Supporting Information

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Synthesis and Blastocyst Implantation Inhibition Potential of Lupeol Derivatives in Female Mice

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S1:

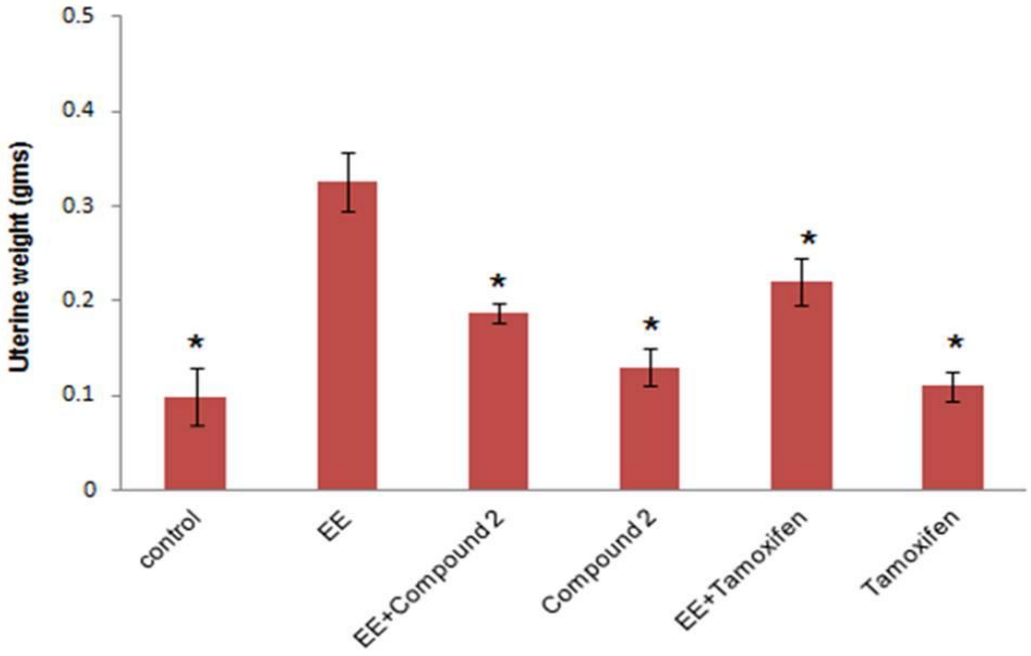
Table 1. Percentage edema protection by synthesised analogues in acute and chronic inflammation

Compounds	% Protection (Acute Inflammation)	% Protection (Chronic Inflammation)				
		1st day	2nd day	3rd day	4th day	5th day
1	70	47	56	62	67	73
2	93	60	67	73	78	85
3	51	NT	NT	NT	NT	NT
4	66	55	58	62	67	69
5	43	NT	NT	NT	NT	NT
6	49	NT	NT	NT	NT	NT
7	42	NT	NT	NT	NT	NT
8	60	NT	NT	NT	NT	NT
9	62	NT	NT	NT	NT	NT
Diclofenac sodium	69	-	-	-	-	-
Dexamethasone	-	46	55	60	67	83

NT: Not Tested

S2:

Figure 3. Uterine weight in control and different groups of treated animals (n =6); *$p < 0.05$ was considered significant when compared to ethinyl estradiol (EE) alone treated animals.



S3: Synthesis of compounds

*Isolation of lupeol (**1**)*

The bark was dried under shade and powdered. The bark powder (800 g) was extracted with *n*-Hexane in a soxhlet apparatus. The extract (21g) was subjected to column chromatography and the titled compound was obtained using hexane to increase polarity of ethyl acetate in hexane as eluting solvent with yield 1.1%. Yield 1.1%; mp 214°C; IR (KBr, cm^{-1}): 3292 (-OH), 2951 (C-H stretching), 1635(C=C), 1377, 1454 , 879 ; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 4.68 and 4.57 (each 1H, 2s, H-29), 3.2 (1H, dd, H-3), 2.38 and 1.92 (each 1H, m, H-19), 1.68 (1H, t, H-15), 1.66 (3H, s, H-30), 1.60 (1H, d, H-2) and 1.59 (1H, q, H-2), 1.42 (1H, d, H-16), 1.39 (1H, q, H-6), 1.36 (1H, t, H-18), 1.33 (1H, m, H-21), 1.20 (1H, m, H-22), 1.03 (1H, q, H-12), 0.99 (3H, s, H-23), 0.97(3H, s, H-27), 0.83, 0.69 (3H, s, H-25, 28, 24); HRMS-ESI *m/z* calcd for $C_{30}H_{50}O$ 449.3715 $[M+Na]^+$, found 449.3752 $[M+Na]^+$. All the data found to exactly matching with the reported values [16].

*General procedure for synthesis of **2** and **3***

To a solution of compound **1** (0.250 g, 0.586 mmol) in dichloromethane, N,N-dicyclohexyl carbodiimide (0.604 g, 2.93 mmol) and N,N-dimethyl amino pyridine (0.360 g, 2.93 mmol) was added followed by appropriate cinnamic acids (1.758 mmol). The mixture was sonicated in an ultrasonicator (35 kHz) for 15 min. Reaction was monitored by thin layer chromatography. The reaction mixture was filtered, evaporated and purified by column chromatography with increasing polarity of ethyl acetate in hexane to obtain the corresponding cinnamic acid esters (**2, 3**).

*3-(p-Chlorocinnamoyl) lupeol (**2**)*: Yield 78%; as a white solid, mp 247°C; IR (KBr) cm^{-1}: 2951, 1712 (C=O), 1489 and 1639 (C=C), 1172, 813; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.60 (1H, d, H-7'), 7.47 (each 2H, d, H-3'and 5', *J*=16 Hz), 7.35 (each 2H, d, H-2', 6'), 7.40 (1H, d, H-8'), 4.63 (1H, dd, H-3), 4.68 and 4.57 (each 1H,2s, H-29), 4.62 (1H, dd, H-3), 2.38 and 1.92 (each 1H, m, H-19); HRMS-ESI *m/z* calcd for $C_{39}H_{55}O_2Cl$ 613.3891 $[M+Na]^+$, found 613.3781 $[M+Na]^+$.

*3-Cinnamoyl lupeol (**3**)*: Yield 91%; as a white solid; mp 236°C; IR (KBr) cm^{-1}: 2949, 1712 (C=O), 1641 (C=C), 1454, 1172, 879 and 761; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.65 (1H, s,H-7', *J*=16 Hz), 7.52 (each 1H, d, H-2' and 6', *J*=8.5 Hz), 7.38 (each 1H, d, H-3' and 5', *J*=8.5 Hz),7.37 (1H, s, H-4'), 6.44 (1H, s,H-8', *J*=16 Hz), 4.68 and 4.57 (each 1H, 2s, H-29), 4.62 (1H, dd, H-3), 2.38 and 1.92 (each 1H, m, H-19); HRMS-ESI *m/z* calcd for $C_{39}H_{56}O_2$ 579.4280 $[M+Na]^+$, found 579.4163 $[M+Na]^+$.

*Lupeol acetate (**4**)*

To Compound **1**(0.250 g, 0.586 mmol) acetic anhydride (0.5 ml) was added in presence of pyridine and kept overnight at room temperature. The reaction was quenched with ice and extracted with chloroform. Chloroform soluble was dried over anh. $NaSO_4$, filtered and concentrated. The compound was crystallized from chloroform and hexane. All the spectral data found to exactly matching with the reported values [16]. Yield 85%; as a white solid; mp 218°C; IR (KBr) cm^{-1}: 2951, 1735 (C=O), 1371 and 1454, 1246, ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 4.68 and 4.57 (each 1H, 2s, H-29), 4.46 (1H, dd, H-3), 2.38 (1H, m, H-19), 2.04 (3H, s, -$OCOCH_3$) and 2.02 (3H, s, -$OCOCH_3$), 2.04 (3H, s, H-1'); HRMS-ESI *m/z* calcd for $C_{32}H_{52}O_2$ 491.3967 $[M+Na]^+$, found 491.3850 $[M+Na]^+$.

*Lupenone (**5**)*: Compound **1** (0.500 g, 1.171 mmol) was stirred with Pyridinium chlorochromate: Silica gel (1:1) (0.505 g, 2.343 mmol) in dichloromethane at room temperature for 4.5 h. Reaction was monitored by TLC. On completion of reaction, it was filtered. The filtrate was concentrated and extracted with hexane. Then it was kept for crystallization to obtain compound **5**. Yield 90%; as a colorless crystalline solid; mp 169°C (lit. mp. 167-169°C); IR (KBr, cm^{-1}): 2939 (C-H of CH_2), 1703 (C=O), 1643 (C=C), 1379 and 1454(C-H of CH_3), 869(=C-H), absence of -OH stretching peak; ^{1}H-NMR(500 MHz, $CDCl_3$): δ 4.68 and 4.57 (each 1H, 2s, H-29), 2.38 and 1.92 (each 1H, m, H-19), 1.68 (1H, t, H-15), 1.66 (3H, s, H-30), 1.60 (1H, d, H-2) and 1.59 (1H, q, H-2), 1.42 (1H, d, H-16), 1.39 (1H, q, H-6), 1.36 (1H, t, H-18), 1.33 (1H, m, H- 21), 1.20 (1H, m, H-22), 1.03 (1H, q, H-12), 0.99 (3H, s, H-23), 0.97 (3H, s, H-27), 0.83, 0.69 (3H, s, H-25, 28, 24), absence of H-3α peak; HRMS-ESI *m/z* calcd for $C_{30}H_{48}O$ 424.3705 $[M]^+$, found 424.3704 $[M]^+$.

*Lupenon-3-oxime (**6**)*: Compound **5** (0.250 g, 0.588 mmol) in dichloromethane was stirred with hydroxylamine hydrochloride (0.102 g, 1.471 mmol) in presence of pyridine at room temperature for 6 h. Reaction was monitored by TLC. Ice-water was added to it and extracted with ethyl acetate (25 mL X 3 times), dried over anhydrous sodium sulphate and concentrated to obtain compound **6**. Yield 80%; as a colorless amorphous solid; mp 244°C (lit. mp. 244-245˚C); IR (KBr, cm^{-1}): 3251 (=N-OH, O-H stretch), 2972 (C-H), 1454 (C=N), 1382 (C-H of CH_3), 1024, 943.16, 877.61 (C-H bending of =C-H), 746, 630 (N=O); ^{1}H-NMR (500MHz, $CDCl_3$):δ 8.12 (1H, s, -OH), 4.68 and 4.57 (each 1H, 2s, H-29), 2.97 (1H, dt, H-3), 2.38 and 1.92 (each 1H, m, H-19), 1.68 (1H, t, H-15), 1.66 (3H, s, H-30), 1.60 (1H, d, H-2), 1.59 (1H, q, H-2), 1.42 (1H, d, H-16), 1.39 (1H, q, H-6), 1.36 (1H, t, H-18), 1.33 (1H, m, H-21), 1.20 (1H, m, H-22), 1.03 (1H, q, H-12), 0.99 (3H, s, H-23), 0.97(3H, s, H-27), 0.83, 0.69 (3H, s, H-25, 28, 24), absence of H-3α peak; HRMS-ESI *m/z* calcd for $C_{30}H_{49}NO$ 440.3893 $[M+H]^+$, found 440.3898 $[M+H]^+$.

*[3,2-b] indole-lupenone (**7**)*: A mixture of **5** (0.250 g, 0.588 mmol), phenylhydrazine (0.066 mL) and glacial acetic acid (2mL) was heated at reflux under N_2 for 1 h. During this, color changes from colorless to bright yellow. Reaction was monitored by TLC. The reaction mixture was pippeted into distilled water and extracted with DCM and combined DCM extracts were washed with 5% aqueous NaOH and brine, dried over anhydrous sodium sulphate and concentrated under vacuum to afford pale yellow solid. Product was purified by column chromatography with increasing polarity of ethyl acetate in hexane to obtain compound **7**. Yield 56%; as a pale yellow amorphous solid; mp 154°C; IR (KBr, cm^{-1}): 3453,

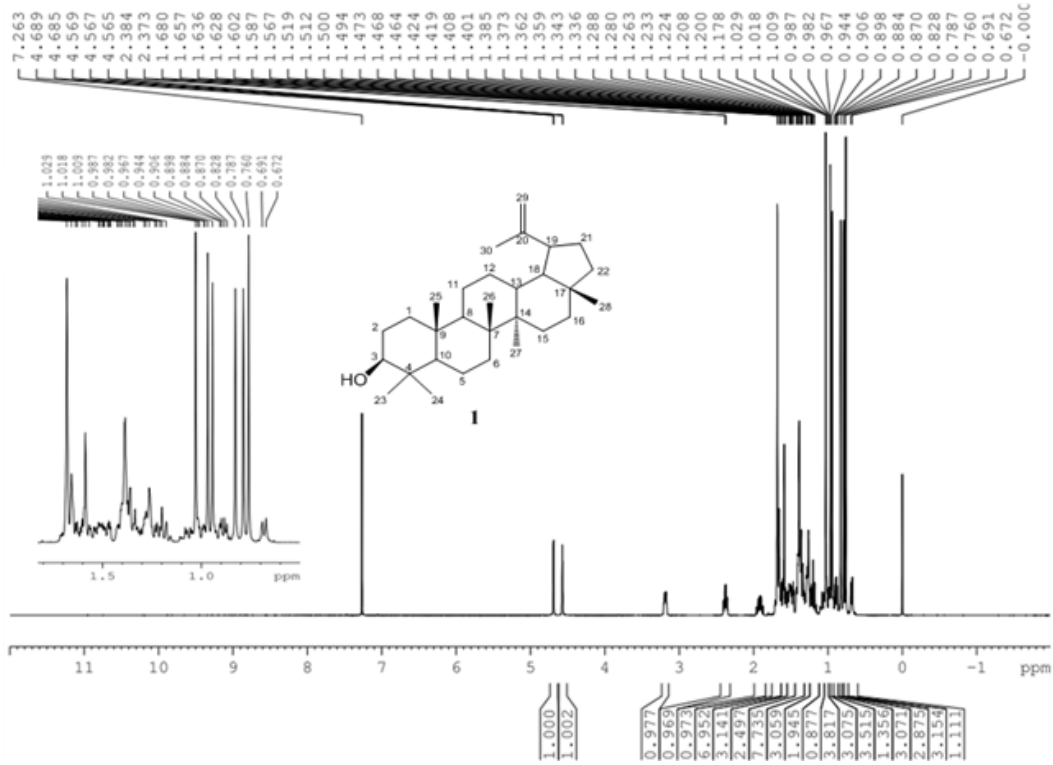
3350 (N-H), 2951 (C-H), 1635 (C=C), 1377, 1454 (C-H of CH_3), 879 (C-H bending); ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.05 (each 1H, bs, -NH), 7.39 (1H, d, H-3', *J*=8 Hz), 7.30 (1H, d, H-6', *J*=8 Hz), 7.10 (1H, t, H-4', *J*=14.5 Hz), 7.05 (1H, t, H-5', *J*=14.5 Hz), 4.72 and 4.60 (each 1H, 2s, H-29), 2.9 and 2.2 (each 1H, dd, H-1), 2.38 and 1.92 (each 1H, m, H-19), 1.68 (1H, t, H-15), 1.66 (3H, s, H-30), 1.42 (1H, d, H-16), 1.39 (1H, q, H-6), 1.36 (1H, t, H-18), 1.33 (1H, m, H-21), 1.20 (1H, m, H-22), 1.03 (1H, q, H-12), 0.99 (3H, s, H-23), 0.97 (3H, s, H-27), 0.69 (3H, s, H-25, 28, 24), absence of H-3α peak; HRMS-ESI *m/z* calcd for $C_{36}H_{51}N$ 498.4100 $[M+H]^+$, found 498.4102 $[M+H]^+$.

*2-Formyl lupenone (**8**)*: Compound **5** (0.250 g, 0.588 mmol) in DCM was stirred with ethyl formate (0.13 mL) in presence of sodium methoxide (0.095 g) under N_2 for 4 h. The reaction mixture was quenched with ice-water, then it was extracted with ethyl acetate. Ethyl acetate layer was dried over anhydrous sodium sulphate, filtered and concentrated, then it was kept for crystallization to obtain compound **8**. Yield 61%; as a colorless amorphous solid; mp 156°C, IR (KBr, cm^{-1}): 3292 (O-H), 2951.09 (C-H), 1703 (C=O), 1635 (C=C), 1377, 1454 (C-H of CH_3), 879 (C-H bending); ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.7 (1H, bs, -OH), 4.68 and 4.57 (each 1H, 2s, H-29), 2.5 (1H, m, H-2'), 2.4 (each 1H, m, H-19), 1.68 (1H, t, H-15), 1.66 (3H, s, H-30), 1.60 (1H, d, H-2), 1.59 (1H, q, H- 2), 1.42 (1H, d, H-16), 1.39 (1H, q, H-6), 1.36 (1H, t, H-18), 1.33 (1H, m, H-21), 1.20 (1H, m, H- 22), 1.03 (1H, q, H-12), 0.99 (3H, s, H-23), 0.97(3H, s, H-27), 0.69 (3H, s, H-25, 28, 24); HRMS-ESI *m/z* calcd for $C_{31}H_{48}O_2$ 452.3654 $[M]^+$, found 452.3657 $[M]^+$.

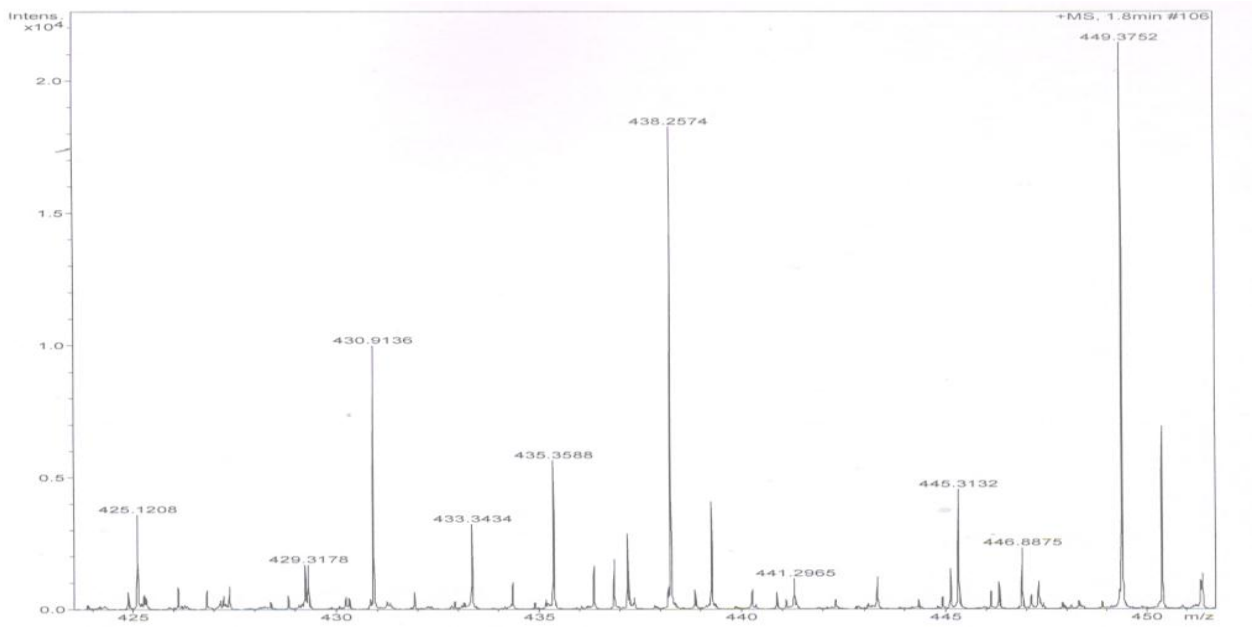
*2-Oxime lupenone (**9**)*: compound **5** (0.250 g, 0.588 mmol) in DCM with conc. HCl (2 mL) was treated with $NaNO_2$ (0.0816 g, 1.177 mmol) in water at 0°C. The reaction mixture was quenched with ice-water, then it was extracted with DCM. DCM layer was dried over anhydrous sodium sulphate, filtered and concentrated, then it was kept for crystallization to obtain compound **9**. Yield 75%; as a pale yellow amorphous solid; mp 235°C; IR (KBr, cm^{-1}): 3251 (=N-OH, O-H stretch), 2972 (C-H), 1703 (C=O), 1454 (C=N), 1382 (C-H of CH_3), 1024, 943, 877(C-H bending of =C-H), 746, 630 (N=O), 540; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.3 (1H, bs, =N-OH), 4.69 and 4.57 (each 1H, 2s, H-29), 2.4 and 1.92 (each 1H, m, H-19), 1.68 (1H, t, H-15), 1.66 (3H, s, H-30), 1.42 (1H, d, H-16), 1.39 (1H, q, H-6), 1.36 (1H, t, H-18), 1.33 (1H, m, H-21), 1.20 (1H, m, H-22), 1.03 (1H, q, H-12), 0.99 (3H, s, H-23), 0.97 (3H, s, H-27), 0.69 (3H, s, H-25, 28, 24); HRMS-ESI *m/z* calcd for $C_{30}H_{47}NO_2$ 453.3685 $[M]^+$, found 453.3439 $[M]^+$.

S4: [1]H-NMR and HRMS Spectra of compounds

S4.1. [1]H-NMR of compound 1



S4.2. HRMS of compound 1 (EXPANDED)



Mass Spectrum List Report

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Sample Name	PSLP-1	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

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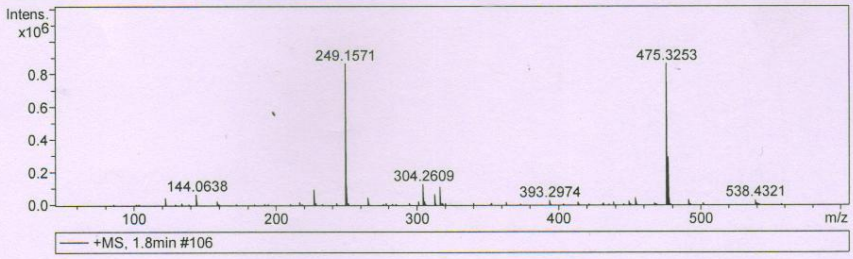

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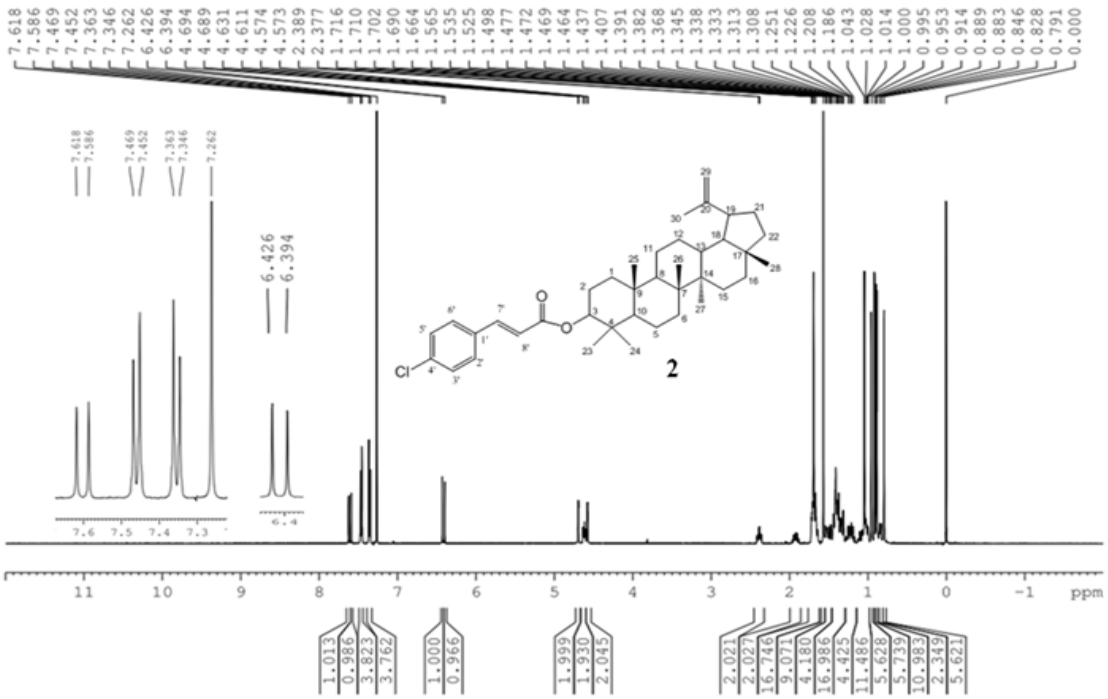
3	144.0638	14587	2928.6	65712	0.0099
4	158.9645	15294	1091.9	25895	0.0104
5	216.9227	16766	431.4	19383	0.0129
6	226.9515	16695	1213.9	63641	0.0136
7	227.1754	16589	1748.2	91937	0.0137
8	249.1571	15697	12449.2	860308	0.0159
9	250.1604	16075	1739.6	121552	0.0156
10	265.1313	16264	732.6	44979	0.0163
11	294.9389	18177	283.4	13645	0.0162
12	301.1409	18040	483.3	23148	0.0167
13	304.2609	17503	2623.2	125232	0.0174
14	305.2640	17996	498.4	23797	0.0170
15	312.2644	17438	1423.5	67561	0.0179
16	313.2669	17826	281.1	13355	0.0176
17	316.1290	18144	2329.1	110204	0.0174
18	317.1323	16641	402.0	19029	0.0191
19	362.9262	18254	481.3	16361	0.0199
20	393.2974	18745	845.2	28127	0.0210
21	413.2662	18200	404.0	16359	0.0227
22	438.2574	19153	329.5	18245	0.0229
23	449.3752	18932	290.9	21429	0.0237
24	453.3436	19188	567.0	45422	0.0236
25	467.1019	19267	127.8	13162	0.0242
26	475.3253	15958	7704.2	861241	0.0298
27	476.3281	18435	2659.0	290746	0.0258
28	477.3312	19092	408.6	43717	0.0250
29	491.2994	18737	452.8	32920	0.0262
30	538.4321	19315	907.1	29867	0.0279

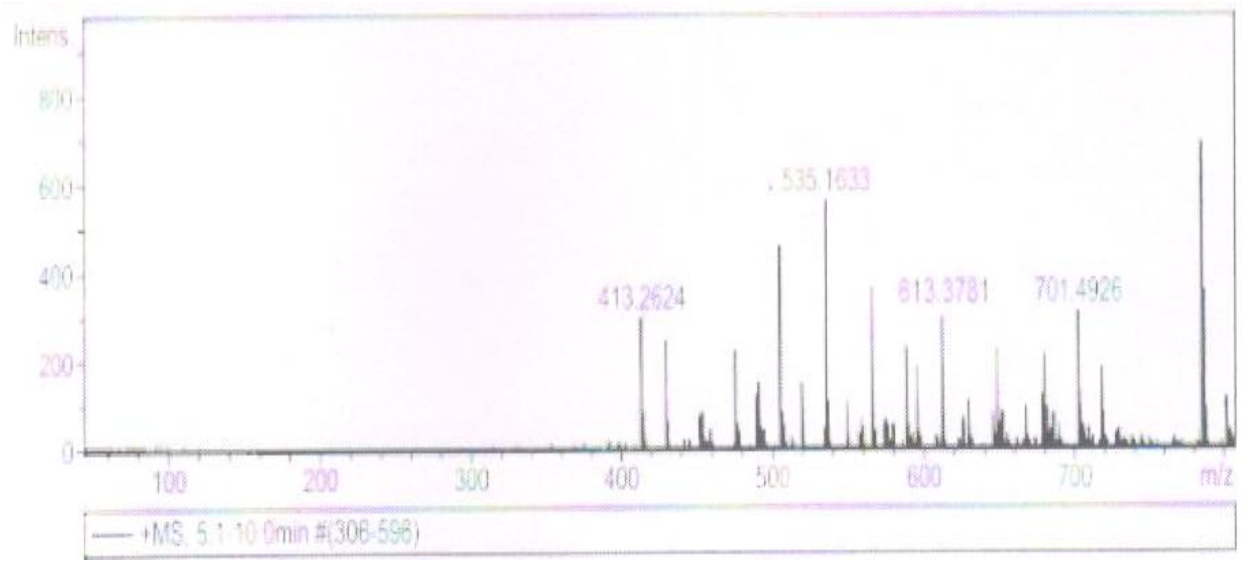
Intensity peak = 449.3759

peak = 426.3861 + 22.9898
= 449.3759

S4.3. ^{1}H-NMR of compound 2



S4.4. HRMS of compound 2



Mass Spectrum List Report

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Comment			

Acquisition Parameter

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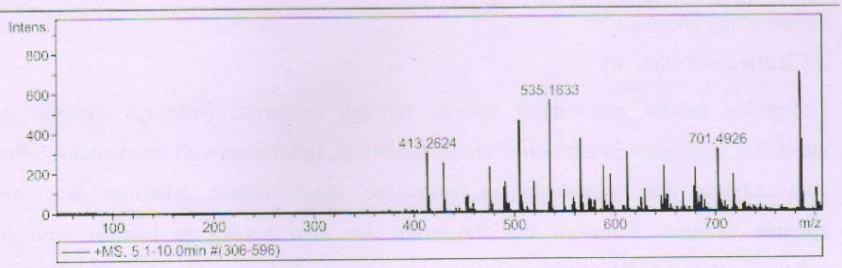

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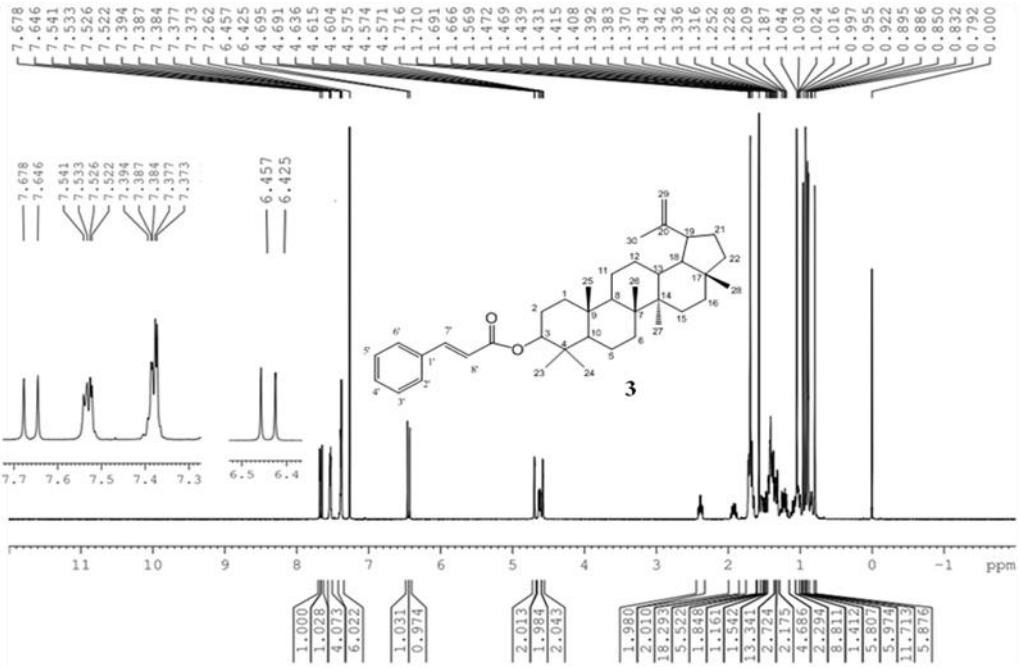
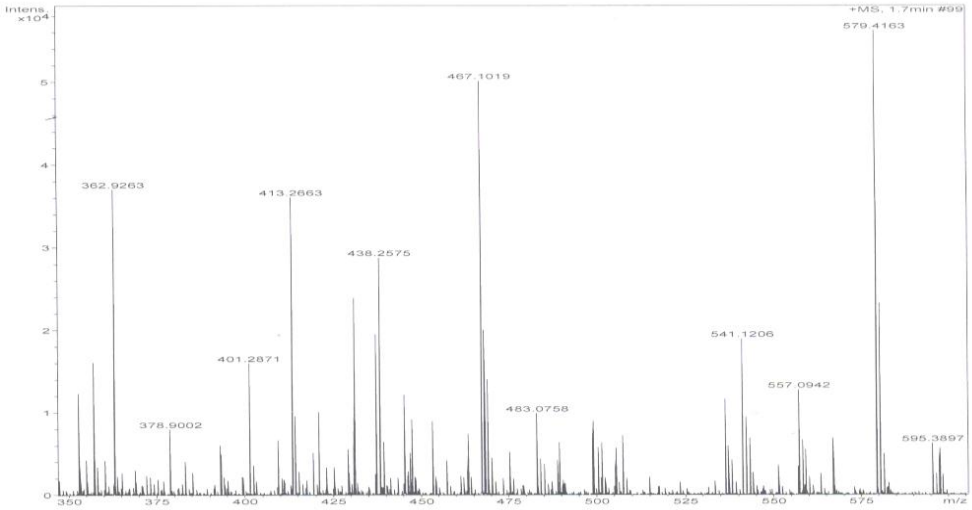
2	429.2370	18902	393.4	250	0.0227
3	475.1410	19297	244.0	181	0.0246
4	475.3246	19218	305.1	225	0.0247
5	489.1782	19541	169.7	127	0.0250
6	491.2986	19117	206.3	153	0.0257
7	505.1524	18948	624.7	461	0.0267
8	519.1893	18930	201.8	150	0.0274
9	535.1633	19721	746.1	563	0.0271
10	536.1668	20131	145.5	112	0.0266
11	549.1999	19265	140.7	112	0.0285
12	565.1741	19389	449.3	367	0.0291
13	588.2705	19494	271.9	232	0.0302
14	595.1833	18929	214.5	184	0.0314
15	613.3781	19646	351.0	306	0.0315
16	629.1518	19135	122.3	110	0.0329
17	648.2914	19033	244.8	228	0.0341
18	678.3012	18306	122.2	124	0.0371
19	679.5109	19182	214.9	216	0.0354
20	701.4093	19028	112.3	116	0.0369
21	701.4926	19772	310.7	316	0.0355
22	702.4954	19375	129.1	133	0.0363
23	717.4666	19320	181.3	188	0.0371
24	784.5265	19294	720.0	694	0.0407
25	785.5300	19222	371.2	360	0.0409
26	800.5844	19847	115.1	114	0.0407

S4.5. ^{1}H-NMR of compound 3



S4.6. HRMS of compound 3(EXPANDED)



Mass Spectrum List Report

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Comment			

Acquisition Parameter

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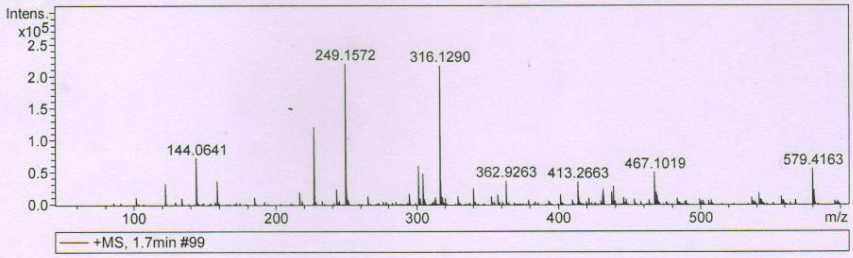
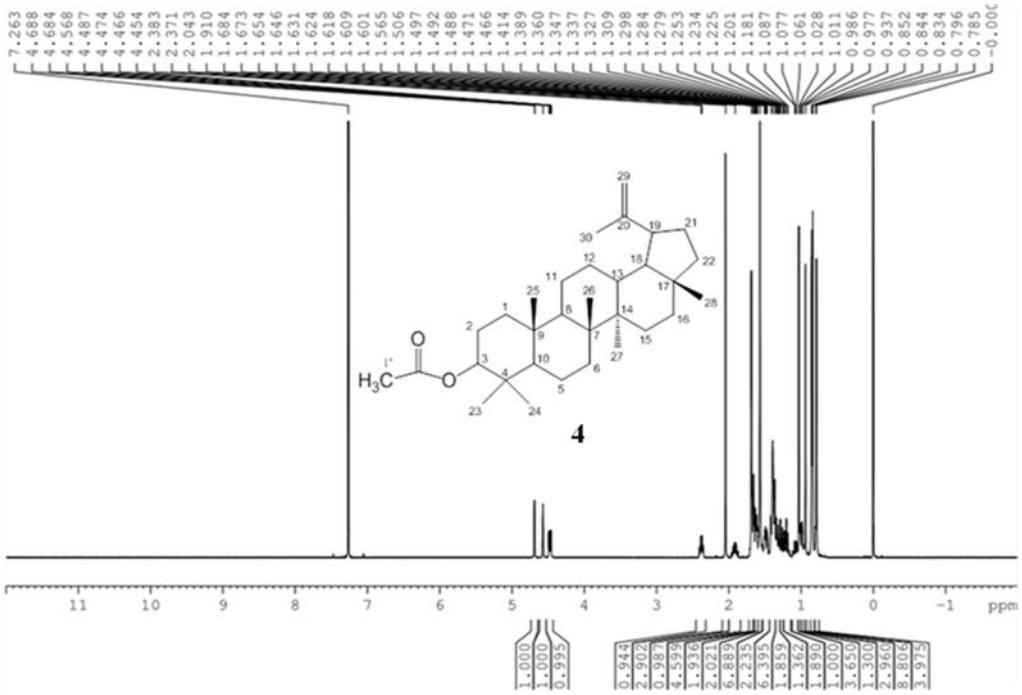
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



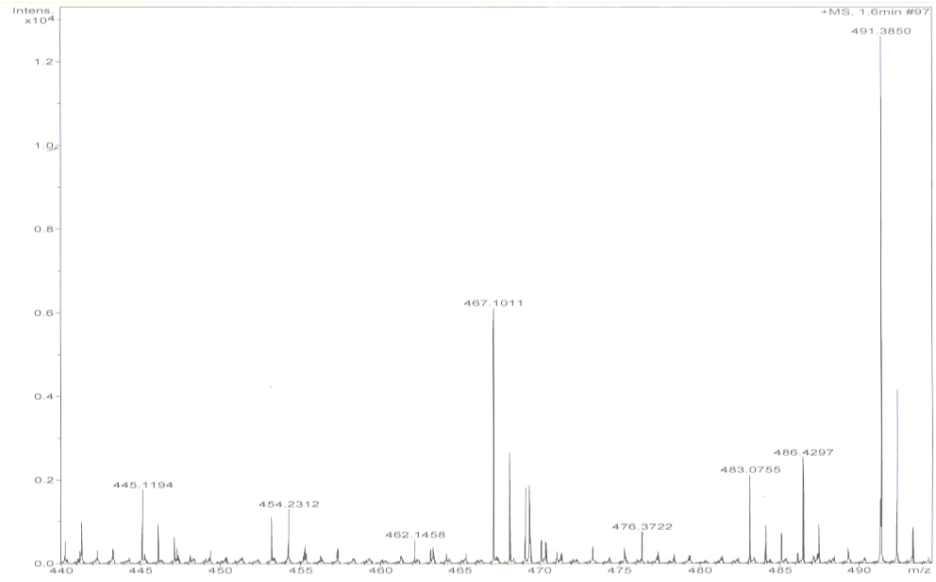
#	m/z	Res.	S/N	I	FWHM
1	122.0829	14291	2315.5	32203	0.0085
2	144.0641	14602	3957.5	72697	0.0099
3	158.9648	15215	1885.4	36694	0.0104
4	216.9226	17067	651.8	20599	0.0127
5	226.9515	16570	3477.3	120856	0.0137
6	227.1753	16948	457.4	15945	0.0134
7	242.9253	16708	599.8	23893	0.0145
8	249.1572	16458	5252.5	219424	0.0151
9	250.1604	16276	682.0	28725	0.0154
10	265.1317	16061	292.0	13087	0.0165
11	294.9388	17915	348.1	17621	0.0165
12	301.1410	17639	1170.8	61064	0.0171
13	304.2611	17813	905.0	47923	0.0171
14	316.1290	17841	3875.0	216802	0.0177
15	317.1315	16931	682.3	38366	0.0187
16	329.1877	17013	232.8	13151	0.0193
17	340.1042	18132	499.2	25865	0.0188
18	357.2611	17631	361.1	16089	0.0203
19	362.9263	18106	874.0	37023	0.0200
20	401.2871	18841	388.1	15987	0.0213
21	413.2663	18392	770.4	36051	0.0225
22	430.9138	19396	433.7	23904	0.0222
23	437.1928	18928	336.8	19511	0.0231
24	438.2575	19453	498.1	28752	0.0225
25	467.1019	19691	947.6	50117	0.0237
26	468.1027	18532	379.3	20017	0.0253
27	469.0994	17479	266.3	14015	0.0268
28	541.1206	19615	490.3	18889	0.0276
29	579.4163	19650	1754.8	56168	0.0295
30	580.4198	19384	731.3	23209	0.0299

peak = 556.428 + 22.9898
. 579.4178

S4.7. ^{1}H-NMR of compound 4



S4.8. HRMS of compound 4(EXPANDED)



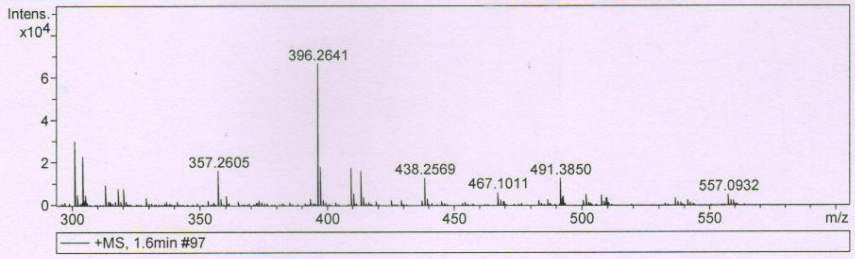
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\Dr. Manjinder Singh\PSLP-4_1-A,7_01_2079.d	Acquisition Date	12/5/2014 3:59:05 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	PSLP-4	Instrument / Ser#	maXis 40
Comment			

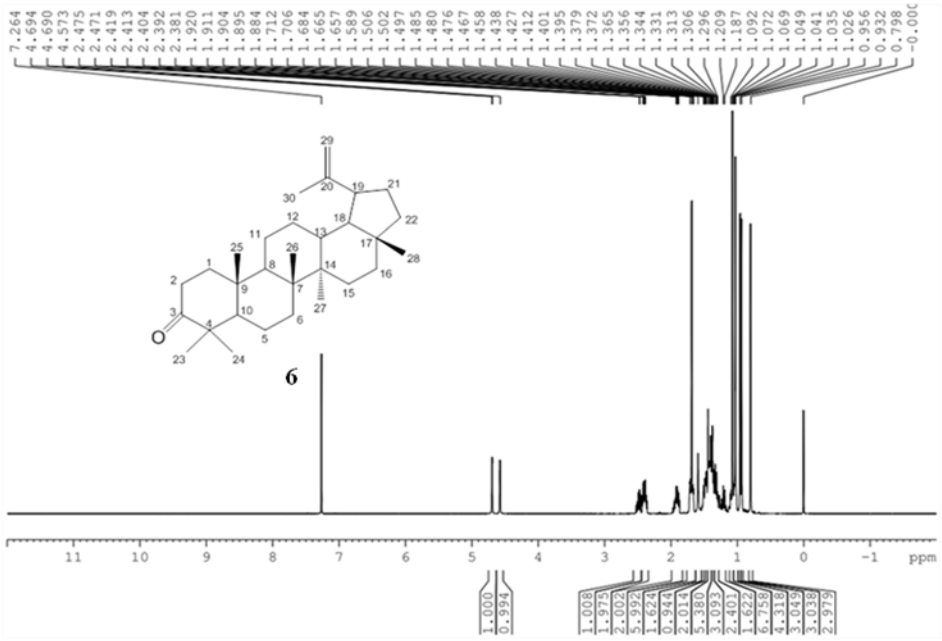
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

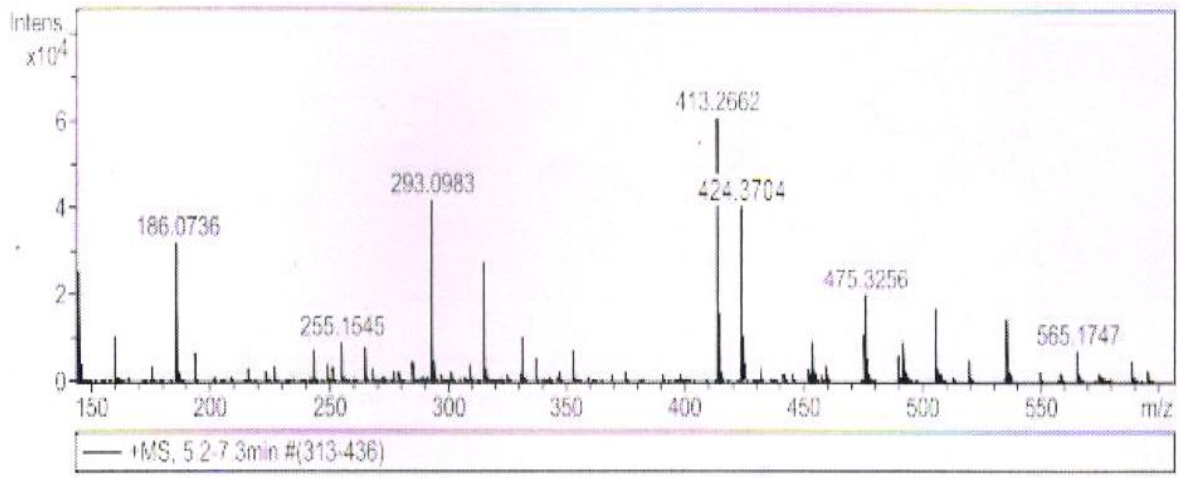


#	m/z	Res.	S/N	I	FWHM
1	301.1408	17726	717.4	29894	0.0170
2	302.1438	16529	119.7	5009	0.0183
3	304.2606	17503	549.5	22902	0.0174
4	305.2629	16810	110.2	4604	0.0182
5	313.2342	17422	245.2	9208	0.0180
6	318.2398	18175	222.8	7796	0.0175
7	320.2580	12503	230.9	7839	0.0256
8	329.1885	13384	116.0	3492	0.0246
9	357.2605	18213	586.5	16311	0.0196
10	358.2638	18243	113.0	3195	0.0196
11	360.3232	18153	151.3	4369	0.0198
12	393.2974	17928	88.0	3008	0.0219
13	396.2641	17961	2016.3	66211	0.0221
14	397.2675	17951	542.9	17654	0.0221
15	398.2706	17441	79.0	2563	0.0228
16	409.3826	18691	618.0	17497	0.0219
17	410.3858	19244	203.7	5730	0.0213
18	413.2658	18807	587.5	16049	0.0220
19	414.2691	18520	147.1	3999	0.0224
20	438.2569	18400	633.2	12959	0.0238
21	439.2599	18099	151.0	3060	0.0243
22	467.1011	18932	312.8	6112	0.0247
23	468.1022	18338	133.7	2643	0.0255
24	491.3850	19116	597.8	12612	0.0257
25	492.3881	18076	197.8	4154	0.0272
26	501.3642	18801	262.7	5112	0.0267
27	507.3588	18811	267.3	4931	0.0270
28	509.3940	17324	193.1	3501	0.0294
29	536.1647	18806	199.8	3570	0.0285
30	557.0932	18956	272.5	5041	0.0294

S4.9. ^{1}H-NMR of compound 5



S4.10. HRMS of compound 5(EXPANDED)



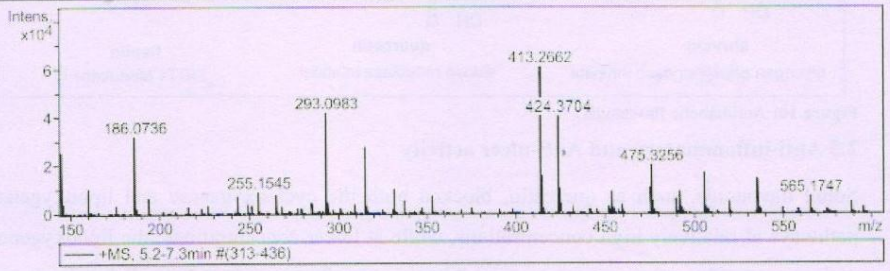
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\IPSINGH\PSLP-6_1-C,7_01_1849.d	Acquisition Date	11/19/2014 10:49:03 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	PSLP-6	Instrument / Ser#	maXis 40
Comment			

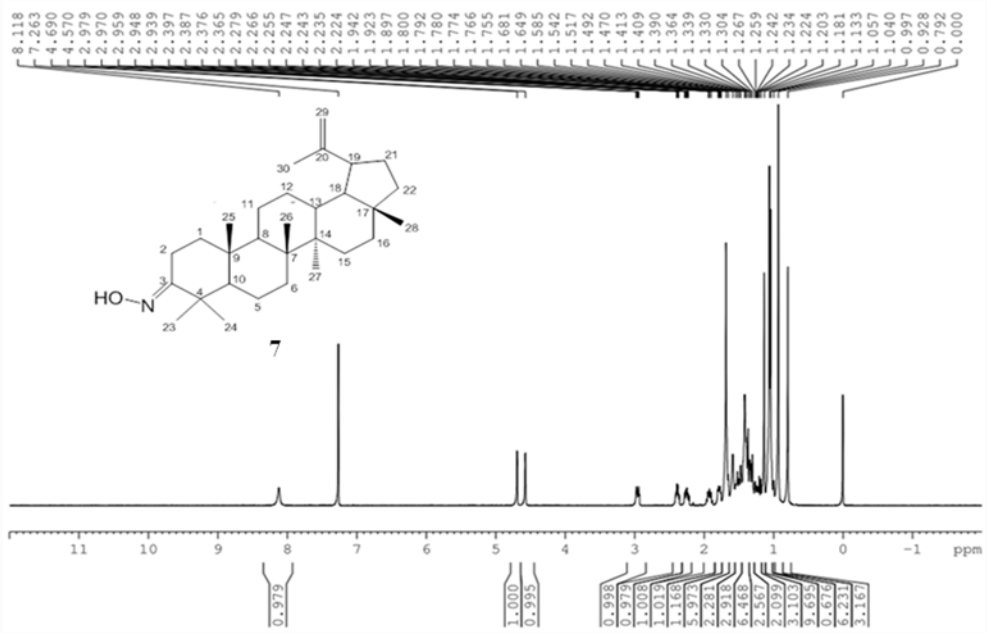
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

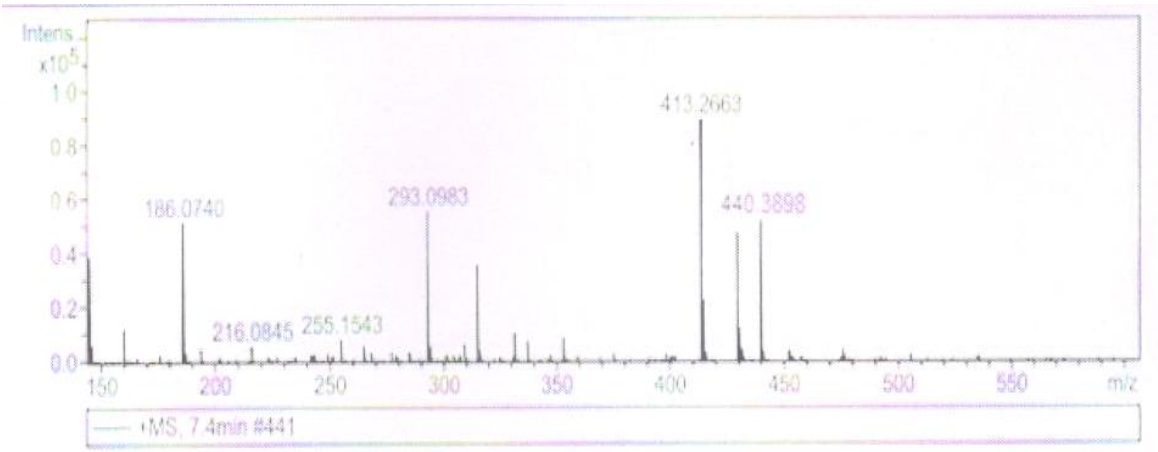


#	m/z	Res.	S/N	I	FWHM
1	145.0658	13715	3871.6	25666	0.0106
2	160.0387	14859	1573.8	10435	0.0108
3	186.0736	15628	4426.6	31995	0.0119
4	194.1025	15683	933.2	6641	0.0124
5	243.1551	16817	881.2	7501	0.0145
6	255.1545	15884	876.7	9042	0.0161
7	265.1369	15408	672.0	7830	0.0172
8	285.1656	17339	353.4	4910	0.0164
9	293.0983	17449	3136.5	41847	0.0168
10	294.1014	16390	352.6	4684	0.0179
11	315.0798	17253	2326.7	27711	0.0183
12	331.0532	17133	888.8	10293	0.0193
13	337.0616	17477	466.1	5342	0.0193
14	353.0351	16633	774.3	7559	0.0212
15	413.2662	18273	3735.7	60648	0.0226
16	414.2697	18774	975.5	15691	0.0221
17	424.3704	17983	2926.5	40347	0.0239
18	425.3732	18021	761.3	10384	0.0239
19	431.2416	16648	314.5	4246	0.0259
20	453.3437	18924	687.4	9395	0.0240
21	475.1427	18864	806.5	11096	0.0252
22	475.3256	18828	1460.3	20062	0.0252
23	476.3286	17959	385.2	5265	0.0265
24	489.1793	19025	504.6	6346	0.0257
25	491.2997	18861	762.7	9451	0.0260
26	505.1532	18408	1615.9	17115	0.0274
27	519.1900	18616	611.2	5031	0.0279
28	535.1639	19007	2257.7	14426	0.0282
29	565.1747	18828	1321.4	7218	0.0300
30	588.2716	19209	823.2	4716	0.0306

S4.11. ^{1}H-NMR of compound 6



S4.12. HRMS of compound 6 (EXPANDED)



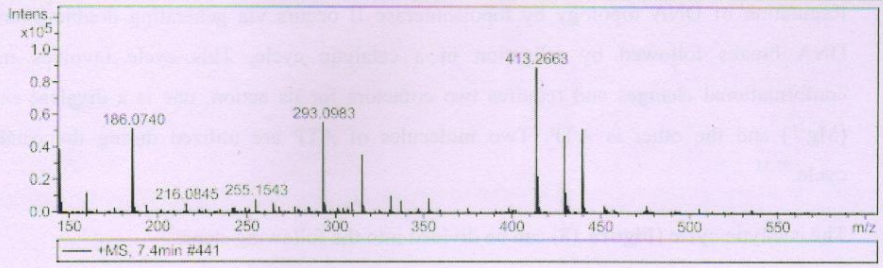
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\IPSINGH\PSLP-7_1-C,8_01_1850.d	Acquisition Date	11/19/2014 11:05:29 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	PSLP-7	Instrument / Ser#	maXis 40
Comment			

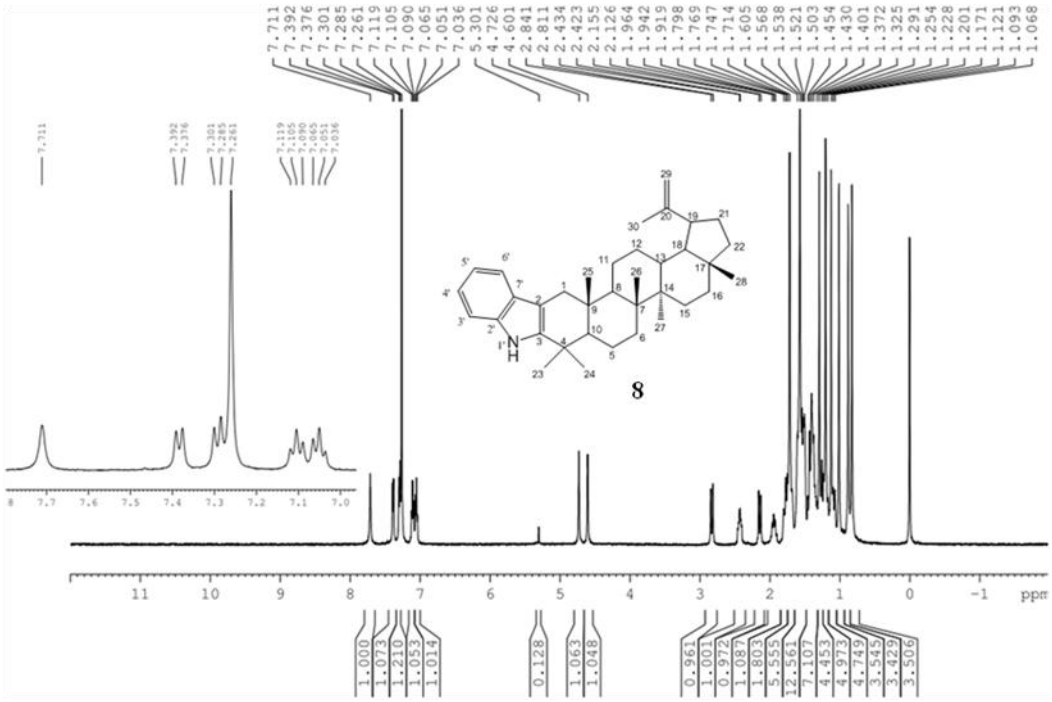
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

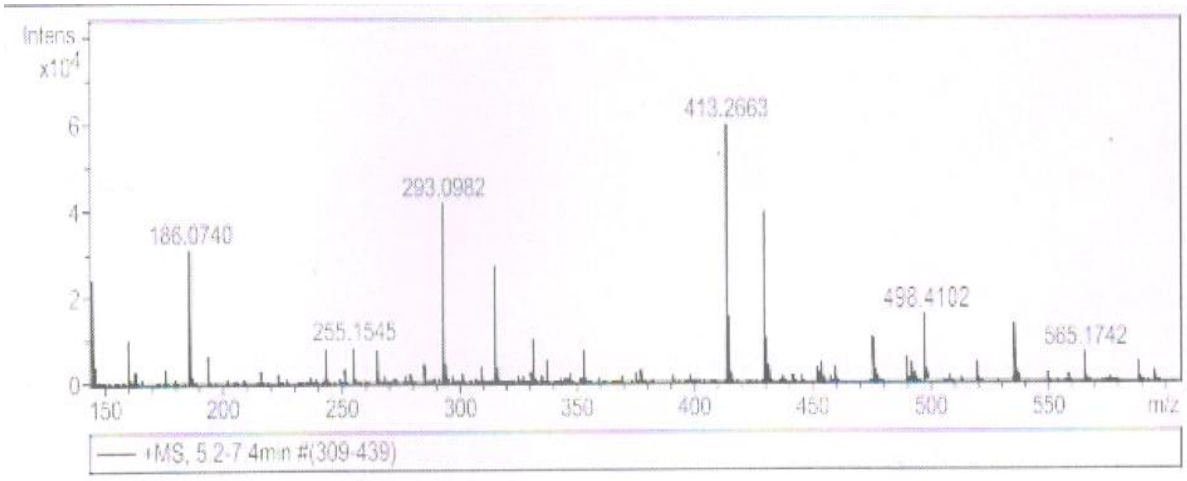


#	m/z	Res.	S/N	I	FWHM
1	145.0668	13433	254.0	38863	0.0108
2	146.0693	14197	43.6	6674	0.0103
3	160.0406	14886	78.8	12059	0.0108
4	160.0589	14317	76.2	11653	0.0112
5	186.0740	15602	304.4	51505	0.0119
6	187.0763	14463	21.1	3583	0.0129
7	194.1032	15456	28.2	4586	0.0126
8	216.0845	16046	60.9	5774	0.0135
9	255.1543	15425	80.2	8293	0.0165
10	265.1369	15585	80.4	5892	0.0170
11	268.0969	16329	52.4	3370	0.0164
12	277.1374	16413	103.2	3819	0.0169
13	285.1658	17356	195.5	3776	0.0164
14	293.0983	17304	2913.5	55438	0.0169
15	294.1015	15988	312.4	5939	0.0184
16	309.0888	17489	341.3	6320	0.0177
17	315.0799	17014	1939.1	35372	0.0185
18	316.0827	16792	230.1	4183	0.0188
19	331.0530	17060	623.1	10591	0.0194
20	337.0619	17510	468.0	7736	0.0192
21	353.0351	16409	244.7	8479	0.0215
22	413.2663	18458	3836.4	89281	0.0224
23	414.2699	18601	977.6	22531	0.0223
24	415.2728	18182	152.1	3478	0.0228
25	429.2404	18152	2441.4	47760	0.0236
26	430.2438	17984	632.7	12235	0.0239
27	440.3898	15602	304.4	51505	0.0119
28	441.2977	18852	191.6	3329	0.0234
29	452.1191	18790	268.9	4335	0.0241
30	475.3255	18719	122.0	3939	0.0254

S4.13. ^{1}H-NMR of compound 7



S4.14. HRMS of compound 7(EXPANDED)



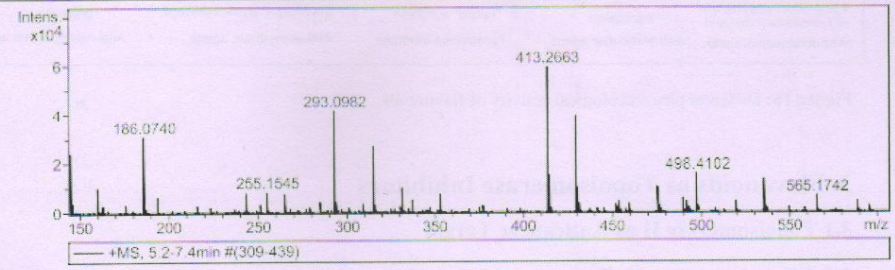
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\IPSINGH\PSLP-8_1-D,1_01_1851.d	Acquisition Date	11/19/2014 11:21:56 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	PSLP-8	Instrument / Ser#	maXis 40
Comment			

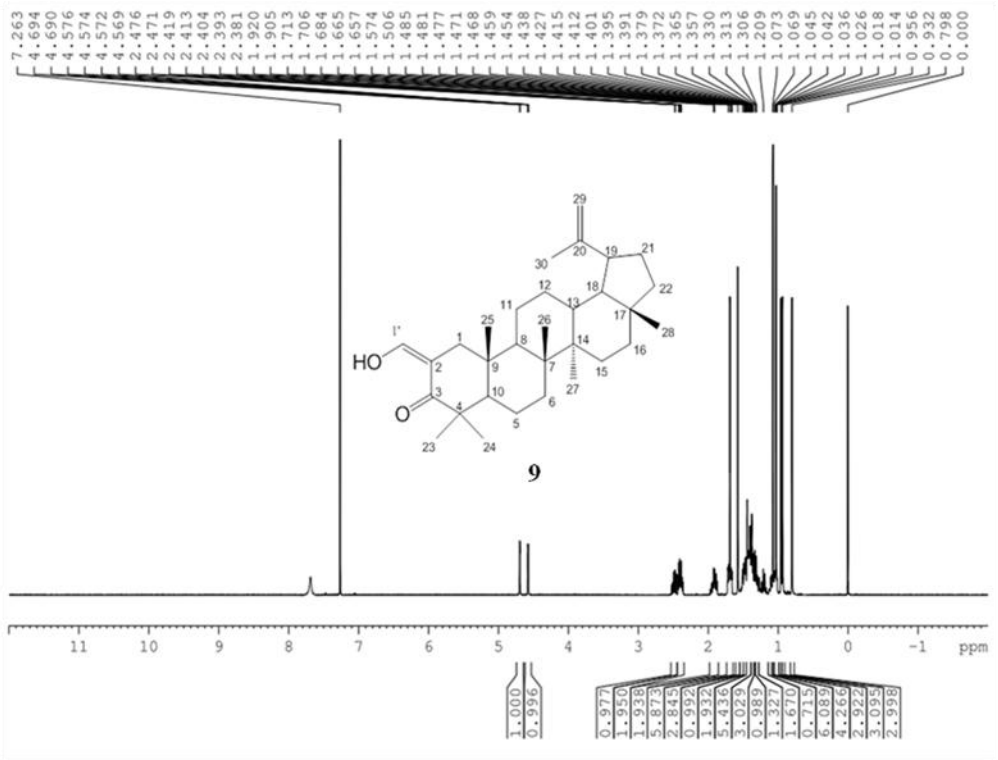
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

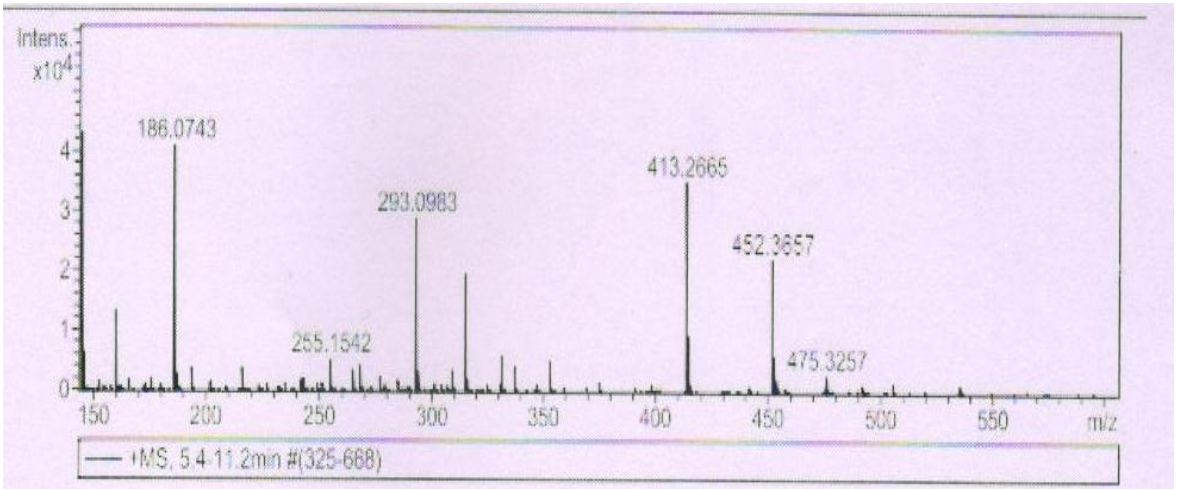


#	m/z	Res.	S/N	I	FWHM
1	145.0669	13577	3399.0	24474	0.0107
2	146.0703	13685	567.2	4086	0.0107
3	160.0395	14921	1435.7	10340	0.0107
4	186.0740	15660	4156.1	31068	0.0119
5	194.1027	15599	903.6	6545	0.0124
6	243.1552	16711	924.0	8178	0.0146
7	255.1545	15574	783.7	8541	0.0164
8	265.1374	16161	629.4	7562	0.0164
9	285.1654	17351	342.3	4774	0.0164
10	293.0982	17330	3043.1	41710	0.0169
11	294.1014	16090	334.5	4579	0.0183
12	315.0798	17079	2094.9	27495	0.0184
13	331.0533	17387	785.6	10402	0.0190
14	337.0617	17784	411.6	5470	0.0190
15	353.0352	16700	653.5	7595	0.0211
16	413.2663	18585	3421.2	59384	0.0222
17	414.2699	18534	880.2	15131	0.0224
18	429.2403	18276	2716.8	39663	0.0235
19	430.2437	18254	712.0	10277	0.0236
20	431.2416	16523	283.8	4052	0.0261
21	453.3437	19081	358.2	4615	0.0238
22	475.1428	18712	882.3	10664	0.0254
23	475.3256	18472	782.2	9448	0.0257
24	489.1794	18908	537.5	6147	0.0259
25	491.2995	18664	399.0	4525	0.0263
26	498.4102	18589	1645.3	16661	0.0272
27	519.1898	18363	564.3	4756	0.0283
28	535.1637	19092	1972.5	13826	0.0280
29	565.1742	18730	1130.1	6766	0.0302
30	588.2710	19145	766.3	4604	0.0307

S4.15. ^{1}H-NMR of compound 8



S4.16. HRMS of compound 8



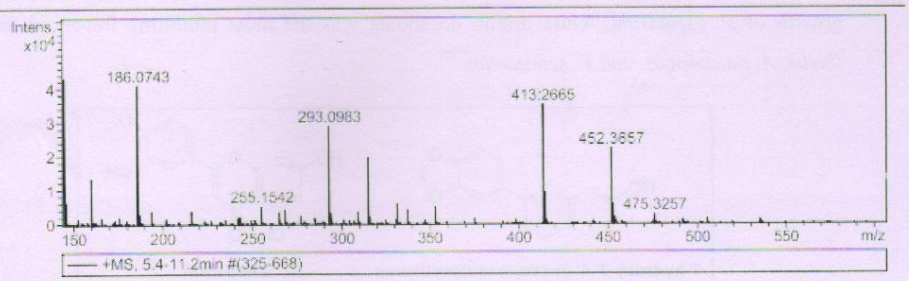
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\IPSINGH\PSLP-9_1-E,1_01_1853.d	Acquisition Date	11/19/2014 12:20:15 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	PSLP-9	Instrument / Ser#	maXis 40
Comment			

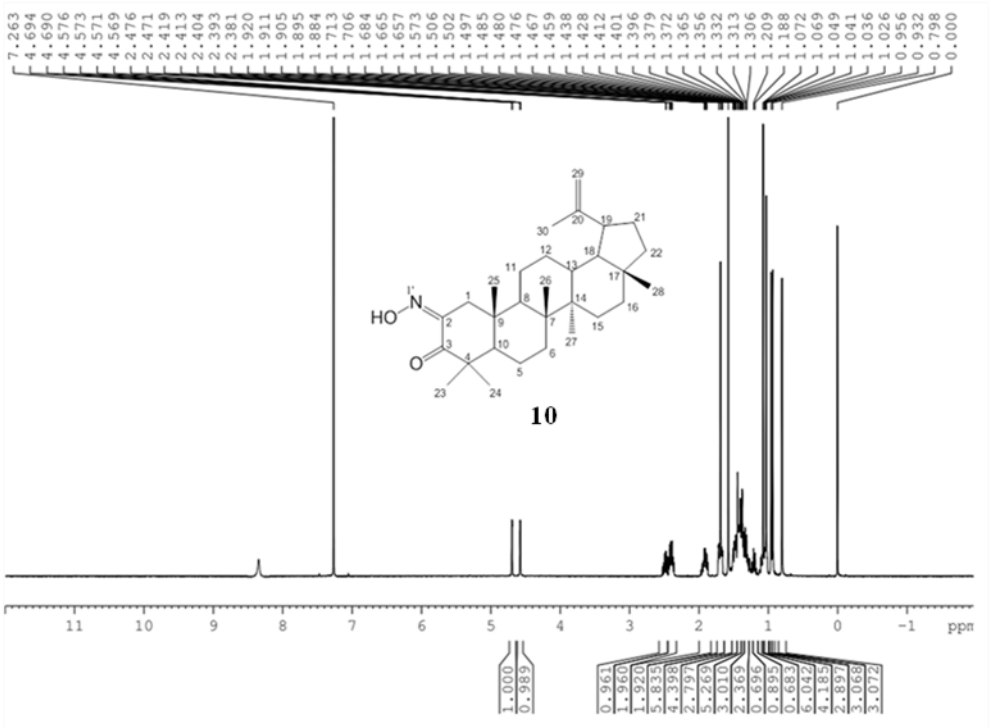
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

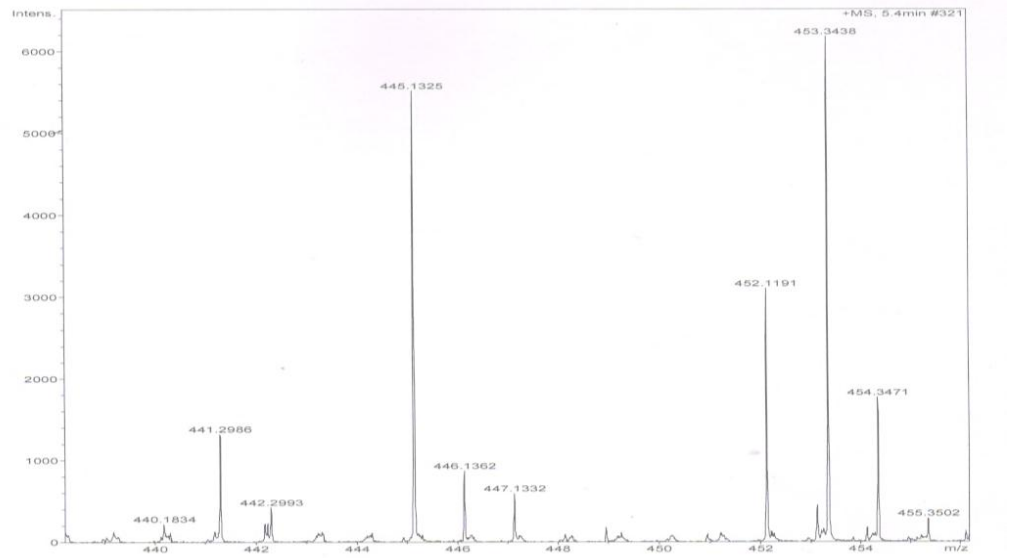


#	m/z	Res.	S/N	I	FWHM
1	145.0678	13687	5157.9	43098	0.0106
2	146.0703	13697	802.2	6704	0.0107
3	160.0402	14561	1633.5	13650	0.0110
4	166.0461	14589	252.4	2079	0.0114
5	176.0927	15228	298.1	2390	0.0116
6	186.0743	15163	5253.2	40945	0.0123
7	187.0763	14012	386.4	3005	0.0134
8	194.1034	15260	526.3	3859	0.0127
9	216.0847	16040	783.5	3801	0.0135
10	242.0612	16729	361.6	1966	0.0145
11	243.1553	16552	388.9	2140	0.0147
12	255.1542	15618	847.4	5338	0.0163
13	265.1372	15808	508.7	3667	0.0168
14	268.0971	17007	610.5	4565	0.0158
15	277.1370	16988	312.4	2593	0.0163
16	285.1656	16576	236.2	2069	0.0172
17	293.0983	17241	3425.2	29005	0.0170
18	294.1015	16561	388.6	3279	0.0178
19	309.0888	17665	460.0	3639	0.0175
20	315.0799	17493	2549.9	19520	0.0180
21	316.0828	16956	300.2	2281	0.0186
22	331.0532	16567	918.6	6103	0.0200
23	337.0618	16872	662.8	4152	0.0200
24	353.0352	16855	1037.7	5169	0.0209
25	413.2665	17780	4521.1	35236	0.0232
26	414.2699	18423	1215.0	9347	0.0225
27	452.3657	18187	3617.5	22297	0.0236
28	453.3635	18282	957.6	5807	0.0235
29	475.3257	18753	726.2	2823	0.0253

S4.17. ^{1}H-NMR of compound 9



S4.18. HRMS of compound 9 (EXPANDED)



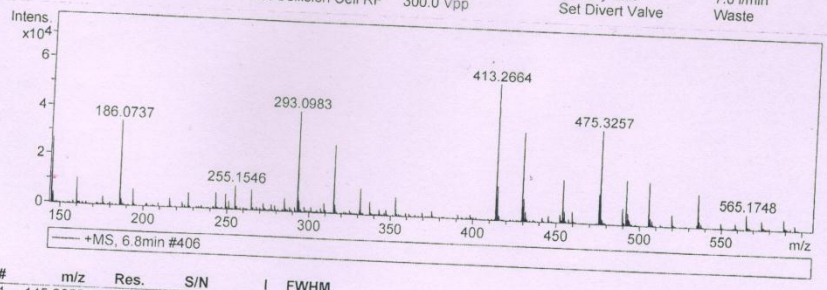
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\IPSINGH\PSLP-10_1-D,2_01_1852.d	Acquisition Date	11/19/2014 11:38:22 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m		
Sample Name	PSLP-10	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	150 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	145.0659	13650	207.6	26954	0.0106
2	160.0388	14992	83.0	10781	0.0107
3	186.0737	15706	249.7	34574	0.0118
4	194.1025	15804	50.4	6755	0.0123
5	227.1755	16626	85.7	6003	0.0137
6	243.1551	16881	176.9	6274	0.0144
7	249.1573	15891	271.8	6109	0.0157
8	255.1546	16005	591.7	9622	0.0159
9	265.1366	15111	444.4	8094	0.0175
10	285.1658	17336	245.4	5275	0.0164
11	293.0983	17156	1977.5	41048	0.0171
12	315.0801	17101	1478.6	27922	0.0184
13	331.0536	17284	559.5	10505	0.0192
14	337.0618	17561	282.4	5293	0.0192
15	353.0352	16495	445.1	7552	0.0214
16	413.2664	18568	2492.3	55320	0.0223
17	414.2697	18800	630.9	13911	0.0220
18	429.2403	17857	1851.8	36492	0.0240
19	430.2439	17893	479.8	9386	0.0240
20	453.3439	19129	769.3	17342	0.0237
21	475.1429	18872	494.6	11958	0.0252
22	475.3257	18629	1584.2	38222	0.0255
23	476.3289	18197	423.9	10154	0.0262
24	489.1795	18894	312.4	6715	0.0259
25	491.2998	19118	859.3	18104	0.0257
26	492.3031	18563	241.1	5041	0.0265
27	505.1532	18579	983.8	17791	0.0272
28	519.1901	18423	335.8	4965	0.0282
29	535.1642	18558	1105.3	13626	0.0288
30	565.1748	18377	538.2	6205	0.0308