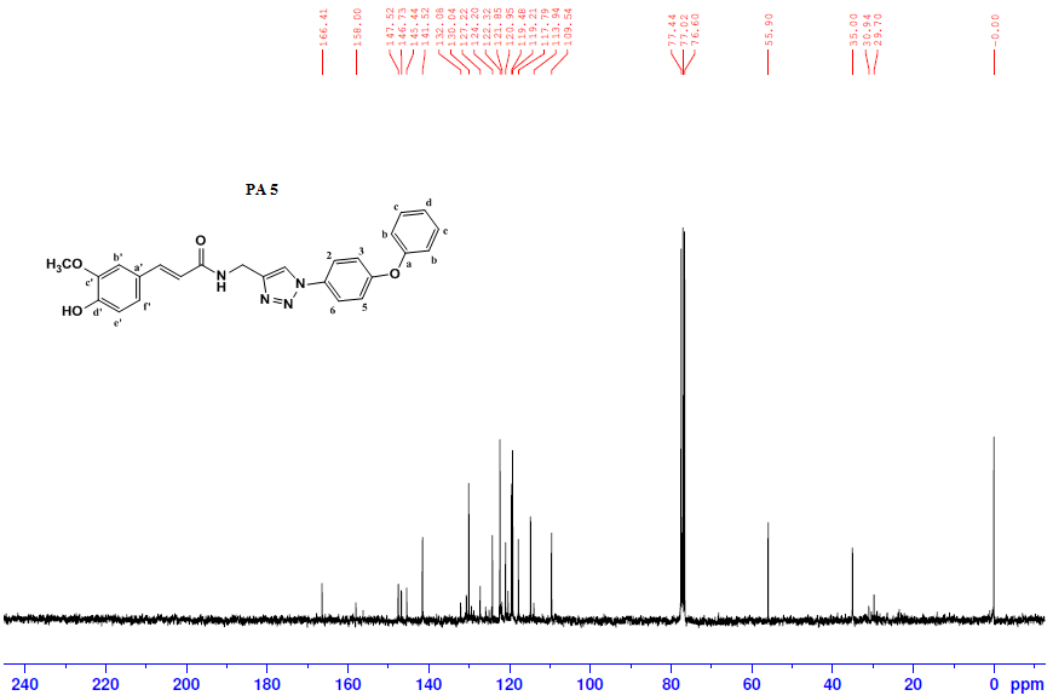
19. ^{13}C-NMR of 4-hydroxy-3-methoxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA4)



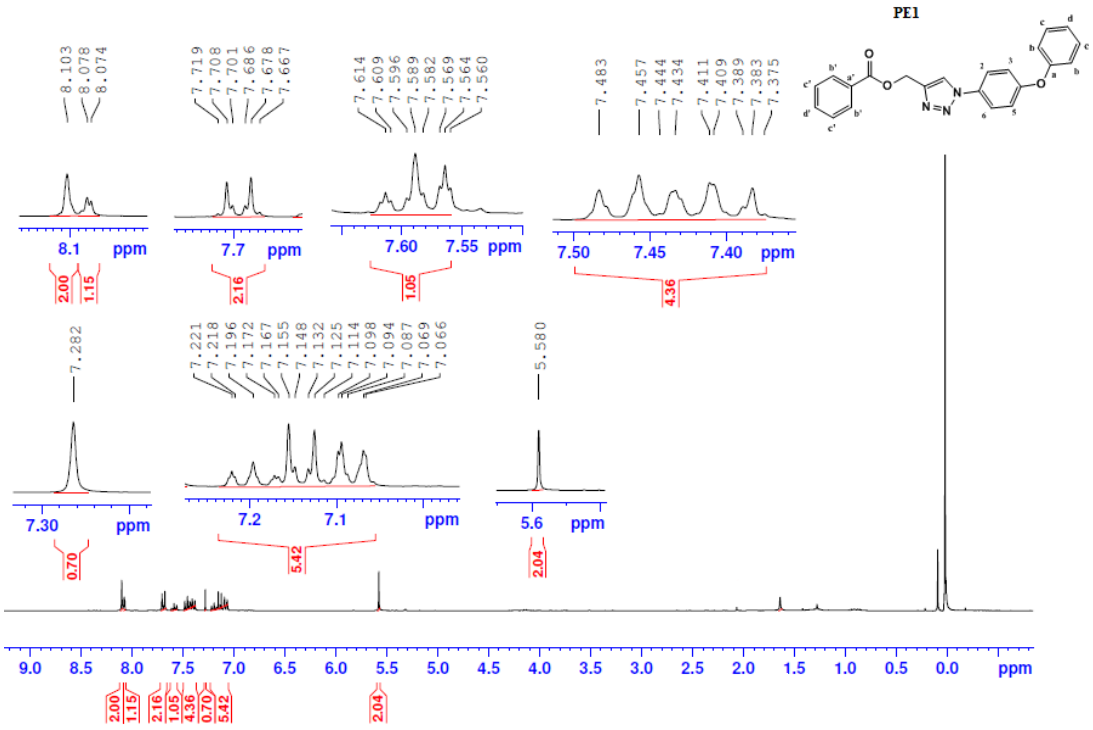
20. ^{1}H-NMR of (*E*)-3-(4-hydroxy-3-methoxyphenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acrylamide (PA5)



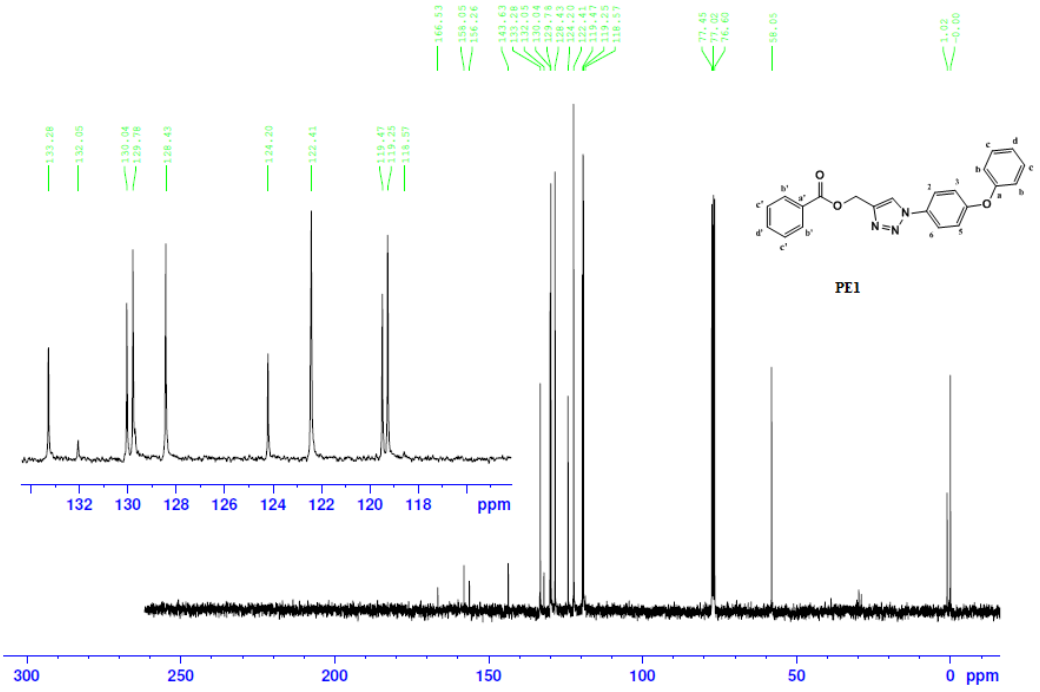
21. ^{13}C-NMR of (*E*)-3-(4-hydroxy-3-methoxyphenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acrylamide (PA5)



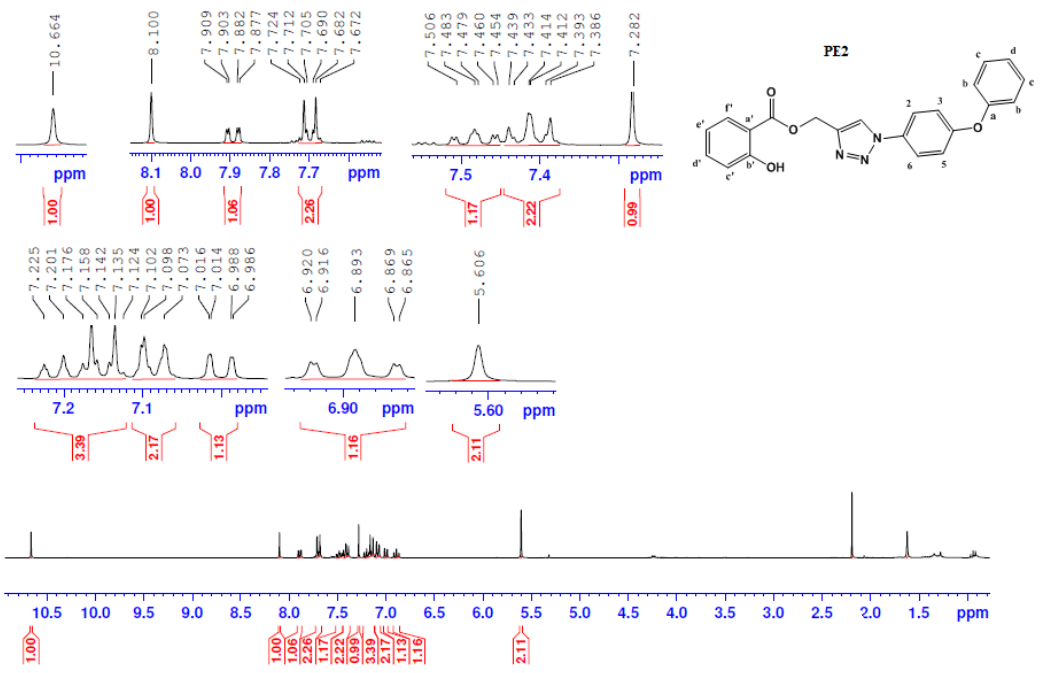
22. ^{1}H-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate (PE1)



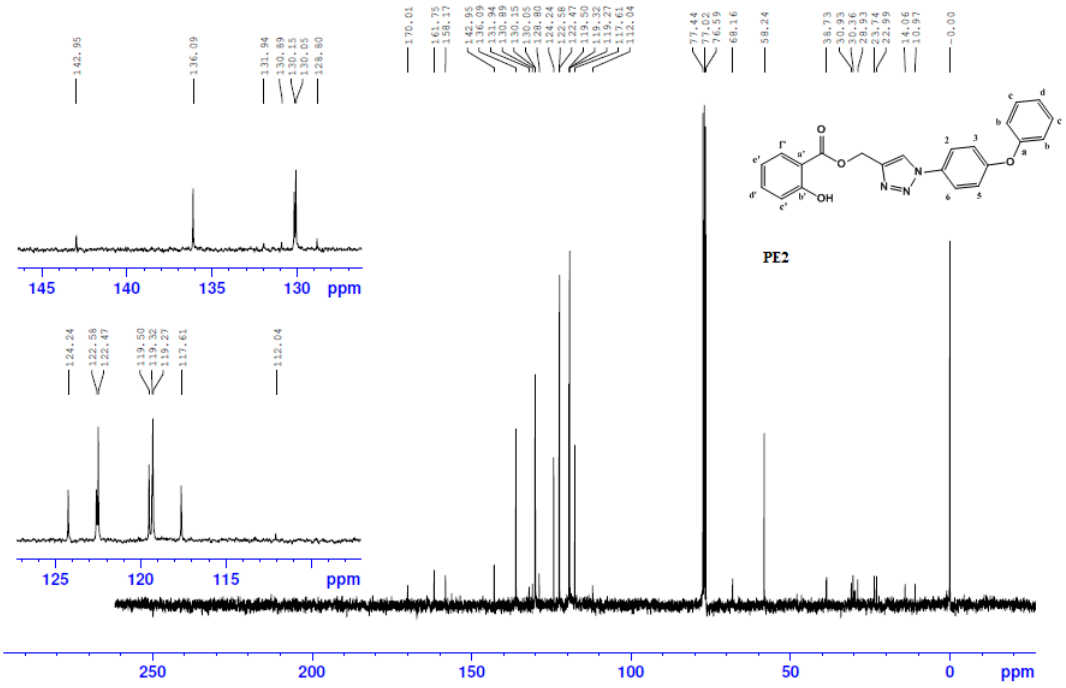
23. ^{13}C-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate (PE1)



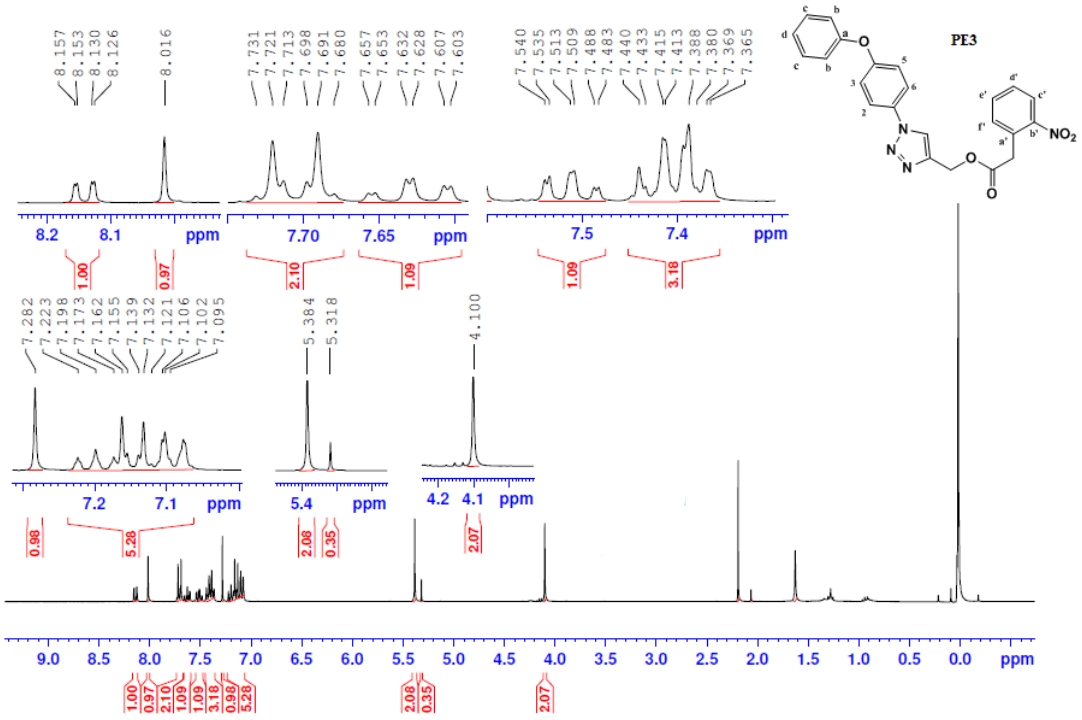
24. ^{1}H-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-hydroxybenzoate (PE2)



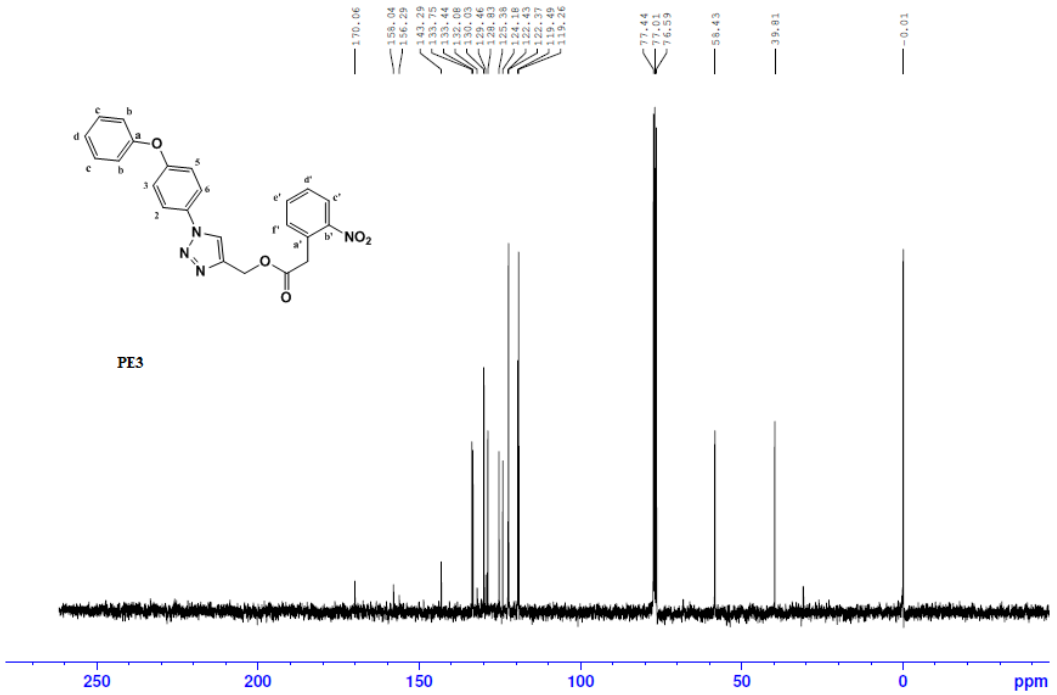
25. ^{13}C-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-hydroxybenzoate (PE2)



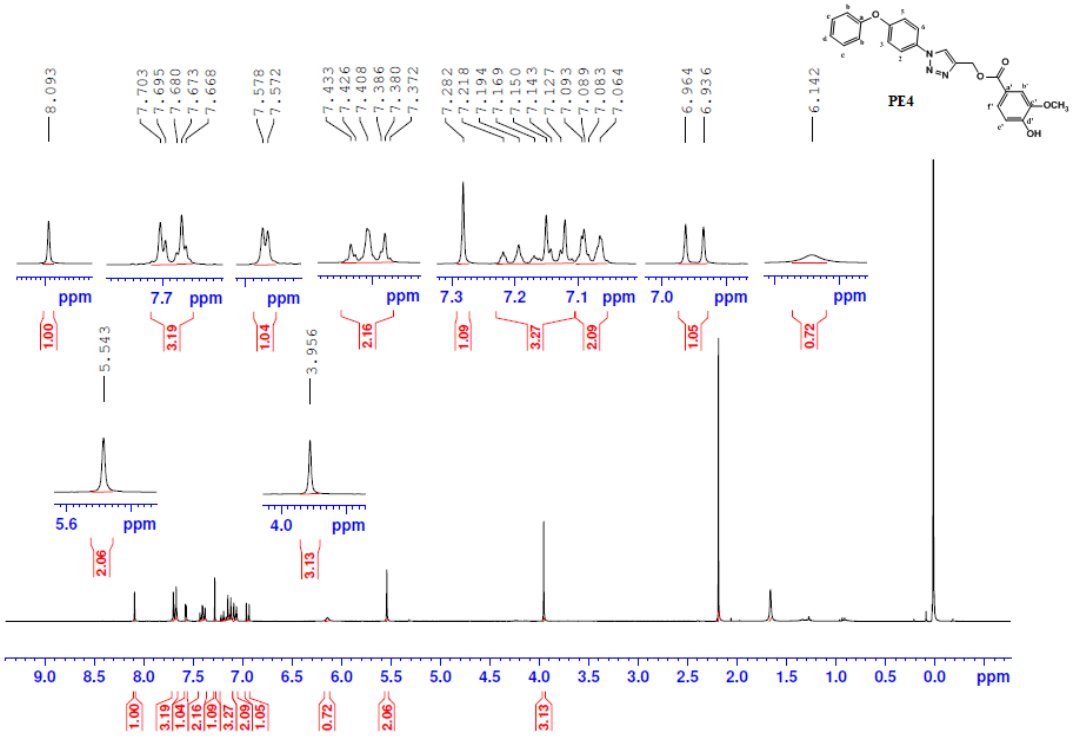
26. ^{1}H-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-(2-nitrophenyl)acetate (PE3)



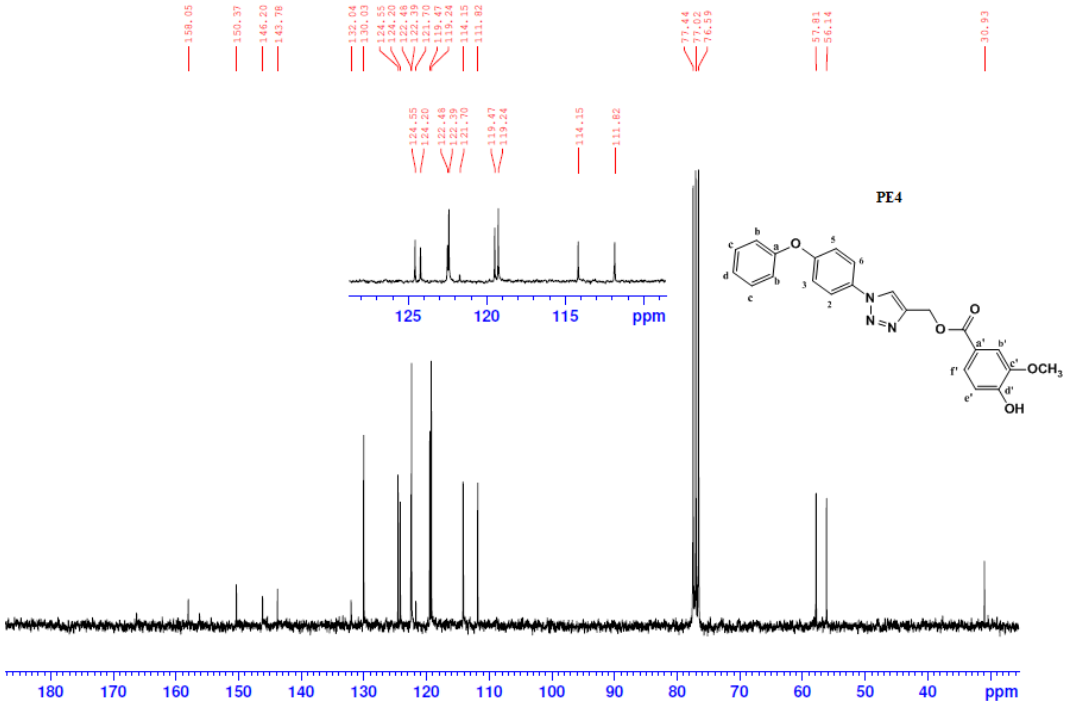
27. ^{13}C-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-(2-nitrophenyl)acetate (PE3)



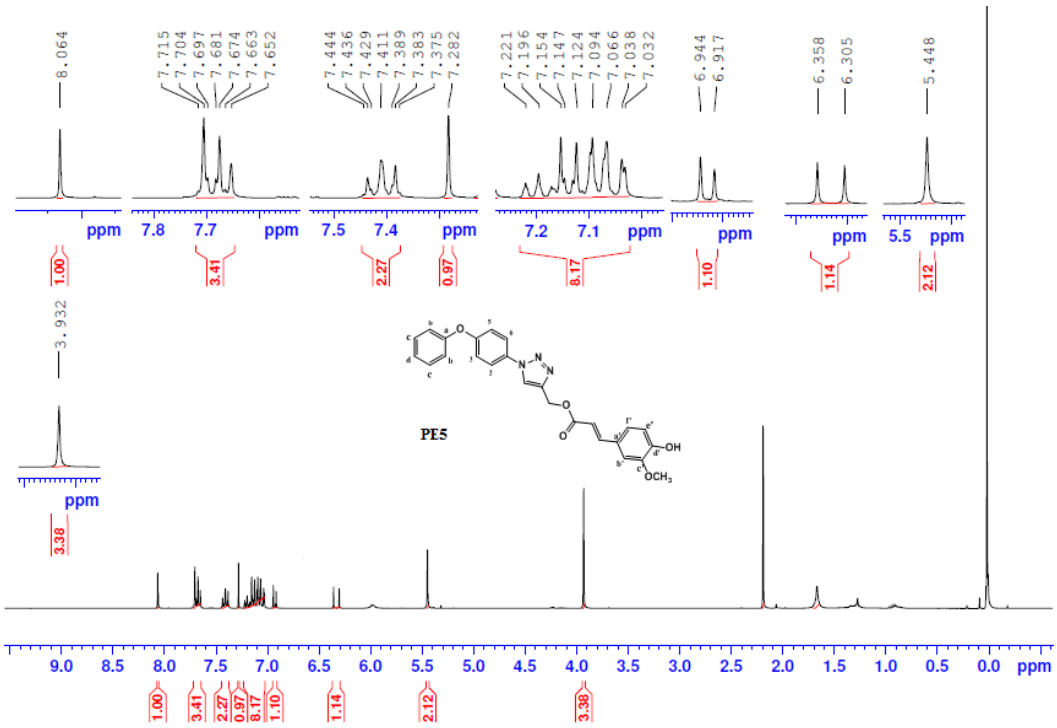
28. ^{1}H-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 4-hydroxy-3-methoxybenzoate (PE4)



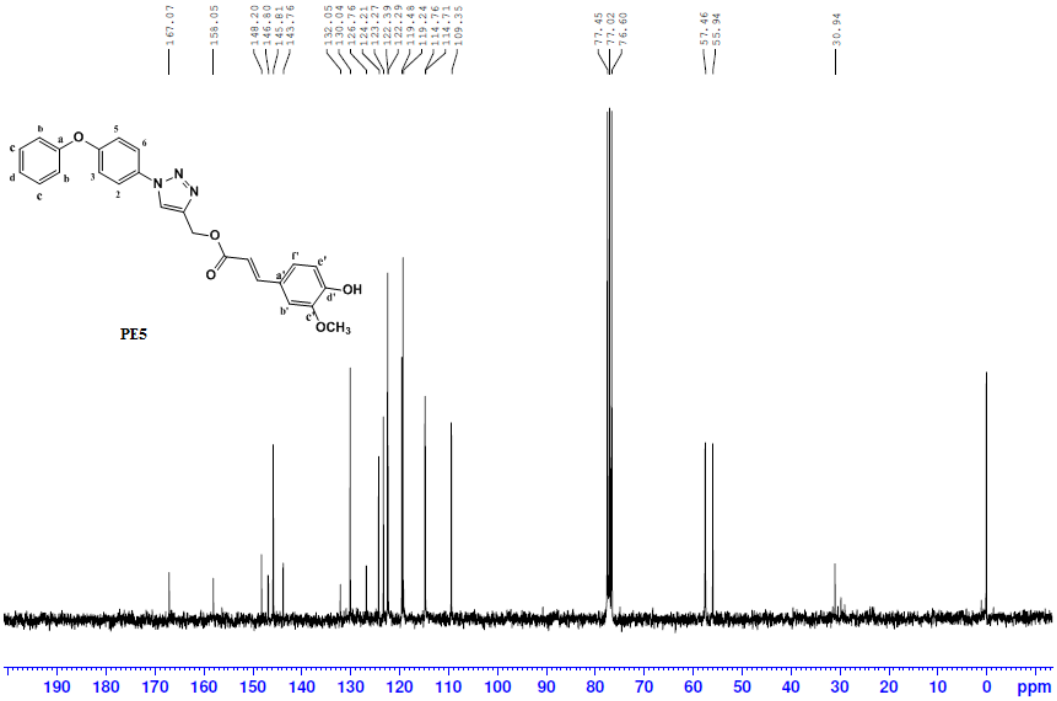
29. ^{13}C-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 4-hydroxy-3-methoxybenzoate (PE4)



30. ^{1}H-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (PE5)

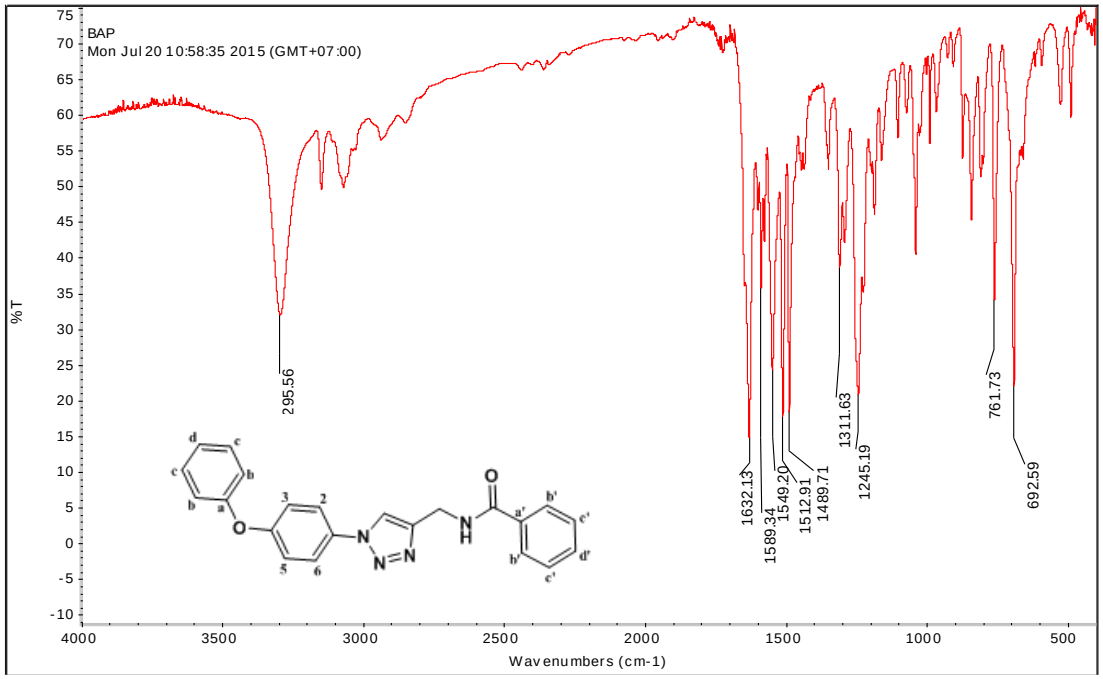


31. ^{13}C-NMR of (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (PE5)

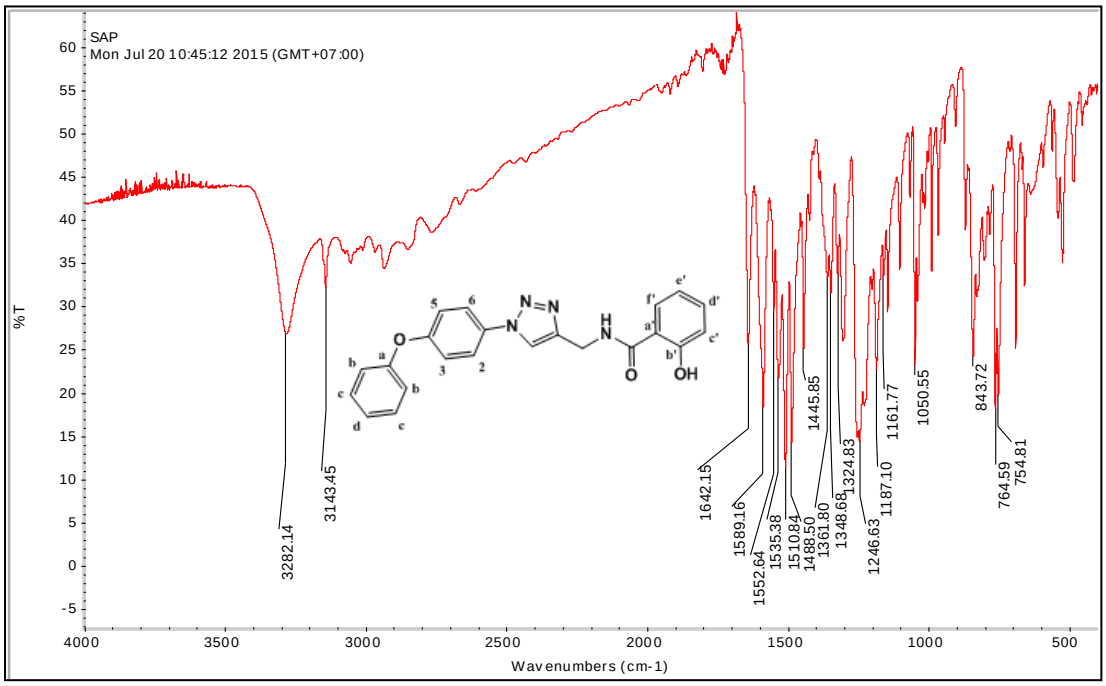


IR spectra

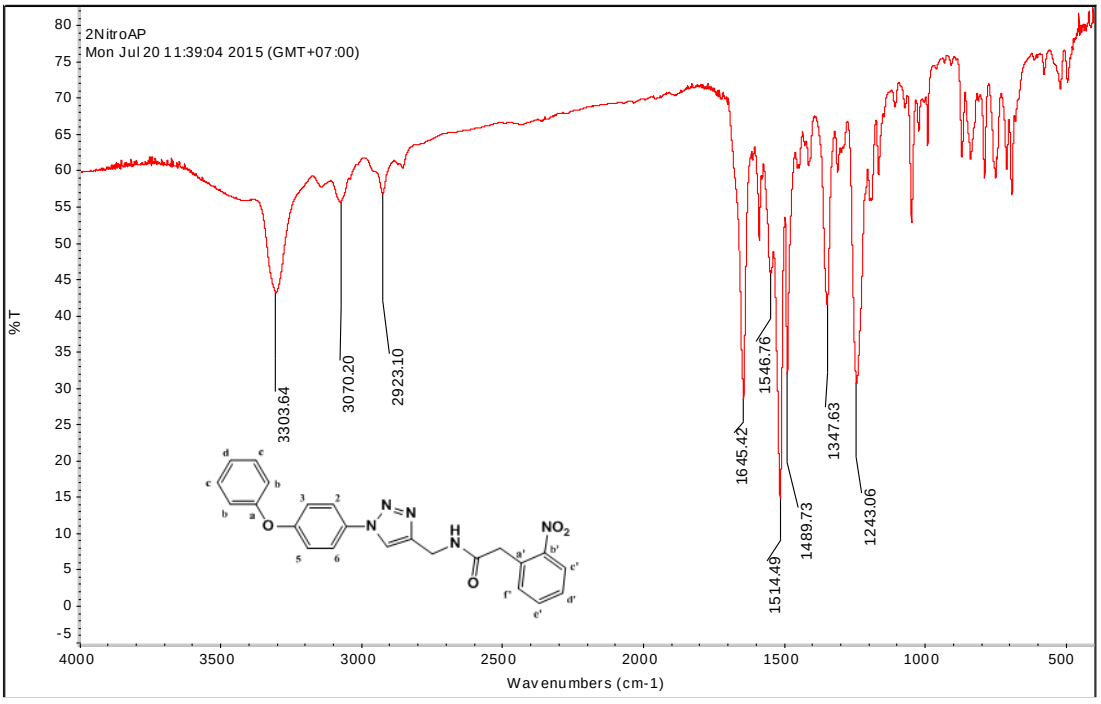
1. *N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA1)



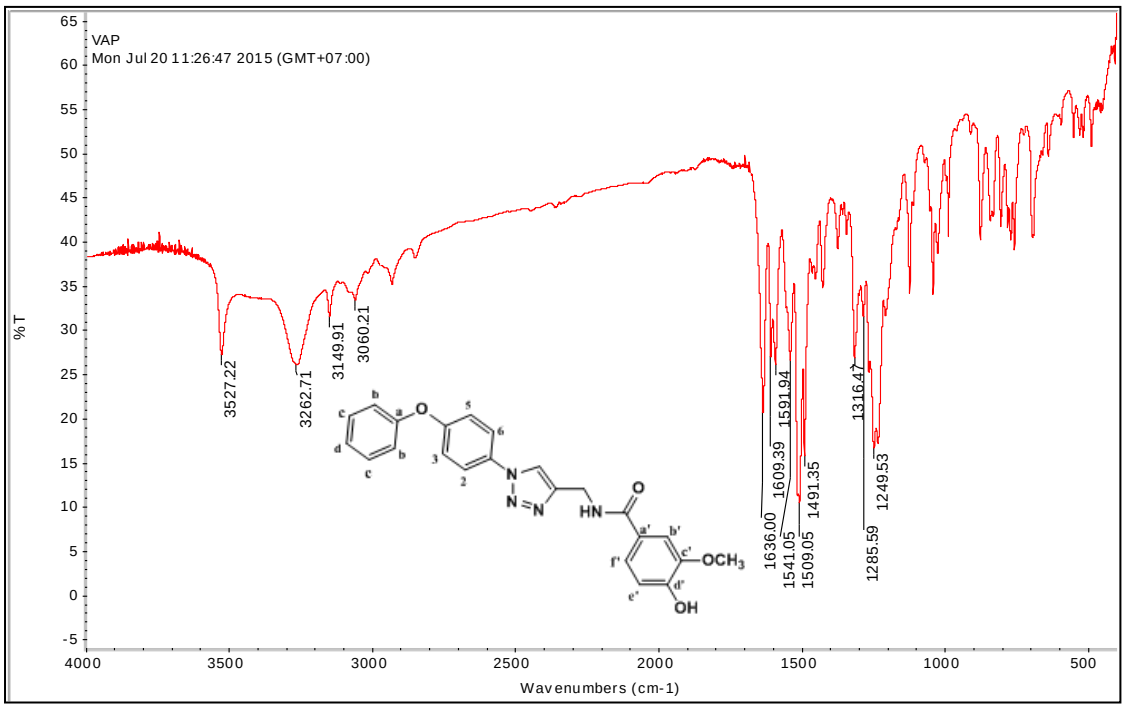
2. 2-Hydroxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA2)



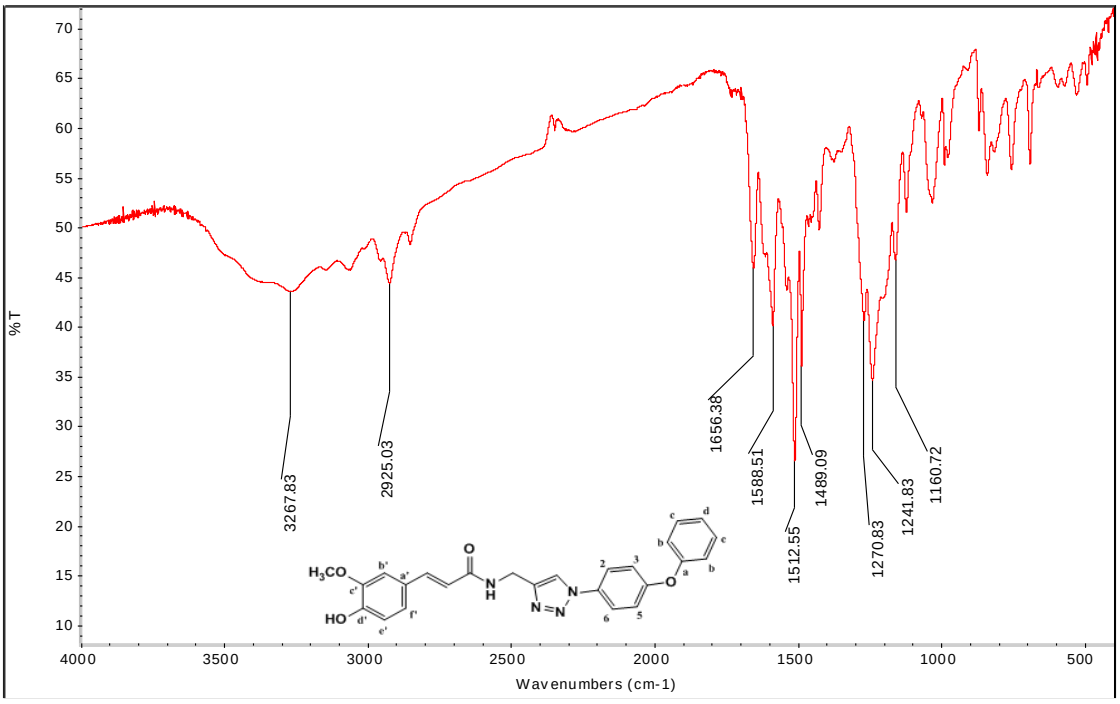
3. 2-(2-nitrophenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide (PA3)



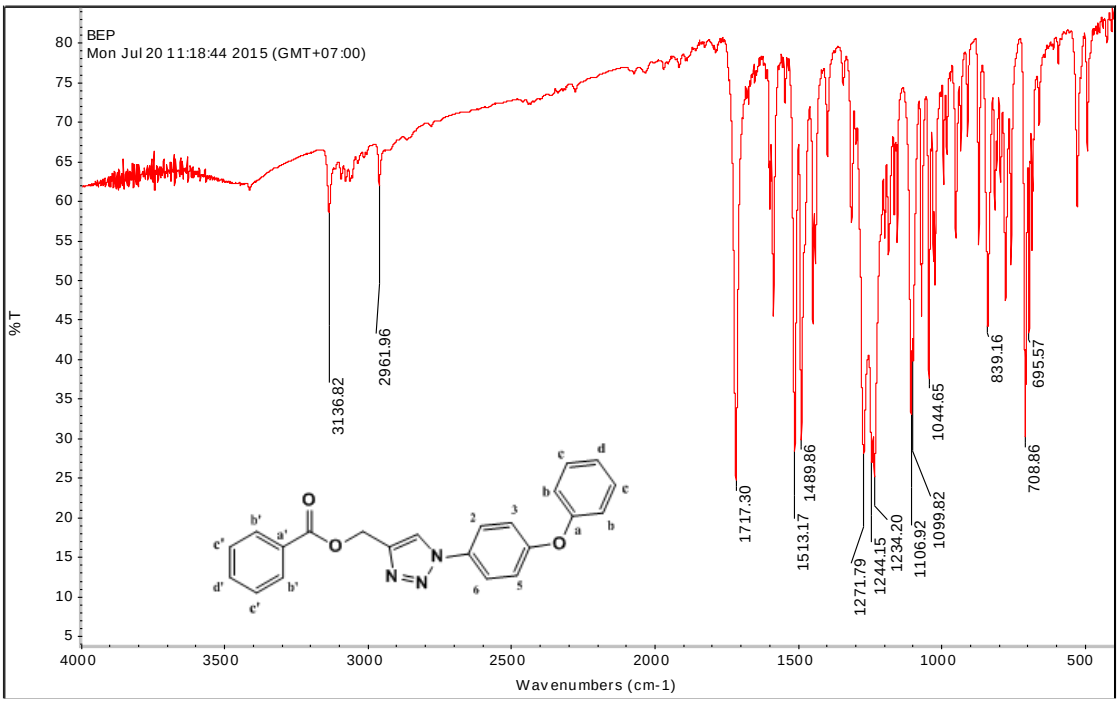
4. 4-Hydroxy-3-methoxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA4)



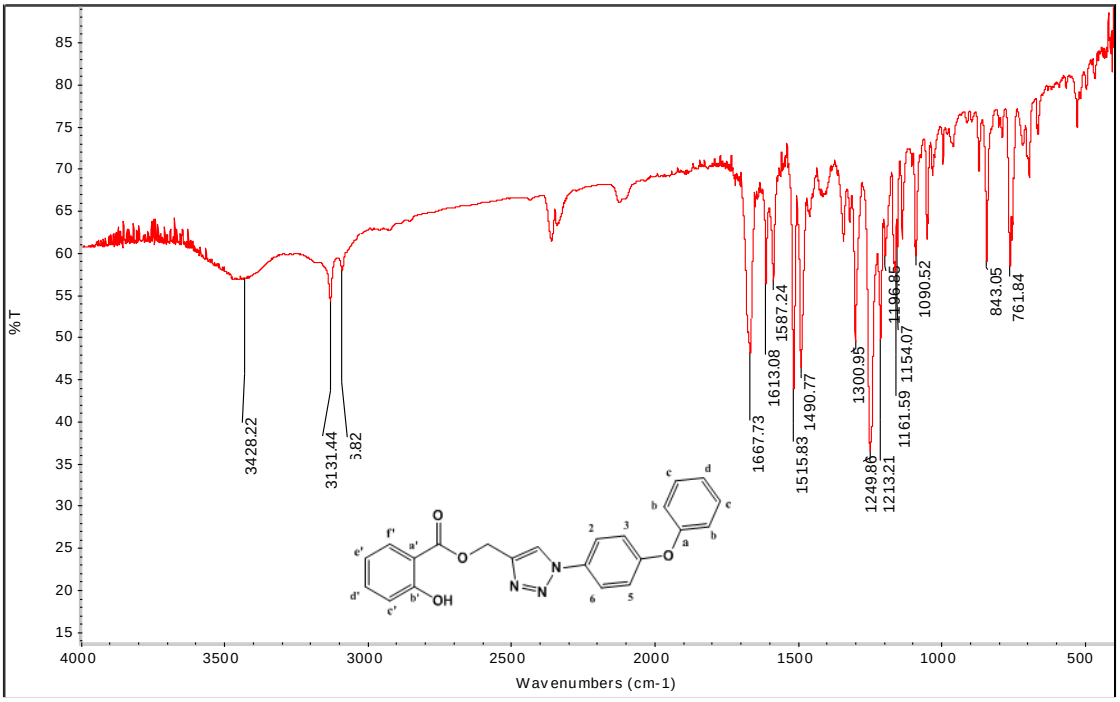
5. (*E*)-3-(4-hydroxy-3-methoxyphenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acrylamide (PA5)



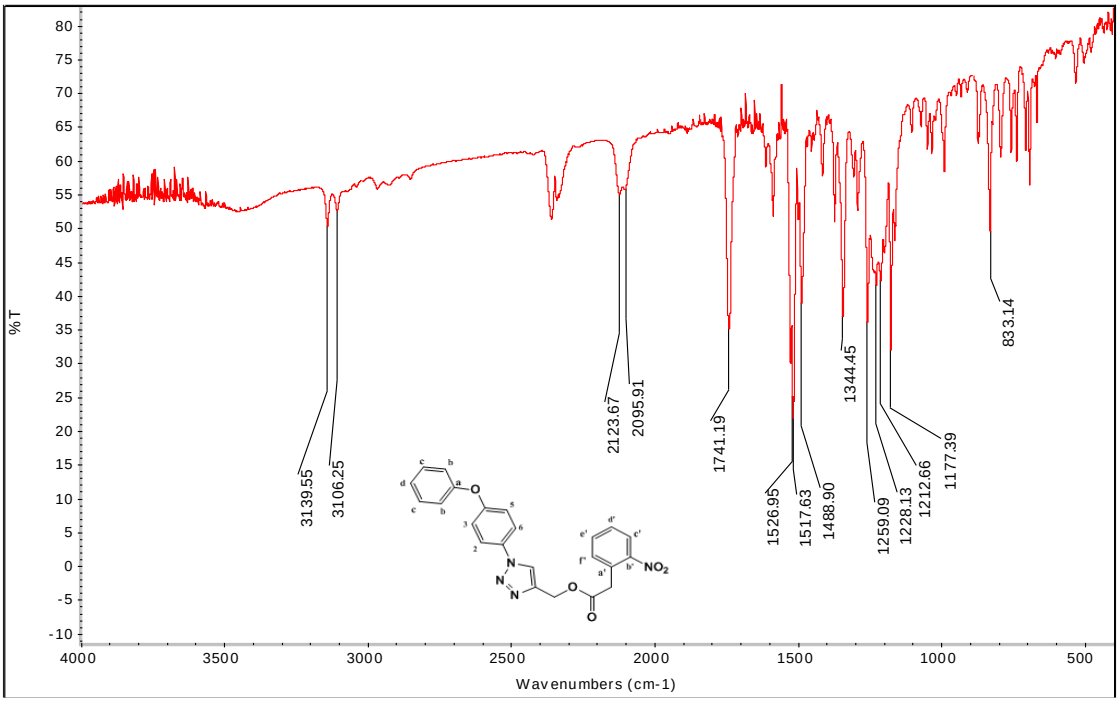
6. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate (PE1)



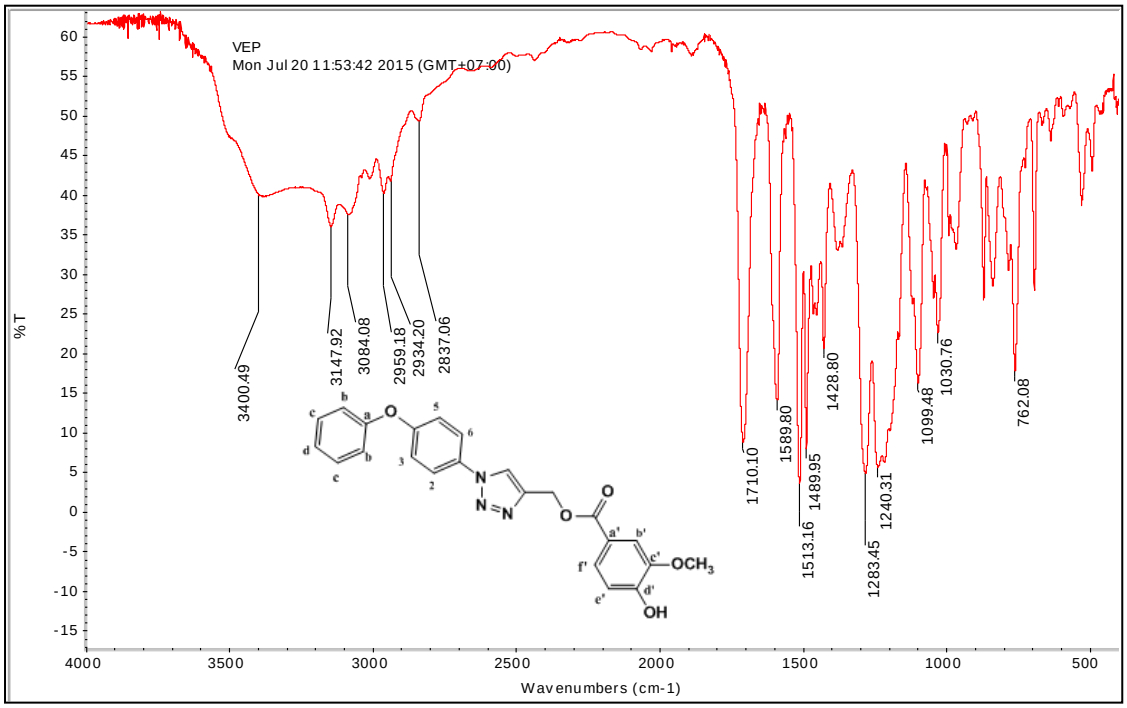
7. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-hydroxybenzoate (PE2)



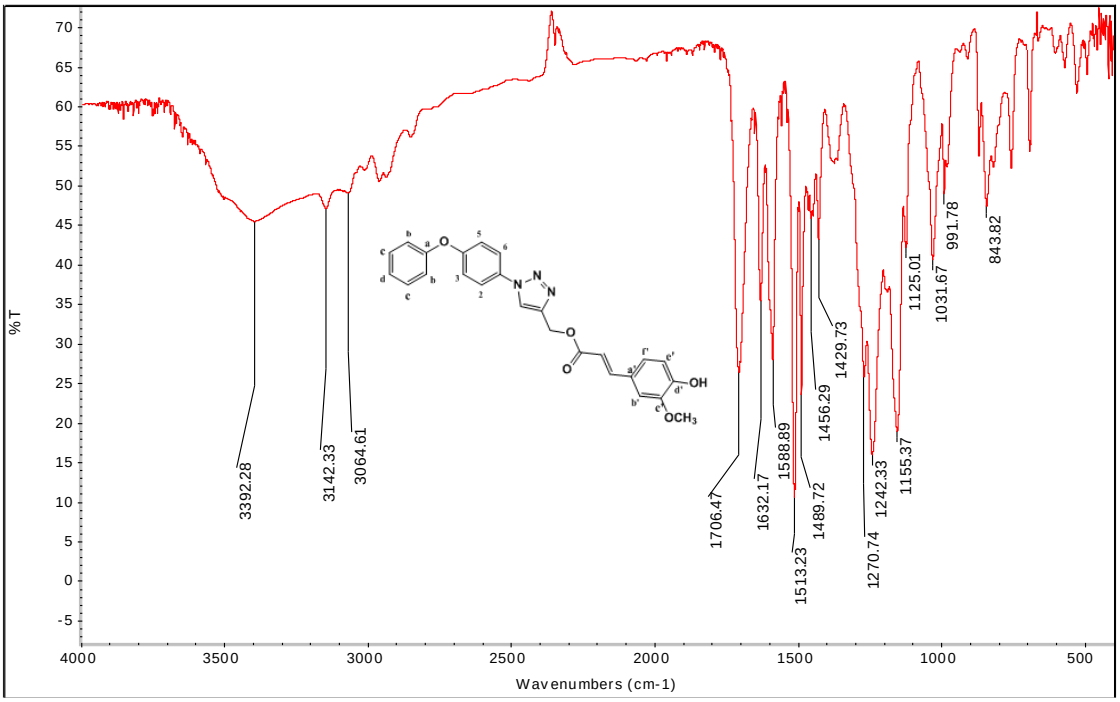
8. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-(2-nitrophenyl)acetate (PE3)



9. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 4-hydroxy-3-methoxybenzoate (PE4)

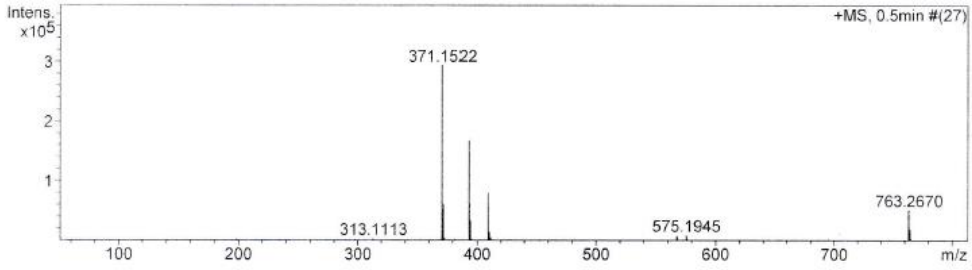


10. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (PE5)

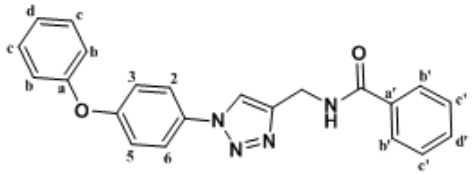


Mass spectra

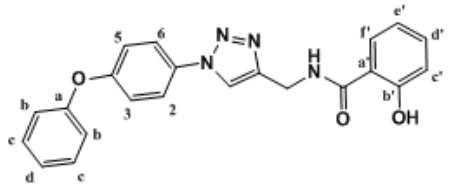
1. *N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA1)

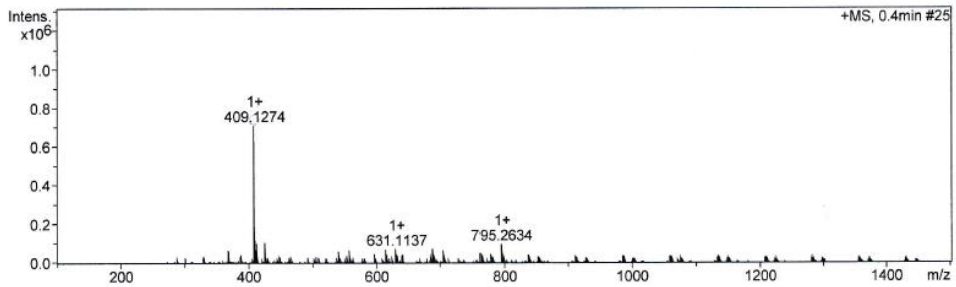


#	m/z	I	I %	S/N	FWHM	Res.
1	149.0238	2420	0.8	26.2	0.0258	5776
2	198.0539	2859	1.0	28.7	0.0371	5345
3	297.6787	2489	0.8	21.7	0.0142	20959
4	301.1388	2259	0.8	19.6	0.0504	5971
5	313.1113	4037	1.4	34.7	0.0509	6154
6	370.0809	3075	1.0	26.7	0.0677	5466
7	371.1522	293780	100.0	2589.5	0.0640	580
8	372.1544	60582	20.6	534.6	0.0576	646
9	373.1575	5153	1.8	45.2	0.0697	535
10	382.1358	3520	1.2	31.3	0.0550	694
11	382.6367	2170	0.7	19.1	0.0553	692
12	393.1344	167685	57.1	1536.4	0.0684	575
13	394.1362	33410	11.4	306.3	0.0608	648
14	395.1403	3206	1.1	29.1	0.0752	525
15	409.1081	80377	27.4	758.0	0.0686	596
16	410.1121	15383	5.2	145.0	0.0665	616
17	411.1105	5875	2.0	55.2	0.0689	5963
18	567.2070	8921	3.0	109.8	0.0904	6272
19	567.7075	7451	2.5	91.6	0.0921	6166
20	568.2085	4098	1.4	50.1	0.1006	5650
21	575.1945	9819	3.3	120.8	0.0961	5984
22	575.6974	7093	2.4	87.1	0.0980	5876
23	576.1983	2963	1.0	36.1	0.0913	6314
24	763.2670	51600	17.6	658.5	0.1468	5200
25	764.2713	19682	6.7	251.4	0.1470	5200
26	765.2769	3753	1.3	47.7	0.1635	4679
27	1038.5959	2243	0.8	41.5	0.0233	44543
28	1080.7210	2425	0.8	45.4	0.0220	49090
29	2351.8749	2816	1.0	56.6	0.0313	75256
30	2352.2411	3123	1.1	62.8	0.0321	73375



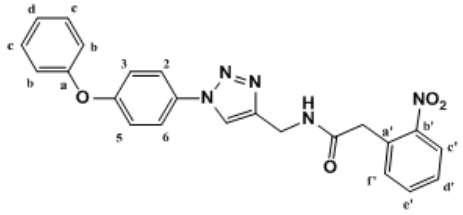
2. 2-Hydroxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA2)

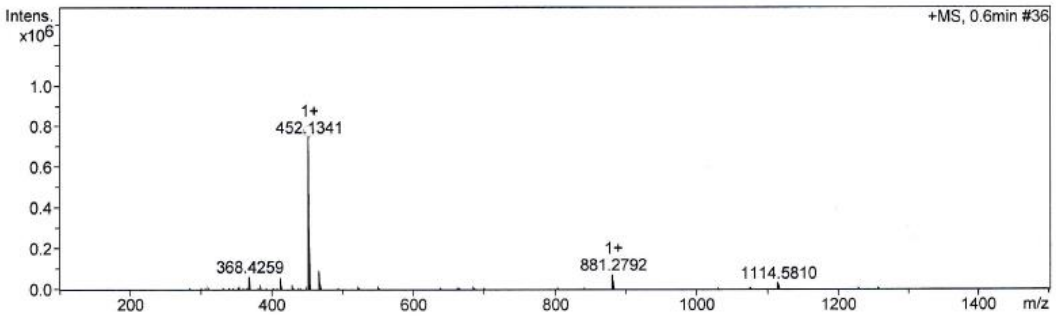




Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
409.127366	1	C22H18N4NaO3	409.127111	0.6	-0.4	15.5	ok	even	2.1	4.2	0.3	1.3	0.6	499.6

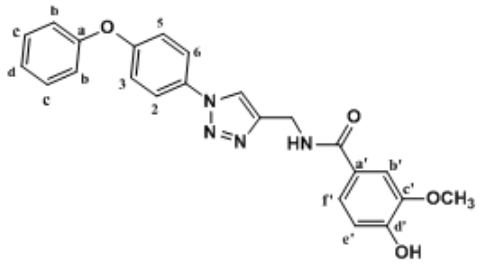
3. 2-(2-nitrophenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide (PA3)

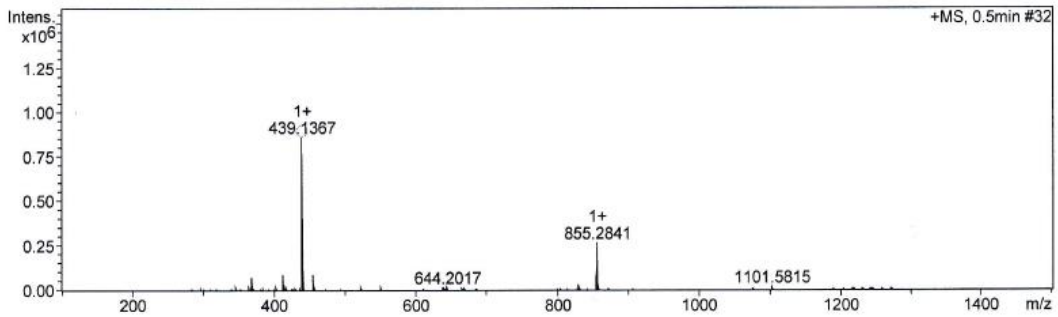




Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
452.134121	1	C23H19N5NaO4	452.132925	-2.6	-2.5	16.5	ok	even	1.5	3.0	1.1	1.0	0.4	659.9

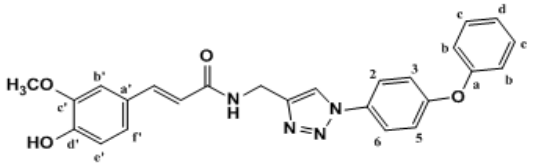
4. 4-Hydroxy-3-methoxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA4)

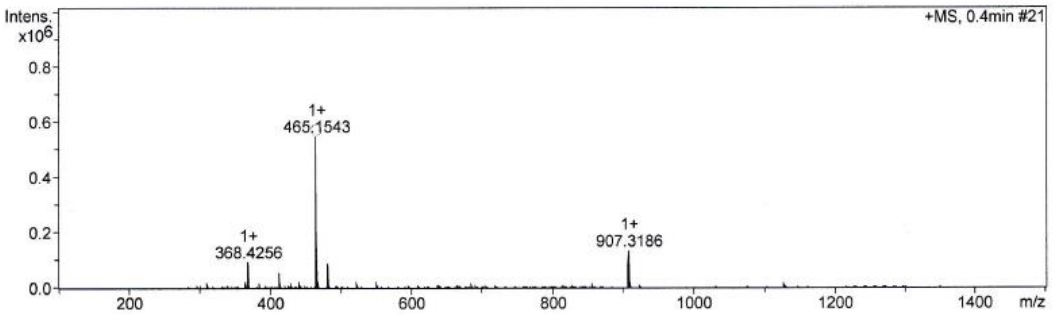




Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
439.136692	1	C23H20N4NaO4	439.137676	-2.2	2.5	15.5	ok	even	0.3	0.6	1.1	0.3	0.5	512.1

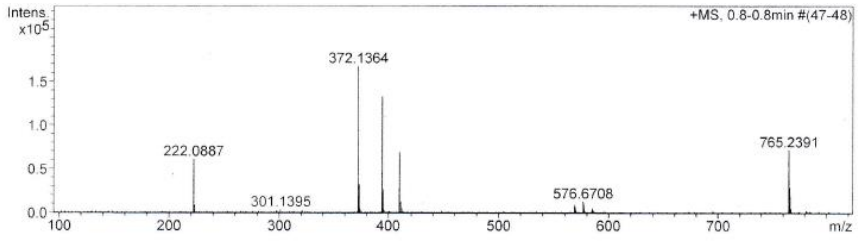
5. (*E*)-3-(4-hydroxy-3-methoxyphenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acrylamide (PA5)



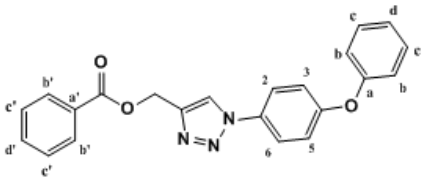


Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
465.154259	1	C25H22N4NaO4	465.153326	2.0	-1.6	16.5	ok	even	5.1	9.0	0.8	2.8	0.9	721.4

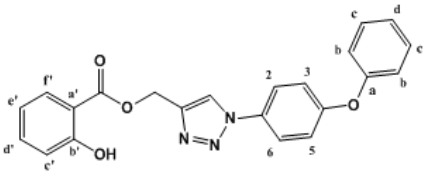
6. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate (PE1)

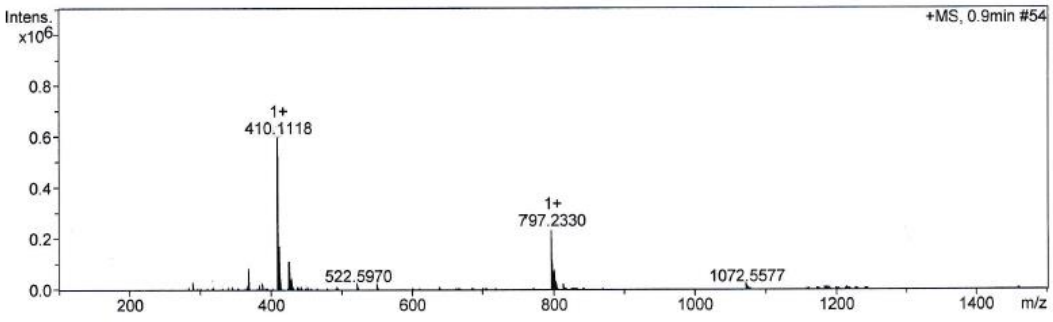


#	m/z	I	I %	S/N	FWHM	Res.
1	101.9299	2278	1.4	24.6	0.0106	9661
2	149.0240	2182	1.3	23.3	0.0224	6662
3	222.0887	60865	36.3	587.7	0.0369	6014
4	223.0929	8948	5.3	86.1	0.0364	6129
5	297.6436	2764	1.6	23.9	0.0118	25175
6	301.1395	3531	2.1	30.5	0.0506	5957
7	372.1364	167528	100.0	1460.4	0.0646	5760
8	373.1377	31972	19.1	278.9	0.0610	6118
9	374.1409	3688	2.2	31.9	0.0556	6728
10	394.1185	132214	78.9	1195.5	0.0653	6035
11	395.1197	26511	15.8	239.8	0.0550	7186
12	396.1253	2550	1.5	22.8	0.0706	5610
13	410.0920	69363	41.4	644.4	0.0708	5791
14	411.0959	12714	7.6	118.0	0.0704	5839
15	412.0954	5086	3.0	47.1	0.0684	6024
16	568.6826	9288	5.5	111.3	0.0901	6311
17	569.1860	8096	4.8	97.0	0.0895	6361
18	569.6851	5057	3.0	60.4	0.0792	7193
19	576.6708	12852	7.7	154.5	0.0960	6006
20	577.1745	9101	5.4	109.3	0.0973	5930
21	577.6748	3669	2.2	43.7	0.0902	6402
22	584.6584	5033	3.0	60.3	0.0891	6560
23	585.1612	3688	2.2	44.0	0.0947	6182
24	585.6596	2487	1.5	29.5	0.0952	6152
25	765.2391	70420	42.0	923.0	0.1584	4832
26	766.2417	28674	17.1	376.3	0.1546	4958
27	767.2421	5094	3.0	66.6	0.1559	4920
28	1080.7246	2377	1.4	46.6	0.0219	49383
29	2351.8719	2854	1.7	53.2	0.0311	75559
30	2352.2354	2845	1.7	53.1	0.0322	73109



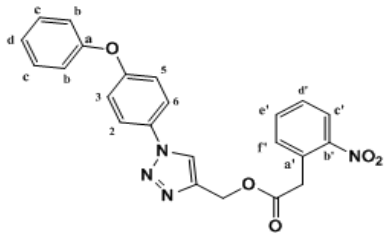
7. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-hydroxybenzoate (PE2)

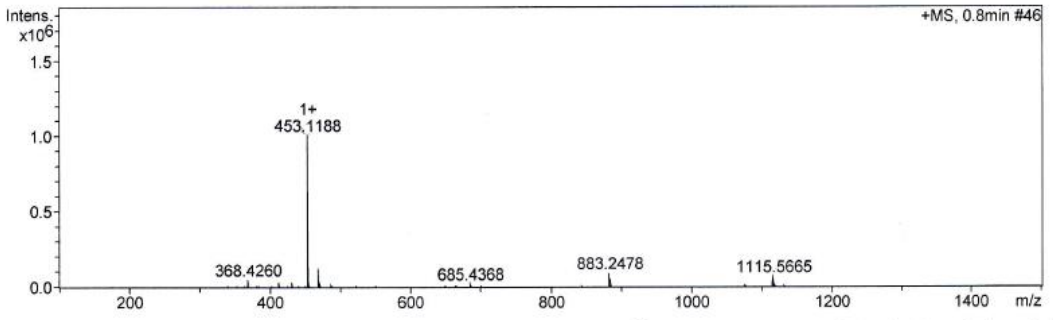




Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
410.111782	1	C22H17N3NaO4	410.111127	-1.6	-1.2	15.5	ok	even	2.2	3.5	0.6	2.4	0.8	577.0

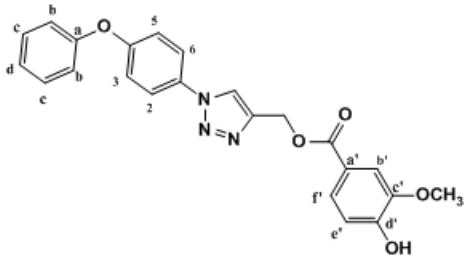
8. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-(2-nitrophenyl)acetate (PE3)

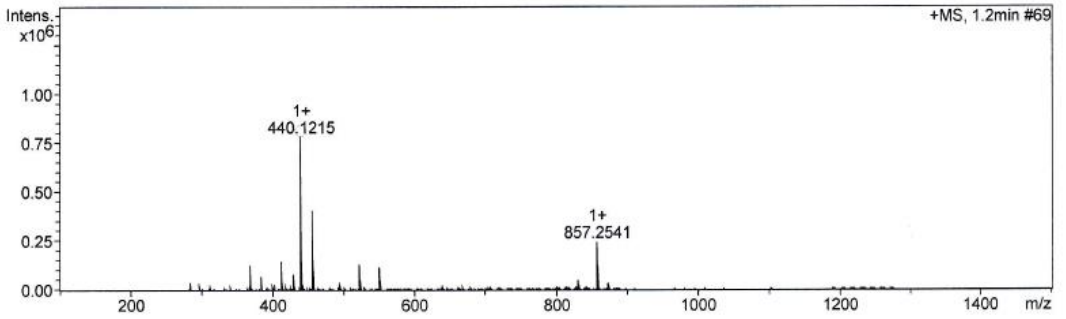




Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
453.118796	1	C23H18N4NaO5	453.116940	4.1	-4.0	16.5	ok	even	4.8	8.7	1.8	2.7	0.3	781.0

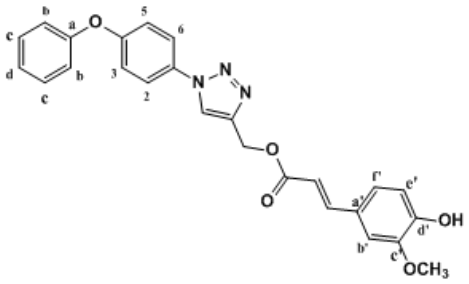
9. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 4-hydroxy-3-methoxybenzoate (PE4)

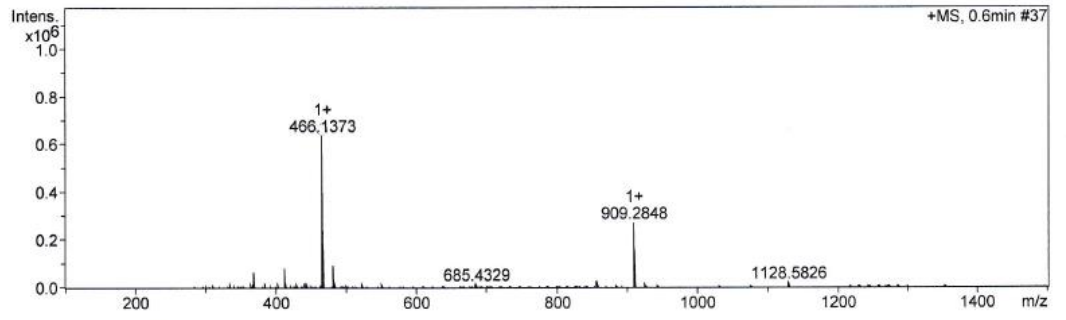




Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
440.121455	1	C23H19N3NaO5	440.121691	-0.5	-0.0	15.5	ok	even	2.7	4.2	0.4	2.9	1.0	544.0

10. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (PE5)



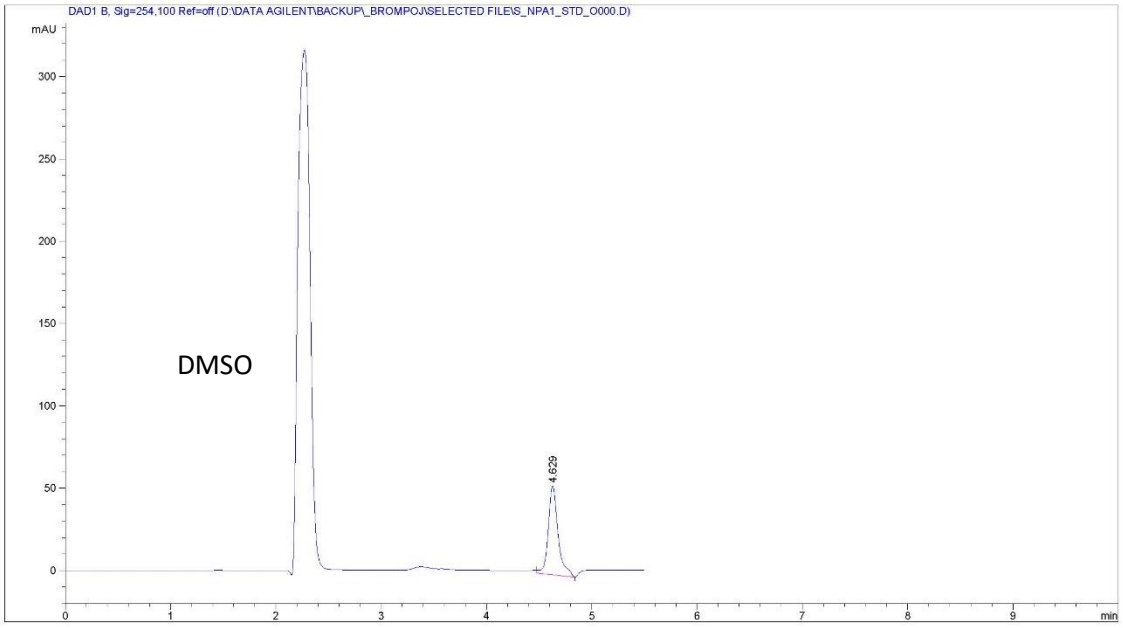


Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
466.137285	1	C25H21N3NaO5	466.137341	0.1	0.3	16.5	ok	even	1.7	3.3	0.3	1.1	0.3	424.6

HPLC Chromatograms

1. *N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA1)

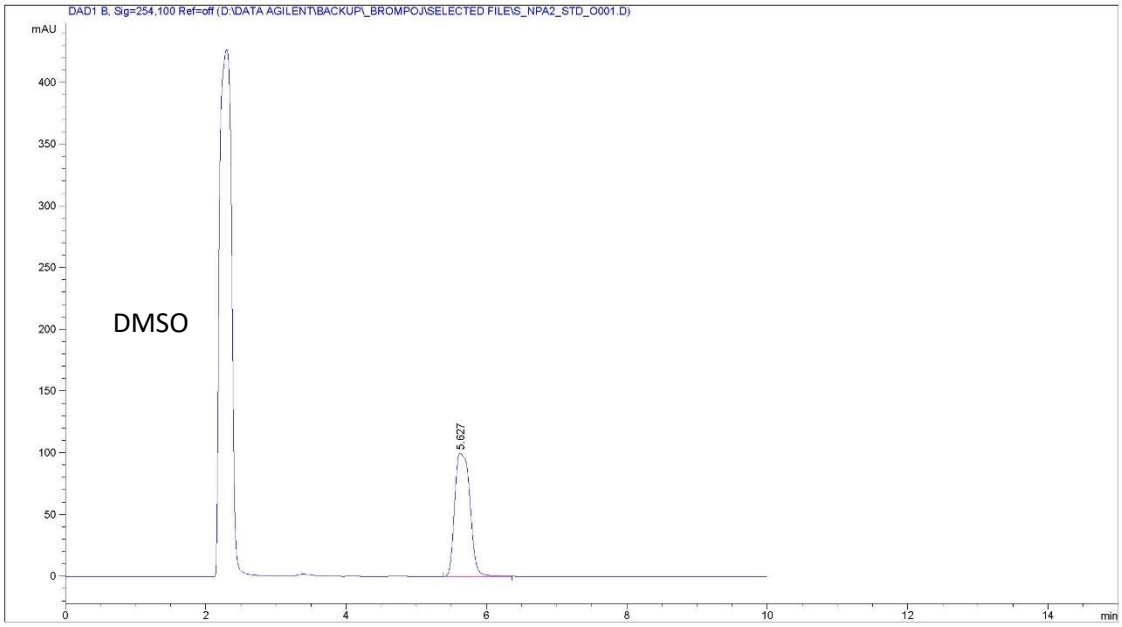
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\S_NPA1_STD_0000.D
Sample Name: NPA1 Std 0

=====================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 2
Injection Date  : 1/17/2023 1:53:03 PM
                                                  Inj Volume : 20.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 1/17/2023 1:58:17 PM by Phuvadol
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 5/23/2024 2:39:02 PM by Thanapat
                  (modified after loading)
Sample Info     : Sample NPA1 Std 0 dilut. to 10 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (20:80); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.629 BV    0.0975  349.22043   53.99437 100.0000

Totals :                   349.22043   53.99437

=====================================================================
                          *** End of Report ***
```

2. *N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA1)

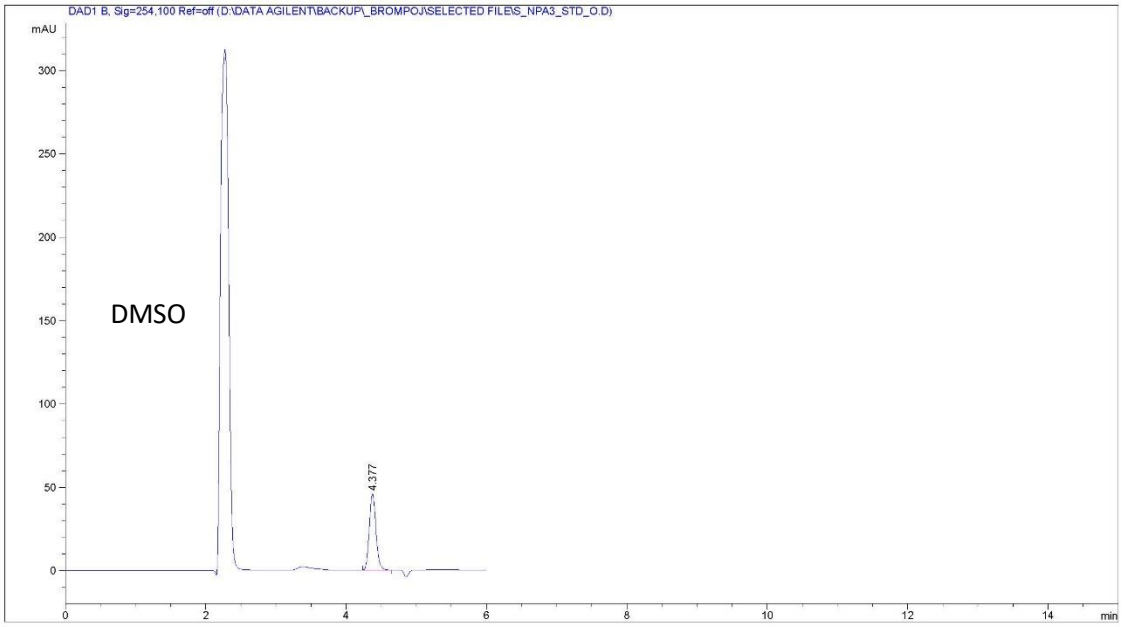
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\S_NPA2_STD_0001.D
Sample Name: NPA2 STD DMSO

=====================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 7
Injection Date  : 2/21/2023 12:40:06 PM
                                                  Inj Volume : 20.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 2/21/2023 12:39:04 PM by Phuvadol
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 5/23/2024 2:40:16 PM by Thanapat
                  (modified after loading)
Sample Info     : Sample NPA2 STD DMSO dilute to 100 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (30:70); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.627 BB    0.2072 1501.22083   99.98650 100.0000

Totals :                  1501.22083   99.98650

=====================================================================
                        *** End of Report ***
```

3. 2-(2-nitrophenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acetamide (PA3)

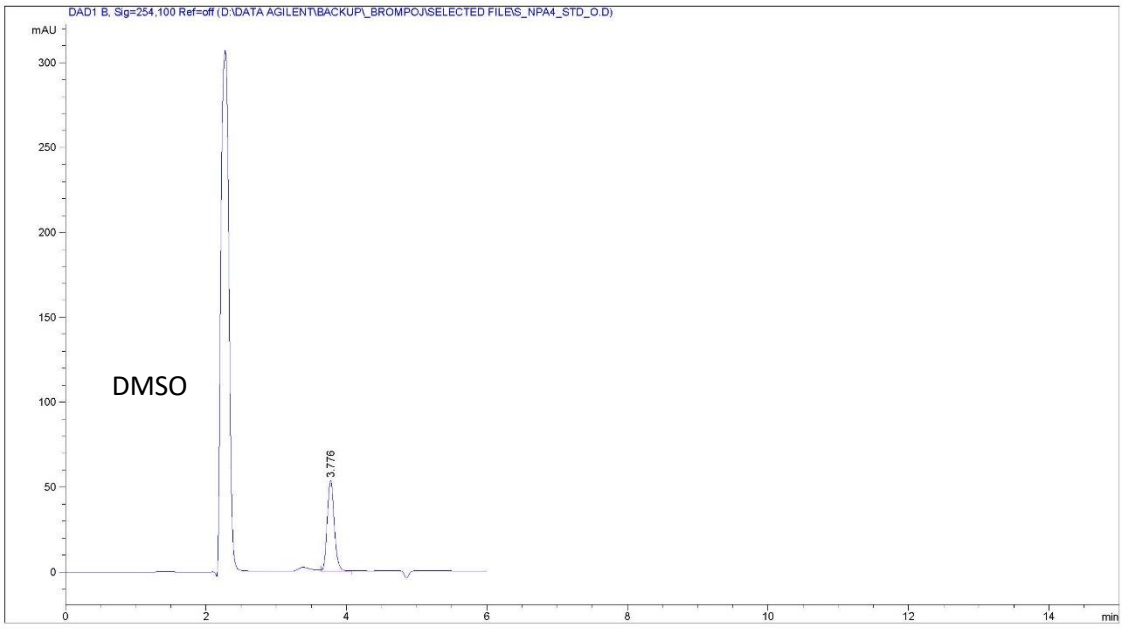
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\S_NPA3_STD_O.D
Sample Name: NPA3 Std O

    ================================================================
    Acq. Operator   : Phuvadol                    Seq. Line :   1
    Acq. Instrument : Instrument 1                 Location : Vial 4
    Injection Date  : 1/17/2023 2:10:08 PM            Inj :   1
                                                  Inj Volume : 20.000 µl
    Acq. Method     : C:\CHEM32\1\DATA\_PHUVADOL\170123\2022-11-10-PM1 2023-01-17 14-09-00\RUN_PARTITION06.M
    Last changed    : 1/17/2023 2:07:29 PM by Phuvadol
    Analysis Method : C:\CHEM32\1\METHODS\ THANAPAT\DATA PROCESS 280 NM.M
    Last changed    : 5/23/2024 2:40:16 PM by Thanapat
                      (modified after loading)
    Sample Info     : Sample NPA3 Std O dil. to 10 uM with 70% MeOH
                      MP: 0.1%v/v Formic acid and MeOH (40:60); Isocratic elu
                      tion at 0.8 mL/min
                      Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                      C; Inj. 5 uL
                      UV: 220 (16); 254 (100); 280/16; 440/8
```




```
    ================================================================
                              Area Percent Report
    ================================================================

    Sorted By             :      Signal
    Multiplier:                   :      1.0000
    Dilution:                     :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=254,100 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.377 BB    0.1026  299.66809   45.65439 100.0000

    Totals :                   299.66809   45.65439

    ================================================================
                              *** End of Report ***
```

4. 4-Hydroxy-3-methoxy-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)benzamide (PA4)

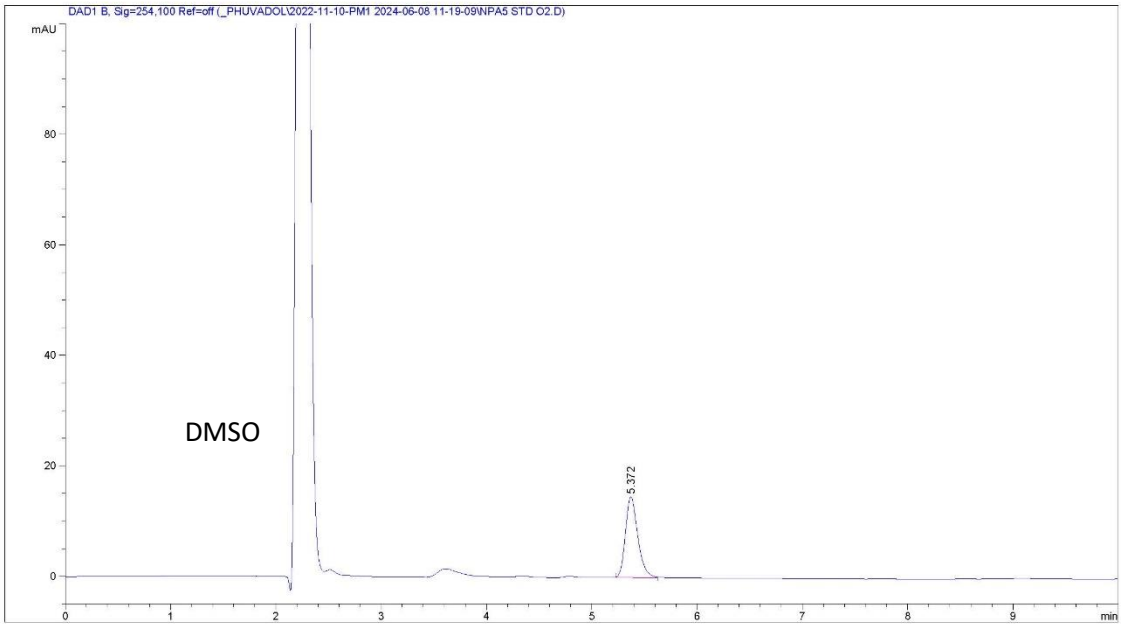
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\S_NPA4_STD_O.D
Sample Name: NPA4 Std O

=====================================================================
Acq. Operator   : Phuvadol                       Seq. Line :   2
Acq. Instrument : Instrument 1                   Location : Vial 5
Injection Date  : 1/17/2023 2:17:18 PM              Inj :   1
                                                 Inj Volume : 20.000 µl
Acq. Method     : C:\CHEM32\1\DATA\_PHUVADOL\170123\2022-11-10-PM1 2023-01-17 14-09-00\RUN_PARTITION06.M
Last changed    : 1/17/2023 2:07:29 PM by Phuvadol
Analysis Method : C:\CHEM32\1\METHODS\ THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 5/23/2024 2:40:16 PM by Thanapat
                  (modified after loading)
Sample Info     : Sample NPA4 Std O dil. to 10 uM with 70% MeOH
                  MP: 0.1%v/v Formic acid and MeOH (40:60); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  C; Inj. 5 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.776 VB    0.1065  367.17117   53.19593 100.0000

Totals :                   367.17117   53.19593

=====================================================================
                        *** End of Report ***
```

5. (*E*)-3-(4-hydroxy-3-methoxyphenyl)-*N*-((1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)acrylamide (PA5)

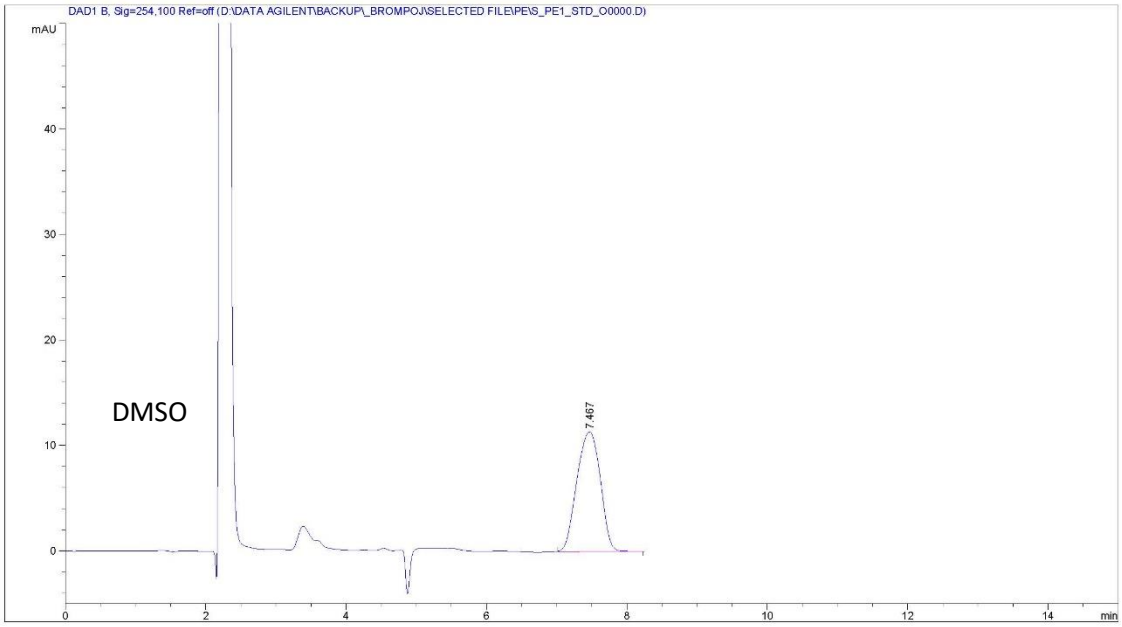
```
Data File C:\CHEM32\1\DATA\_PHUVADOL\2022-11-10-PM1 2024-06-08 11-19-09\NPA5 STD O2.D
Sample Name: NPA5 Std O

=====================================================================
Acq. Operator   : Phuvadol                      Seq. Line :   1
Acq. Instrument : Instrument 1                  Location : Vial 1
Injection Date  : 6/8/2024 11:31:12 AM             Inj :   2
                                                Inj Volume : 20.000 µl
Acq. Method     : C:\CHEM32\1\DATA\_PHUVADOL\2022-11-10-PM1 2024-06-08 11-19-09\RUN_PARTITION06.M
Last changed    : 6/8/2024 11:13:09 AM by Phuvadol
Analysis Method : C:\CHEM32\1\METHODS\ THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 6/8/2024 11:44:22 AM by Phuvadol
                  (modified after loading)
Sample Info     : Sample NPA5 Std O dil. to 10 uM with 70% MeOH
                  MP: 0.1%v/v Formic acid and MeOH (40:60); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.372 BB    0.1222  117.97494   14.81239 100.0000

Totals :                   117.97494   14.81239

=====================================================================
                        *** End of Report ***
```

6. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate (PE1)

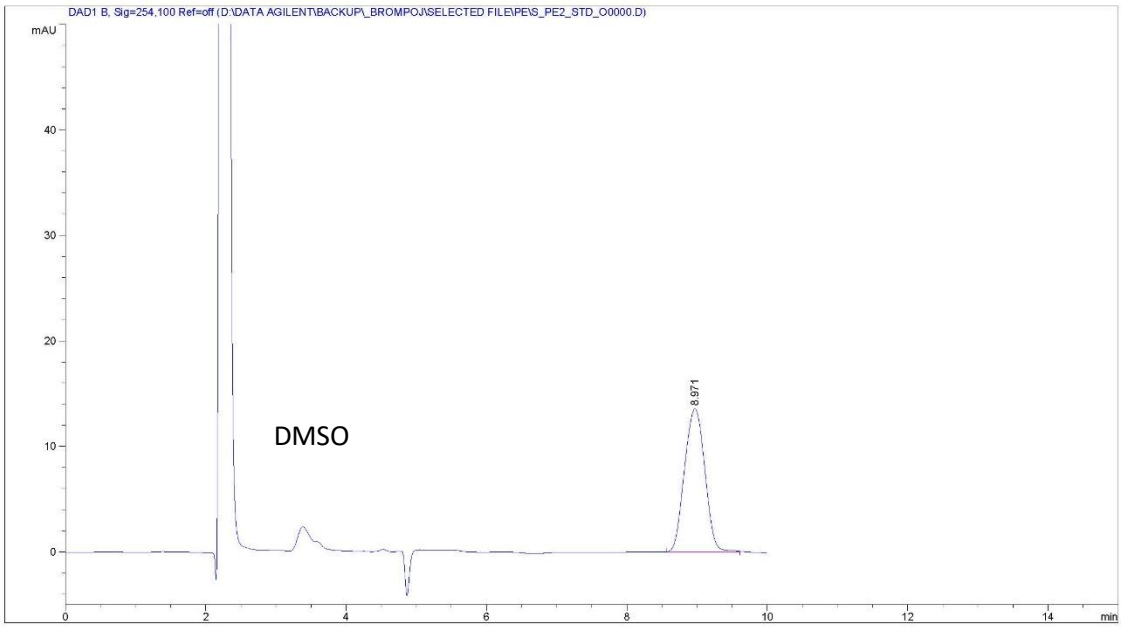
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\PE\S_PE1_STD_O0000.D
Sample Name: PE1 Std O

=====================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 2
Injection Date  : 1/16/2023 11:53:26 AM
                                                  Inj Volume : 20.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 1/16/2023 11:52:42 AM by Phuvadol
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 6/8/2024 11:15:01 AM by Phuvadol
                  (modified after loading)
Sample Info     : Sample PE1 Std O dilut. to 50 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (20:80); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; @ 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.467 BBA   0.3914  263.77896   11.34002 100.0000

Totals :                   263.77896   11.34002

=====================================================================
                        *** End of Report ***
```

7. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-hydroxybenzoate (PE2)

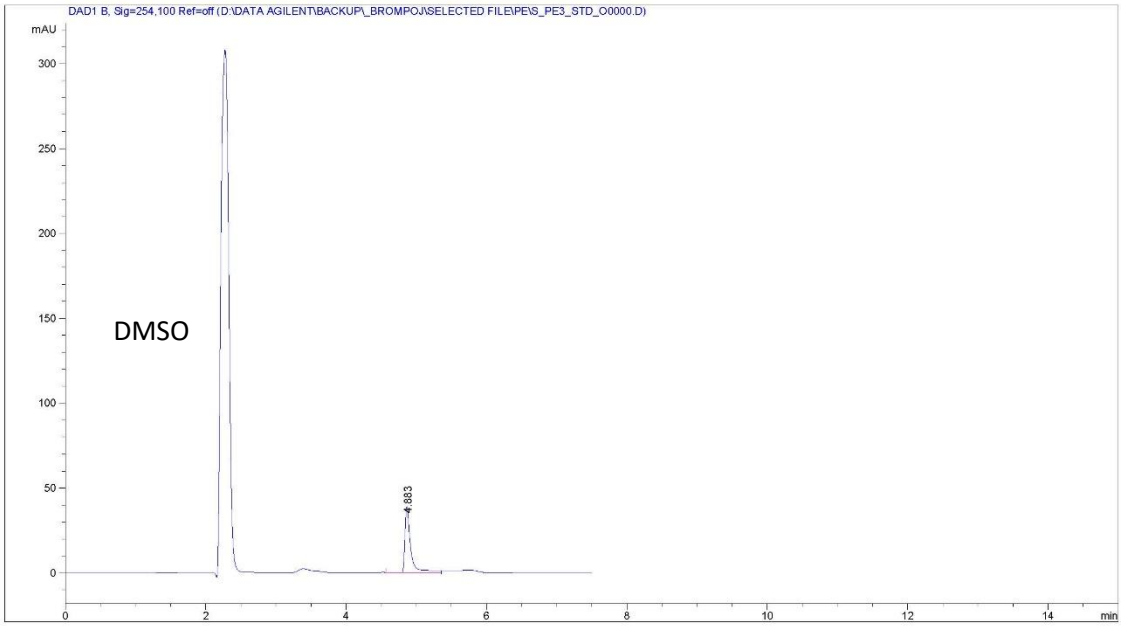
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\PE\S_PE2_STD_O0000.D
Sample Name: PE2 Std O

================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 3
Injection Date  : 1/16/2023 12:04:37 PM
                                                  Inj Volume : 20.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 1/16/2023 12:03:34 PM by Phuvadol
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 6/8/2024 11:15:01 AM by Phuvadol
                  (modified after loading)
Sample Info     : Sample PE2 Std O dilut. to 50 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (20:80); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
================================================================
                      Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.971 BB    0.3308  272.68188   13.55027 100.0000

Totals :                   272.68188   13.55027

================================================================
                      *** End of Report ***
```

8. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 2-(2-nitrophenyl)acetate (PE3)

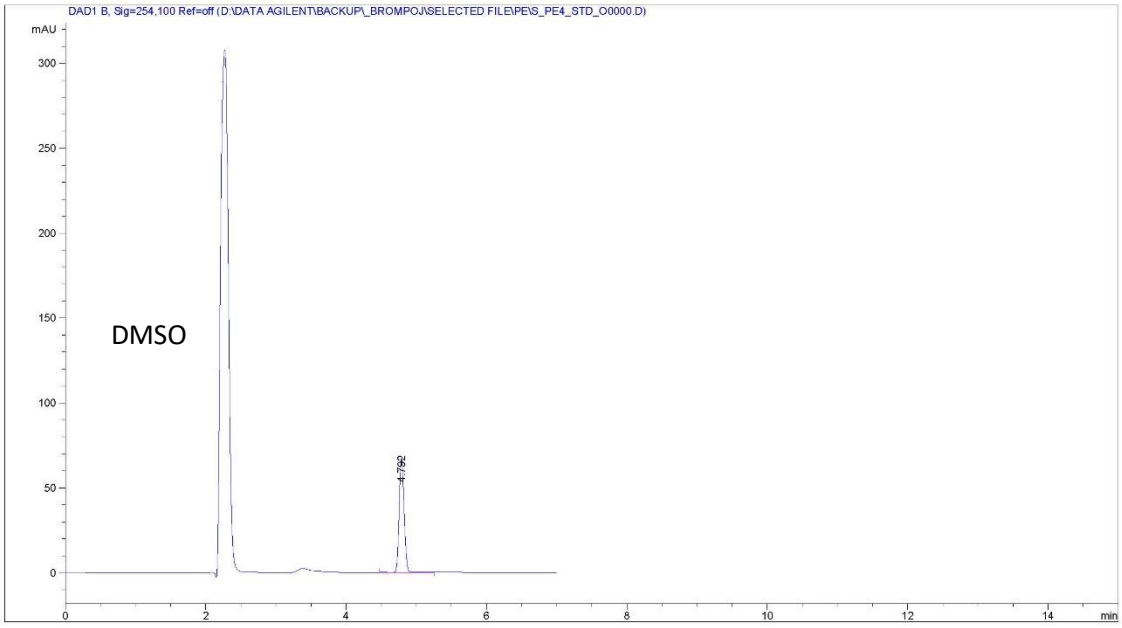
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\PE\S_PE3_STD_O0000.D
Sample Name: PE3 Std O

================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 4
Injection Date  : 1/16/2023 12:35:08 PM
                                                  Inj Volume : 20.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 1/16/2023 12:34:19 PM by Phuvadol
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 5/23/2024 2:55:32 PM by Thanapat
                  (modified after loading)
Sample Info     : Sample PE3 Std O dilut. to 50 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (20:80); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.883 BB    0.1406  218.25984   33.25533 100.0000

Totals :                   218.25984   33.25533

================================================================
                        *** End of Report ***
```

9. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl 4-hydroxy-3-methoxybenzoate (PE4)

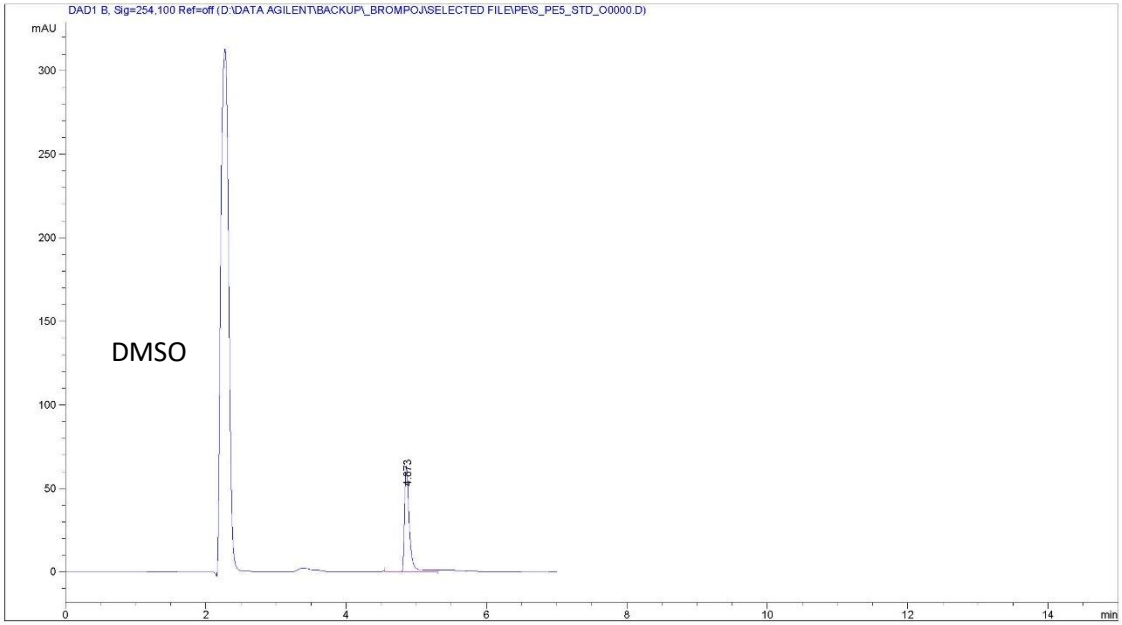
```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\PE\S_PE4_STD_O0000.D
Sample Name: PE4 Std O

=====================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 5
Injection Date  : 1/16/2023 12:25:50 PM
                                                  Inj Volume : 20.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 1/16/2023 12:24:07 PM by Phuvadol
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 5/23/2024 2:57:04 PM by Thanapat
                  (modified after loading)
Sample Info     : Sample PE4 Std O dilut. to 50 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (20:80); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; T 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.792 BB    0.1398  334.10324   51.43027 100.0000

Totals :                   334.10324   51.43027

=====================================================================
                        *** End of Report ***
```

10. (1-(4-phenoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (PE5)

```
Data File D:\DATA AGILENT\BACKUP\_BROMPOJ\SELECTED FILE\PE\S_PE5_STD_O0000.D
Sample Name: PE5 Std O

=====================================================================
Acq. Operator   : Phuvadol
Acq. Instrument : Instrument 1                    Location : Vial 6
Injection Date  : 1/16/2023 12:17:02 PM
                                                  Inj Volume : 20.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\_PHUVADOL\RUN_PARTITION06.M
Last changed    : 1/16/2023 12:23:30 PM by Phuvadol
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\_THANAPAT\DATA PROCESS 280 NM.M
Last changed    : 5/23/2024 2:57:04 PM by Thanapat
                  (modified after loading)
Sample Info     : Sample PE5 Std O dilut. to 50 uM with 70%MeOH
                  MP: 0.1%v/v Formic acid and MeOH (20:80); Isocratic elu
                  tion at 0.8 mL/min
                  Column: C18 (YMC- Pack Pro), 150- x 4.6-mm; 3-um; @ 25
                  C; Inj. 20 uL
                  UV: 220 (16); 254 (100); 280/16; 440/8
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,100 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.873 BB    0.1344  297.74475   49.32880 100.0000

Totals :                   297.74475   49.32880

=====================================================================
                        *** End of Report ***
```