SUPPORTING INFORMATION

Leonurenones A-C: Labdane Diterpenes from *Leonotis leonurus*

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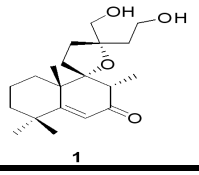


Qualitative Compound Report

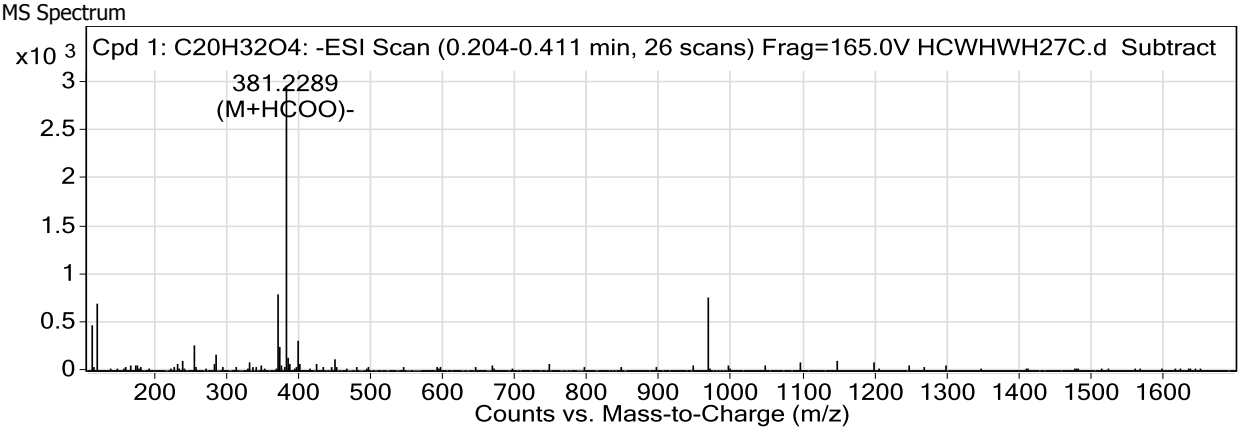
Data File	HCWHWH27C.d	**Sample Name**	FH-1-56B
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method		**Acquired Time**	9/29/2010 1:16:51 PM
IRM Calibration Status	Success	**DA Method**	HCEmpirical1.m
Comment	EM=318.2195 EM=HC ESI Pos Small Molecule No HPLC.m		

Compound Table

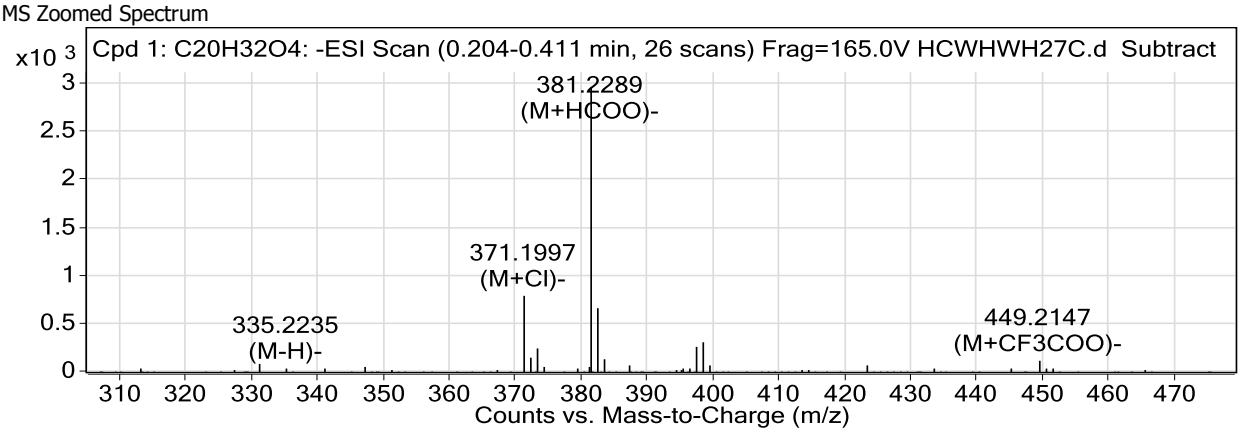
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C20H32O4	0.27	336.2307	2967	C20H32O4	336.2301	1.86

Compound Label	RT	Algorithm	Mass
Cpd 1: C20H32O4	0.27	Find By Formula	336.2307

MS Spectrum



MS Zoomed Spectrum



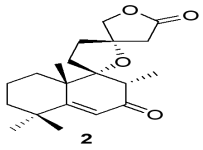
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
335.2235	335.2228	2.04	-1	52	C20 H31 O4	(M-H)-
371.1997	371.1995	0.51	-1	806	C20 H32 Cl O4	(M+Cl)-
372.2037	372.2029	2.31	-1	161	C20 H32 Cl O4	(M+Cl)-
373.1982	373.1973	2.36	-1	254	C20 H32 Cl O4	(M+Cl)-
374.2016	374.2003	3.34	-1	57	C20 H32 Cl O4	(M+Cl)-
377.1993				15		
379.2104				41		

Qualitative Compound Report

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
380.9777				65		
381.2289	381.2283	1.69		2967	C21 H33 O6	(M+HCOO)-
381.4058				22		
382.2313	382.2317	-0.88		678	C21 H33 O6	(M+HCOO)-
383.2329	383.2343	-3.43		140	C21 H33 O6	(M+HCOO)-
385.1869				17		
449.2147	449.2156	-2.05	-1	127	C22 H32 F3 O6	(M+CF3COO)-
450.2137	450.2191	-11.85	-1	40	C22 H32 F3 O6	(M+CF3COO)-

--- End Of Report ---



Qualitative Compound Report

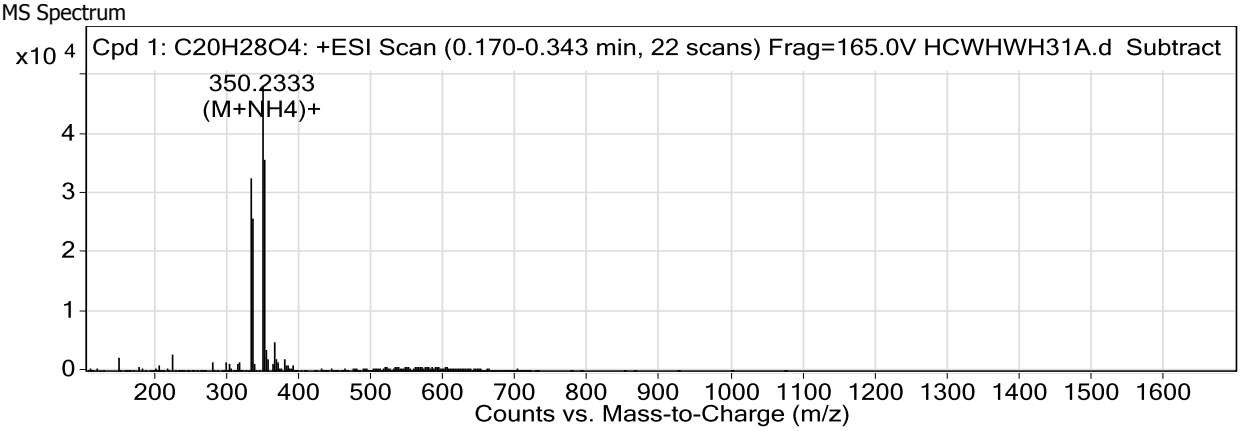
Data File	HCWHWH31A.d	**Sample Name**	FH-1-54B
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method		**Acquired Time**	11/3/2010 7:55:28 PM
IRM Calibration Status	Success	**DA Method**	HCEmpirical1.m
Comment	EM=332.1988 EM=HC HC ESI Pos Small Molecule No HPLC.m modified		

Compound Table

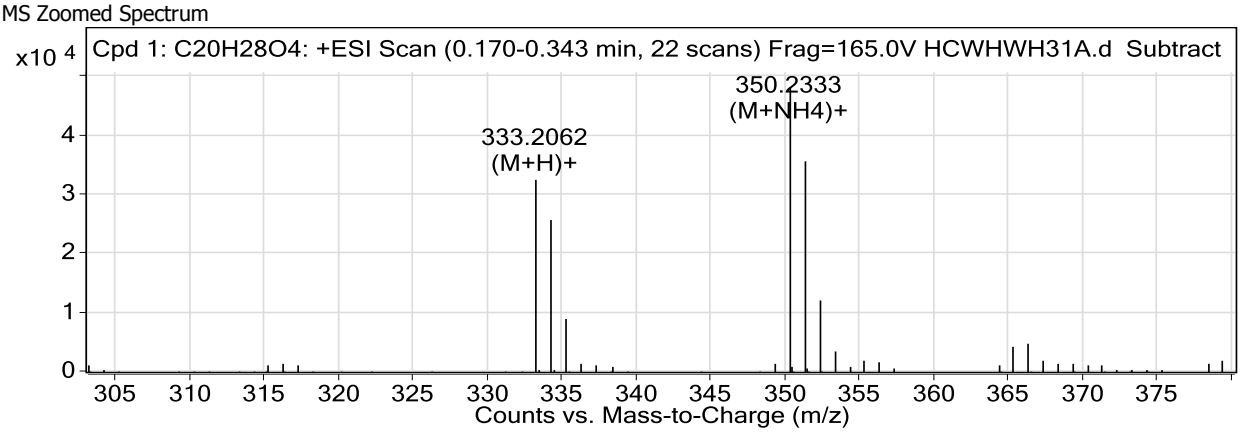
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C20H28O4	0.219	332.1994	32645	C20H28O4	332.1988	1.79

Compound Label	RT	Algorithm	Mass
Cpd 1: C20H28O4	0.219	Find By Formula	332.1994

MS Spectrum



MS Zoomed Spectrum



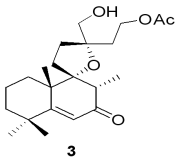
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
333.2062	333.206	0.55	1	32645	C20 H29 O4	(M+H)+
348.2239				256		
349.2037				1587		
350.2333	350.2326	2.06		48217	C20 H32 N O4	(M+NH4)+
350.4016				1017		
350.4727				179		

Qualitative Compound Report

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
351.239				35874		
351.4067				828		
351.4688				281		
351.7579				130		
352.2419				12231		
352.41				255		
353.2389				3763		
354.2646				1160		
355.1899				2214		

--- End Of Report ---



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Qualitative Compound Report

Data File	HCWHWH57A.d	**Sample Name**	FH-1-95
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method		**Acquired Time**	3/23/2011 7:48:56 PM
IRM Calibration Status	Success	**DA Method**	HCEmpirical1.m
Comment	EM=378.2406 M=HC ESI Pos Small Molecule No HPLC.m		

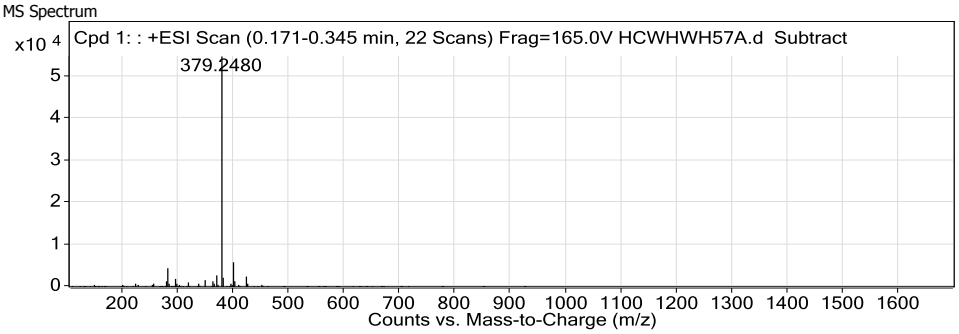
Sample Group	**Info.**
User Defined 1	**User Defined 2**

Compound Table

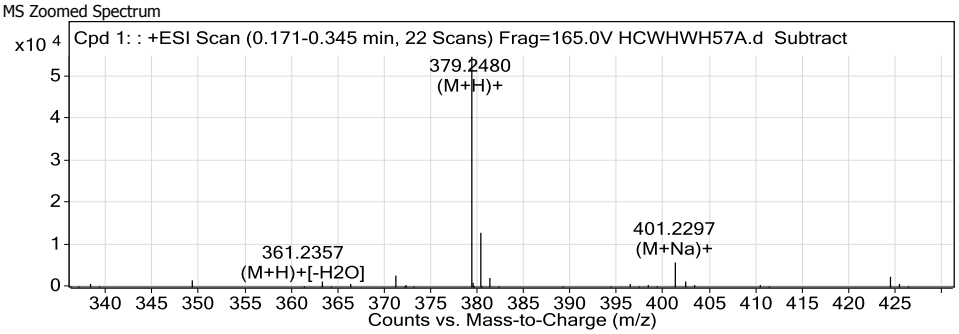
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1:	0.229	378.2407	54741	C22H34O5	378.2406	0.14	C22H34O5	C22H34O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1:	402.2337	0.229	Find By Formula	378.2407

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
361.2357	361.2373	-4.45	1	357.8	C22H33O4	(M+H)+[-H2O]
362.2313	362.2407	-25.96	1	82.6	C22H33O4	(M+H)+[-H2O]
379.248				54740.9		
379.248	379.2479	0.16	1	54740.9	C22H35O5	(M+H)+
380.2509	380.2513	-1.13	1	13100.3	C22H35O5	(M+H)+
381.2523	381.254	-4.53	1	2209.3	C22H35O5	(M+H)+
382.2585	382.2567	4.56	1	332	C22H35O5	(M+H)+
383.2669	383.2594	19.5	1	34.6	C22H35O5	(M+H)+
396.2734	396.2744	-2.55	1	892.8	C22H38NO5	(M+NH4)+
397.2687	397.2778	-22.71	1	46.9	C22H38NO5	(M+NH4)+
398.2549	398.2805	-64.29	1	472.9	C22H38NO5	(M+NH4)+
401.2297	401.2298	-0.42	1	6021.3	C22H34NaO5	(M+Na)+
402.2337	402.2333	1.03	1	1445.9	C22H34NaO5	(M+Na)+

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