

Natural Hydrophobic Deep Eutectic Solvent-Based Enhanced Extraction of Bioactive Compounds from *Cannabis sativa* L. Leaf for Pharmaceutical Applications

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Table S1. % Yield comparison of actual, and predicted values generated by experimental analysis along with RSM and ANN predictions

Std	Run	A: shaking speed	B: Ratio	C: Temperature	D: time	% Yield Experimental	% Yield RSM predicted	% Yield ANN predicted
		rpm	DES/Ethanol	°C	min			
20	1	225	5.5	55	107.5	1.30	1.20	1.23

6	2	175	2.5	75	82.5	0.05	0.03	0.04
5	3	275	2.5	35	132.5	0.02	0.00	0.02
15	4	225	5.5	55	70	1.30	1.34	1.30
19	5	225	5.5	55	107.5	1.20	1.20	1.23
9	6	150	5.5	55	107.5	0.50	0.54	0.50
2	7	275	8.5	35	82.5	1.12	1.10	1.12
1	8	275	8.5	75	82.5	1.06	1.04	1.06
7	9	175	8.5	75	132.5	1.02	1.00	1.02
4	10	175	8.5	35	132.5	1.41	1.39	1.41
21	11	225	5.5	55	107.5	1.20	1.20	1.23
8	12	175	2.5	35	82.5	0.55	0.53	0.55
3	13	275	2.5	75	132.5	0.33	0.31	0.37
18	14	225	5.5	55	107.5	1.20	1.20	1.23
10	15	300	5.5	55	107.5	1.00	1.04	1.00
12	16	225	10	55	107.5	1.10	1.14	1.08
17	17	225	5.5	55	107.5	1.24	1.20	1.23
14	18	225	5.5	85	107.5	0.85	0.89	0.85
16	19	225	5.5	55	145	0.66	0.70	0.66
11	20	225	1	55	107.5	0.44	0.48	0.44
13	21	225	5.5	25	107.5	1.10	1.13	1.10

The design matrix was generated following a partially rotatable central composite design ($\alpha=1.5$), std indicates standard randomization order.

Table S2 : GC-MS library match and predicted chemical identity of components

Library Search Report

Data Path : C:\GCMS Data\05-06-2024\
Data File : S678.D
Acq On : 06 Jun 2024 19:14
Operator :
Sample : S-6, 7, 8
Misc :
ALS Vial : 7 Sample Multiplier: 1

Search Libraries: C:\MassHunter\LIBRARY\NIST0.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	4.174	0.01	C:\MassHunter\LIBRARY\NIST0.L Bicyclo[3.1.0]hexane, 4-methylene- 1-(1-methylethyl)- Cyclohexene, 4-methylene-1-(1-methylethyl)- Bicyclo[3.1.0]hexane, 4-methylene- 1-(1-methylethyl)-	18240 18182 18245	003387-41-5 000099-84-3 003387-41-5	97 91 91
2	4.360	0.00	C:\MassHunter\LIBRARY\NIST0.L .beta.-Myrcene .beta.-Pinene Bicyclo[3.1.0]hexane, 4-methylene- 1-(1-methylethyl)-	18031 18023 18243	000123-35-3 000127-91-3 003387-41-5	93 87 86
3	4.458	0.00	C:\MassHunter\LIBRARY\NIST0.L 3-Octanol 3-Octanol 3-Octanol	15662 15663 15660	000589-98-0 000589-98-0 000589-98-0	72 72 72
4	4.932	0.06	C:\MassHunter\LIBRARY\NIST0.L D-Limonene D-Limonene Limonene	18009 18005 17995	005989-27-5 005989-27-5 000138-86-3	99 94 91
5	5.144	0.00	C:\MassHunter\LIBRARY\NIST0.L .beta.-Ocimene 1,3,6-Octatriene, 3,7-dimethyl-, (Z)- 1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	18026 18141 18140	013877-91-3 003338-55-4 003338-55-4	97 97 90
6	5.923	0.04	C:\MassHunter\LIBRARY\NIST0.L Propane, 2-fluoro-2-methyl- Glycerin Methanamine, N-methoxy-	1114 2719 360	000353-61-7 000056-81-5 001117-97-1	9 9 5
7	6.184	0.01	C:\MassHunter\LIBRARY\NIST0.L Pyrimidine, 2-ethoxy-4,6-dimethyl- Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (E)- (3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	29890 29363 29282	007781-21-7 026532-25-2 206115-88-0	64 55 46
8	7.070	0.13	C:\MassHunter\LIBRARY\NIST0.L Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- (+)-2-Bornanone (+)-2-Bornanone	29380 29115 29114	000464-48-2 000464-49-3 000464-49-3	98 97 96
9	7.252	0.15	C:\MassHunter\LIBRARY\NIST0.L Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- L-Menthone Camphor	29381 30920 29049	000464-48-2 014073-97-3 000076-22-2	93 83 83

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Search Libraries: C:\MassHunter\LIBRARY\NIST20.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
10	7.473	0.05	C:\MassHunter\LIBRARY\NIST20.L Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- Camphor	29373 29381 29042	000464-48-2 000464-48-2 000076-22-2	93 93 93
11	7.610	0.09	C:\MassHunter\LIBRARY\NIST20.L Cyclohexane, 1-methyl-4-(1-methylthylidene)- Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, (1.alpha.,3.alpha.,6.alpha.)- Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1.alpha.,3.beta.,6.alpha.)]-	19538 19560 19563	001124-27-2 018968-23-5 002778-68-9	93 92 70
12	8.362	19.93	C:\MassHunter\LIBRARY\NIST20.L dl-Menthol Levomenthol dl-Menthol	32850 32859 32851	000089-78-1 002216-51-5 000089-78-1	91 91 91
13	8.503	9.67	C:\MassHunter\LIBRARY\NIST20.L Levomenthol dl-Menthol dl-Menthol	32859 32851 32850	002216-51-5 000089-78-1 000089-78-1	91 91 91
14	8.717	4.87	C:\MassHunter\LIBRARY\NIST20.L dl-Menthol Cyclohexanol, 5-methyl-2-(1-methylethyl)- dl-Menthol	32850 32983 32851	000089-78-1 001490-04-6 000089-78-1	91 91 91
15	8.817	15.80	C:\MassHunter\LIBRARY\NIST20.L dl-Menthol Levomenthol dl-Menthol	32851 32859 32850	000089-78-1 002216-51-5 000089-78-1	91 91 91
16	10.339	0.01	C:\MassHunter\LIBRARY\NIST20.L Dehydroelsholtzia ketone 2,3-Dimethyltricyclo[2.2.1.02,6]heptane-3-carboxylic acid 2-(1-Hydroxybut-2-enylidene)cyclohexanone	39249 41300 41224	006138-88-1 000562-66-3 1000186-18-9	83 44 42
17	12.468	46.48	C:\MassHunter\LIBRARY\NIST20.L 4-Hydroxy-3-methylacetophenone 4-Hydroxy-3-methylacetophenone 2,5-Diethylphenol	28353 28357 27461	000876-02-8 000876-02-8 000876-20-0	70 70 68
18	12.620	0.19	C:\MassHunter\LIBRARY\NIST20.L 2-Methyl-6-propylphenol Phenol, 4-(1-methylpropyl)-	27487 27512	003520-52-3 000099-71-8	90 86

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Phenol, 2-(1-methylpropyl)-	27504	000089-72-5	80
19	12.852	0.02	C:\MassHunter\LIBRARY\NIST0.L			
			Phenol, 2-methyl-5-(1-methylethyl)	27579	000499-75-2	90
			3-Methyl-4-isopropylphenol	27496	003228-02-2	87
			Phenol, 2-methyl-5-(1-methylethyl)	27581	000499-75-2	87
20	13.018	0.04	C:\MassHunter\LIBRARY\NIST0.L			
			Phenol, 5-methyl-2-(1-methylethyl)	66733	000528-79-0	93
			-, acetate			
			Phenol, 2-ethyl-4,5-dimethyl-	27532	002219-78-5	76
			Phenol, 5-methyl-2-(1-methylethyl)	66732	000528-79-0	76
			-, acetate			
21	13.407	0.03	C:\MassHunter\LIBRARY\NIST0.L			
			3-tert-Butyl-2-hydroxybenzaldehyde	52595	024623-65-2	60
			6-tert-Butyl-2,4-dimethylphenol	52844	001879-09-0	58
			6-tert-Butyl-2,4-dimethylphenol	52840	001879-09-0	49
22	13.698	0.04	C:\MassHunter\LIBRARY\NIST0.L			
			2-Methoxybenzoic acid, allyl ester	66356	031994-79-3	74
			1-(2-Methyl-4-propoxy-phenyl)-etha	66674	1000187-58-2	70
			none			
			3-(2-Methoxy-5-methylphenyl)propio	68801	061371-44-6	70
			nic acid			
23	13.916	0.02	C:\MassHunter\LIBRARY\NIST0.L			
			Benzene, 1,2,4,5-tetraethyl-	64876	000635-81-4	91
			2-Acetyl-3-methylbenzo[b]thiophene	64489	018781-31-2	78
			2-Acetyl-4-methylbenzo(b)thiophene	64490	001467-88-5	60
24	14.095	0.02	C:\MassHunter\LIBRARY\NIST0.L			
			8,9-Dehydrothymol	26187	018612-99-2	96
			Benzene, 1-ethyl-3-(1-methylethyl)	26395	004920-99-4	76
			Benzene, 1-methoxy-2-(1-methylethe	26313	010278-02-1	74
			nyl)-			
25	14.519	0.04	C:\MassHunter\LIBRARY\NIST0.L			
			Caryophyllene	80121	000087-44-5	99
			Bicyclo[5.2.0]nonane, 2-methylene-	80294	242794-76-9	98
			4,8,8-trimethyl-4-vinyl-			
			Caryophyllene	80124	000087-44-5	96
26	14.638	0.02	C:\MassHunter\LIBRARY\NIST0.L			
			5-Methyl-2,4-diisopropylphenol	66876	040625-96-5	91
			5-Methyl-2,4-diisopropylphenol	66875	040625-96-5	87
			1,3-Benzodioxol-2-one, 5-(1,1-dime	66411	054815-21-3	76
			thylethyl)-			
27	14.762	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			(Z,Z)-.alpha.-Farnesene	80225	1000293-03-1	70
			Bicyclo[3.1.1]hept-2-ene, 2,6-dime	80319	017699-05-7	70
			thyl-6-(4-methyl-3-pentenyl)-			
			1,3,6,10-Dodecatetraene, 3,7,11-tr	80268	026560-14-5	70

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Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
imethyl-, (Z,E)-						
28	14.928	0.00	C:\MassHunter\LIBRARY\NIST0.L			
			Aromandendrene	80136	000489-39-4	55
			Benzamide, 3-methoxy-N-methyl-N-propyl-	83785	1000421-51-8	53
			Benzeneacetaldehyde, 2-methoxy-	28361	033567-59-8	50
29	15.139	0.02	C:\MassHunter\LIBRARY\NIST0.L			
			1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z-	80275	1000062-61-9	98
			Humulene	80087	006753-98-6	97
			Humulene	80088	006753-98-6	96
30	15.365	0.00	C:\MassHunter\LIBRARY\NIST0.L			
			Cycloheptasiloxane, tetradecamethyl-	340529	000107-50-6	64
			Cycloheptasiloxane, tetradecamethyl-	340530	000107-50-6	64
			Benzamide, 3-methoxy-N-[4-(1-methylcyclopropyl)phenyl]-	174740	1000351-11-1	46
31	15.454	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecyclodeca-1,6-diene	80314	317819-80-0	80
			Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-	80351	000483-75-0	52
			Naphthalene, decahydro-1,6-bis(methylene)-4-(1-methylethyl)-, (4.alpha.,4a.alpha.,8a.alpha.)-	80462	030021-46-6	51
32	15.681	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-, [4aR-(4a.alpha.,7.alpha.,8a.beta.)].beta.-Humulene	80481	017066-67-0	99
			Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-, [4aR-(4a.alpha.,7.alpha.,8a.beta.)]	80147	000116-04-1	97
			Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-, [4aR-(4a.alpha.,7.alpha.,8a.beta.)]	80473	017066-67-0	96
33	15.791	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethylidene)-, (4aR-trans)-	80431	000515-17-3	95
			1H-Cyclopropa[a]naphthalene, decahydro-1,1,3a-trimethyl-7-methylene-, [1aS-(1a.alpha.,3a.alpha.,7a.beta.,7b.alpha.)]-	80537	020071-49-2	91
			Spiro[5.5]undec-2-ene, 3,7,7-trimethyl-11-methylene-, (-)-	80303	018431-82-8	90
34	16.055	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			Aromandendrene	80135	000489-39-4	25
			1H-Pyrazol-5-amine, 3-methyl-1-phe	48232	001131-18-6	15

Library Search Report

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Unknown Spectrum: Apex
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PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			nyl- 4-(2-Hydroxyethyl)-5-oxo-3-phenyl- 2-pyrazoline	79534	010244-77-6	15
35	16.443	0.00	C:\MassHunter\LIBRARY\NIST0.L Cyclohexene, 4-[(1E)-1,5-dimethyl- 1,4-hexadien-1-yl]-1-methyl- Bicyclo[2.2.1]heptane, 7,7-dimethy 1-2-methylene- cis-.alpha.-Bisabolene	80317 18226 80218	025532-79-0 000471-84-1 029837-07-8	97 60 58
36	16.586	0.05	C:\MassHunter\LIBRARY\NIST0.L p-Cymene-2,5-diol Ethanone, 1-(2-hydroxy-6-methoxyph enyl)- Ethanone, 1-(2-hydroxy-6-methoxyph enyl)-	41078 42248 42256	002217-60-9 000703-23-1 000703-23-1	95 86 86
37	17.043	0.01	C:\MassHunter\LIBRARY\NIST0.L Caryophyllene oxide 2-((2R,4aR,8aS)-4a-Methyl-8-methyl enedecahydronaphthalen-2-yl)prop-2 -en-1-ol 1-Methyl-6-(3-methylbuta-1,3-dieny l)-7-oxabicyclo[4.1.0]heptane	99191 99331 52943	001139-30-6 000515-20-8 1000185-67-2	76 76 70
38	17.410	0.01	C:\MassHunter\LIBRARY\NIST0.L Tricyclo[4.4.1.0(1,6)]undecane 3-Methoxybenzyl alcohol 1H-3a,7-Methanoazulene, 2,3,6,7,8, 8a-hexahydro-1,4,9,9-tetramethyl-, (1.alpha.,3a.alpha.,7.alpha.,8a.b eta.)-	27751 19909 80506	006571-73-9 006971-51-3 000560-32-7	42 35 30
39	17.659	0.01	C:\MassHunter\LIBRARY\NIST0.L 1-Pyridin-3-yl-1,4-diazepane 6-Acetaminoflavanone Spiro[benzo-1,3-dioxolane-2,3'-pyr rolidine]	51755 174630 51711	223796-20-1 1000423-07-5 024476-94-6	38 38 18
40	17.986	0.00	C:\MassHunter\LIBRARY\NIST0.L .gamma.-Elemene .gamma.-Elemene .beta.-Humulene	80157 80148 80147	029873-99-2 029873-99-2 000116-04-1	64 64 59
41	18.174	0.00	C:\MassHunter\LIBRARY\NIST0.L 4-Hydroxy-3-methylacetophenone p-Cymen-7-ol Icosa-9,11-diyne	28353 27440 166403	000876-02-8 000536-60-7 028393-07-9	38 30 30
42	18.355	0.00	C:\MassHunter\LIBRARY\NIST0.L Levomenol .alpha.-Bisabolol (1S,2R,5R)-2-Methyl-5-((R)-6-methy	101922 101962 102057	023089-26-1 000515-69-5 058319-05-4	68 64 58

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PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			1hept-5-en-2-yl)bicyclo[3.1.0]hexa n-2-ol			
43	19.492	0.01	C:\MassHunter\LIBRARY\NIST0.L Tricyclo[3.3.1.1(3,7)]decane-1-met hanamine, N-(4-fluorophenyl)- Fumaric acid, 2-methoxyphenyl dode c-2-en-1-yl ester Succinic acid, dec-2-yl 3-methoxyp henyl ester	147143 294103 273512	1000337-10-7 1000405-94-1 1000390-98-5	58 43 43
44	20.064	0.01	C:\MassHunter\LIBRARY\NIST0.L Neophytadiene Bicyclo[3.1.1]heptane, 2,6,6-trime thyl- 3,7,11,15-Tetramethyl-2-hexadecen- 1-ol	171299 19511 194565	000504-96-1 000473-55-2 102608-53-7	99 50 46
45	20.341	0.00	C:\MassHunter\LIBRARY\NIST0.L 10.alpha.-Eremophilane Naphthalene, decahydro-1,8a-dimeth yl-7-(1-methylethyl)-, [1R-(1.alph a.,4a.beta.,7.beta.,8a.alpha.)]- Tricyclo[4.4.1.0(1,6)]undecane	85361 85389 27751	003242-05-5 015404-63-4 006571-73-9	38 38 30
46	20.553	0.00	C:\MassHunter\LIBRARY\NIST0.L 3-Chloropropionic acid, undec-2-en yl ester 2-Decylfuran cis-3-Methyl-endo-tricyclo[5.2.1.0 (2.6)]decane	148058 85239 27784	1000299-21-9 083469-85-6 1000215-29-0	58 38 30
47	21.579	0.01	C:\MassHunter\LIBRARY\NIST0.L n-Hexadecanoic acid n-Hexadecanoic acid n-Hexadecanoic acid	143510 143511 143507	000057-10-3 000057-10-3 000057-10-3	99 96 95
48	22.201	0.00	C:\MassHunter\LIBRARY\NIST0.L 1-[4-Acetyl-1-(2-amino-4,5-dimethy l-phenyl)-2,5-dimethyl-1H-pyrrol-3 -yl]-ethanone 4-Isopropylbenzenethiol, S-pentafl uoropropionyl- Flavone, 5-hydroxy-7,8-dimethoxy-	197109 195987 196657	1000300-66-6 1000353-28-9 003570-62-5	64 53 43
49	22.627	0.00	C:\MassHunter\LIBRARY\NIST0.L p-Acetophenetide, o-amino, N,N'-bi s-methyl O-Cresol, .alpha.,.alpha.'-(tetram ethylenedinitrilo)bis[6-methoxy- 7-Chloro-2,3-dihydrofuro(2,3-b)qui noline	101255 265622 81289	1000511-93-8 104978-24-7 064124-91-0	38 38 35
50	23.517	0.00	C:\MassHunter\LIBRARY\NIST0.L			

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			3-Amino-4,6-dimethylthieno[2,3-b]p yridine-2-carbonitrile	78573	052505-57-4	50
			Silane, diethylethoxy(2-methylpent -3-yloxy)-	113554	1000363-77-1	47
			Acetamide, N-(3-methylphenyl)- 2,2-trifluoro-	79271	1000307-30-9	47
51	24.291	0.02	C:\MassHunter\LIBRARY\NIST0.L Phytol	194551	000150-86-7	86
			Phytol	194548	000150-86-7	50
			4-Fluorobenzoic acid, 2-tetrahydro furylmethyl ester	103841	1000279-07-0	47
52	24.736	0.00	C:\MassHunter\LIBRARY\NIST0.L 9,12-Octadecadienoic acid (Z,Z)- 7-Pentadecyne	173583	000060-33-3	91
			1,8,11-Heptadecatriene, (Z,Z)-	85355	022089-89-0	86
				116386	056134-03-3	50
53	24.868	0.02	C:\MassHunter\LIBRARY\NIST0.L 9,12,15-Octadecatrien-1-ol, (Z,Z,Z)-	153474	000506-44-5	43
			Docosapentaenoic Acid methyl ester	253739	108698-02-8	38
			6,4'-Dimethoxy-3-hydroxyflavone	196652	093176-02-4	30
54	25.507	0.00	C:\MassHunter\LIBRARY\NIST0.L 9-Cyano-7,8-dimethyl-2-oxo-1H-2,3, 4,5-tetrahydropyrrolo[1,2-a]-1,3-d iazepine	78609	060138-29-6	46
			1-Phenyl-3-methyl-4-oximido-2-pyra zolin-5-one	78551	001080-89-3	38
			Bis(3,3,5,5-tetramethylcyclohexyl) diethylpyrophosphonate (isomer 2)	333579	1000510-34-6	38
55	26.445	0.05	C:\MassHunter\LIBRARY\NIST0.L Cannabidiol	181829	024274-48-4	99
			p-Heptylacetophenone	96751	037593-03-6	64
			Eupatoriachromene	96442	019013-03-7	59
56	26.865	0.04	C:\MassHunter\LIBRARY\NIST0.L 2-Methyl-6,7-methylenedioxy-4[1H]q uinolone	78653	1000227-48-2	64
			4-Hydrazino-6-pyridin-2-yl-[1,3,5] triazin-2-ylamine	79159	175204-69-0	64
			4H-Pyrazolo[3,4-b]pyrane-5-carboni trile, 6-amino-4-phenyl-3-propyl-	173183	300393-93-5	50
57	27.160	0.01	C:\MassHunter\LIBRARY\NIST0.L Phenanthrene, 1,2,3,4,4a,10a-hexah ydro-7-methoxy-1,1,4a-trimethyl-8- (1-methylethyl)-	197473	054833-49-7	55
			3-(2,5-Dimethylthiophen-3-yl)-2-(4 -methoxyphenyl)cyclopent-2-en-1-on	196958	1000444-65-9	38
			5-Isopentyl-6-methyl-2-(methylsulf anyl)-4-pyrimidinol, TMS derivativ	196253	1000297-98-3	38

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Data File : S678.D
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Sample : S-6, 7, 8
Misc :
ALS Vial : 7 Sample Multiplier: 1

Search Libraries: C:\MassHunter\LIBRARY\NIST0.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
58	27.388	0.00	C:\MassHunter\LIBRARY\NIST0.L 3-Chloro-8-methylthio-11H-indolo[3 ,2-c]quinoline 1,2,3-Trimethoxy-5-[2-(4-methoxyph enyl)ethynyl]benzene Bisphenol C, acetate	196451 197046 197221	155249-85-7 208347-68-6 1000462-16-1	38 38 27
59	27.572	0.01	C:\MassHunter\LIBRARY\NIST0.L 1H-4-Oxabenzo(f)cyclobut(cd)inden- 8-ol, 1a-.alpha.,2,3,3a,8b-.alpha. ,8c-.alpha.-hexahydro-1,1,3a-trime thyl-6-pentyl- Cannabichromene Cannabidiol	217712 217656 217644	021366-63-2 020675-51-8 013956-29-1	87 87 83
60	27.847	0.02	C:\MassHunter\LIBRARY\NIST0.L Dimethyl 2,4-quinolinedicarboxylat 2-Amino-4-(4-chlorophenyl)-7-hydro xy-4H-chromene-3-carbonitrile Pyrido[3,4-d]pyrimidin-4(3H)-one, 2,6,8-trimethyl-	129287 196449 63536	007170-24-3 1000468-82-0 022378-52-5	30 30 27
61	28.061	0.34	C:\MassHunter\LIBRARY\NIST0.L .delta.9-Tetrahydrocannabivarin 9-Oxabicyclo[4.3.0]non-6-en-8-one, 7-[2-methylenebicyclo[3.3.0]octan e-3,6-dione-1-yl]- 1-(2-Methoxyphenyl)-2,5-dihydro-1H -pyrrole-2,5-dione	181849 181622 78674	031262-37-0 1000160-28-9 017392-68-6	99 60 59
62	28.260	0.00	C:\MassHunter\LIBRARY\NIST0.L Indole, TMS derivative Benzeneethanol, .beta.-methoxy-.be ta.-(trifluoromethyl)-, (S)- Thiazole, 4-methyl-2-(phenylmethyl)-	63751 98144 63740	017983-42-5 052356-17-9 007210-74-4	43 43 43
63	28.358	0.01	C:\MassHunter\LIBRARY\NIST0.L 1H-4-Oxabenzo(f)cyclobut(cd)inden- 8-ol, 1a-.alpha.,2,3,3a,8b-.alpha. ,8c-.alpha.-hexahydro-1,1,3a-trime thyl-6-pentyl- 1H-4-Oxabenzo(f)cyclobut(cd)inden- 8-ol, 1a-.alpha.,2,3,3a,8b-.alpha. ,8c-.alpha.-hexahydro-1,1,3a-trime thyl-6-pentyl- Cannabidiol	217711 217712 217643	021366-63-2 021366-63-2 013956-29-1	70 70 62
64	28.479	0.01	C:\MassHunter\LIBRARY\NIST0.L 8-Acetyl-6-(4-nitrophenyl)-2,3-dih ydroindolizin-5(1H)-one 2,4-Dimethyl-6-(1-phenylethyl)phen ol, trimethylsilyl ether	196509 197268	1000482-06-5 1000462-25-6	80 80

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Search Libraries: C:\MassHunter\LIBRARY\NIST0.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			8-Acetyl-6-(3-nitrophenyl)-2,3-dihydroindolizin-5(1H)-one	196508	1000482-06-4	64
65	28.644	0.02	C:\MassHunter\LIBRARY\NIST0.L Cannabispiran	130823	061262-81-5	95
			6-(2-Methylbutyl)oxy-4-methylcoumarin	130830	1000395-87-1	64
			6-(Neopentyl)oxy-4-methylcoumarin	130829	1000395-92-4	64
66	28.844	0.09	C:\MassHunter\LIBRARY\NIST0.L 6H-Dibenzo[b,d]pyran-1-ol, 6,6,9-trimethyl-3-propyl-1H-Trindene, 2,3,4,5,6,7,8,9-octahydro-1,1,4,4,7,7-hexamethyl-6-Aminonicotinic acid,N,O di-TMS	176320	033745-21-0	94
				176422	040650-56-4	72
				175212	1000472-37-7	72
67	29.141	0.00	C:\MassHunter\LIBRARY\NIST0.L 2-Ethylhydroquinone, bis(trimethylsilyl) ether	175513	1000463-15-0	70
			9-Ethyl-N-(trimethylsilyl)-9H-carbazol-3-amine	176078	1000473-81-1	70
			9-Ethyl-N-(trimethylsilyl)-9H-carbazol-3-amine	176077	1000473-81-1	70
68	29.256	0.00	C:\MassHunter\LIBRARY\NIST0.L 2-(4-Methoxyphenyl)-6-methyl-1-(pyridin-3-yl)indole	217620	1000435-25-2	52
			Pyrene, 1,6-bis(1,1-dimethylethyl)-2-Nitrofluorenone, 4-methylphenylamine	217751	055044-29-6	45
				217542	111796-34-0	43
69	29.440	0.13	C:\MassHunter\LIBRARY\NIST0.L Cannabidiol	217645	013956-29-1	99
			Cannabidiol	217646	013956-29-1	98
			Cannabidiol	217639	013956-29-1	98
70	29.623	0.18	C:\MassHunter\LIBRARY\NIST0.L Cannabichromene	217655	020675-51-8	97
			Cannabichromene	217657	020675-51-8	96
			Cannabichromene	217653	020675-51-8	95
71	29.926	0.02	C:\MassHunter\LIBRARY\NIST0.L Pregn-17(20)-en-16-one, (5.alpha., 17Z)-4a(2H)-Phenanthrenecarboxaldehyde, 1,3,4,9,10a-hexahydro-6-methoxy-1,1-dimethyl-7-(1-methylethyl)-, (4aR-trans)-Morphinan-6-one, 4,5-epoxy-2-hydroxy-N-methyl-, (5.alpha.)-	200066	054548-12-8	64
				217710	057397-33-8	60
				180164	076786-92-0	46
72	30.171	0.01	C:\MassHunter\LIBRARY\NIST0.L exo-THC	217632	027179-28-8	64
			.DELTA.8-Tetrahydrocannabinol	217676	005957-75-5	45

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Search Libraries: C:\MassHunter\LIBRARY\NIST0.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Benz[b]-1,4-oxazepine-4(5H)-thione , 2,3-dihydro-2,8-dimethyl-	83671	1000258-63-4	44
73	30.366	0.00	C:\MassHunter\LIBRARY\NIST0.L Cannabidiol	217640	013956-29-1	41
			Ethyl 5-(4-methylphenyl)-1,3-oxazo le-2-carboxylate	112607	033115-91-2	41
			Cannabidiol	217641	013956-29-1	41
74	30.574	0.63	C:\MassHunter\LIBRARY\NIST0.L Dronabinol	217638	001972-08-3	99
			Dronabinol	217637	001972-08-3	99
			Dronabinol	217635	001972-08-3	99
75	30.877	0.01	C:\MassHunter\LIBRARY\NIST0.L 4-((Bis(trimethylsilyl)amino)methy l)-N-(trimethylsilyl)benzenesulfon amide	303288	1000485-72-1	38
			Silane, diethylheptadecyloxy(2-met hoxyethoxy)-	311456	1000363-54-6	38
			Skullcapflavone II, dimethyl ether	303499	074670-18-1	32
76	31.192	0.17	C:\MassHunter\LIBRARY\NIST0.L Cannabinol	212244	000521-35-7	99
			Cannabinol	212246	000521-35-7	98
			Cannabinol	212247	000521-35-7	97
77	31.495	0.01	C:\MassHunter\LIBRARY\NIST0.L 3-Bromo-5,6,7,8-tetrahydro-1,6-nap hthyridine, N-trifluoroacetyl-	208480	1000506-47-2	56
			7-Ethoxy-3-(4-methoxyphenyl)-4-met hylcoumarin	211972	263364-88-1	52
			2-Propanone, 1-phenyl-1-(5-phenyl- 3H-1,2-dithiol-3-ylidene)-	211733	038489-98-4	49
78	31.772	0.00	C:\MassHunter\LIBRARY\NIST0.L Tetrasiloxane, decamethyl-	210888	000141-62-8	43
			N-(3-Phenylpropyl)pyridine-3-carbo xamide, TMS derivative	214408	1000510-98-3	38
			N-(2-Hydroxyethyl)pyridine-3-carbo xamide, 2TMS derivative	211233	1000485-24-9	38
79	31.968	0.01	C:\MassHunter\LIBRARY\NIST0.L 4-(2,4-Dichlorophenyl)-5-methyl-2- thiazolamine, TMS	235995	1000512-01-0	60
			4-Ethoxy-N-(3,4,5-trimethoxybenzyl idene)aniline	218497	158319-78-9	25
			Benzo[f]quinolin-3(2H)-one, 1,4-di hydro-1-(4-isopropylphenyl)-	218758	1000272-51-8	25
80	32.076	0.01	C:\MassHunter\LIBRARY\NIST0.L Anthracene, 1,2,3,4,5,6,7,8-octahy dro-1,1,4,4,5,5,8,8-octamethyl- Spiro[2,5-cyclohexadiene-1,7'(1'H)	197476	022306-30-5	38
				177365	002241-43-2	35

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PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			-cyclopent[ij]isoquinolin]-4-one, 2',3',8',8'a-tetrahydro-5'-hydroxy -6'-methoxy-, (R)- Ethoxy(phenyl)silanediol, 2TMS	233553	1000496-86-0	25
81	32.236	0.01	C:\MassHunter\LIBRARY\NIST0.L 6-Hydroxyflavone, trimethylsilyl ether 7-Hydroxyflavone, trimethylsilyl ether 6-Hydroxyflavone, trimethylsilyl ether	211811 211814 211806	1000454-60-4 039273-05-7 1000454-60-4	78 78 78
82	32.337	0.01	C:\MassHunter\LIBRARY\NIST0.L Eicosane Heneicosane Heptacosane	176384 194590 287976	000112-95-8 000629-94-7 000593-49-7	97 93 91
83	32.939	0.00	C:\MassHunter\LIBRARY\NIST0.L 2-Methyl-7-phenylindole Arsenous acid, tris(trimethylsilyl) ester 1,2-Benzisothiazol-3-amine, TBDMS derivative	84013 251605 152650	001140-08-5 055429-29-3 1000332-57-2	43 38 38
84	33.214	0.00	C:\MassHunter\LIBRARY\NIST0.L Tetrasiloxane, decamethyl- Methyltris(trimethylsiloxy)silane 2-Methyl-7-phenylindole	210886 210890 84013	000141-62-8 017928-28-8 001140-08-5	47 47 46
85	33.724	0.01	C:\MassHunter\LIBRARY\NIST0.L 2-Propanesulfonamide, N-[2-(4'-cya no[1,1'-biphenyl]-4-yl)propyl]- 9,10-Methanoanthracen-11-ol, 9,10- dihydro-9,10,11-trimethyl- 2-Bromo-4,5-dimethoxycinnamic acid	250811 136133 180502	211311-95-4 126615-74-5 051314-72-8	45 41 38
86	33.830	0.00	C:\MassHunter\LIBRARY\NIST0.L (E)-3-(3,4-Dimethoxyphenyl)prop-2- enamide 1,1,1,3,5,5,5-Heptamethyltrisiloxa ne Indolizine, 2-(4-methylphenyl)-	83611 102314 84034	130973-10-3 001873-88-7 007496-81-3	35 35 30
87	33.924	0.03	C:\MassHunter\LIBRARY\NIST0.L Eicosane Octadecane Pentacosane	176384 141057 262013	000112-95-8 000593-45-3 000629-99-2	97 97 93
88	34.890	0.02	C:\MassHunter\LIBRARY\NIST0.L Cyclotrisiloxane, hexamethyl- Methyltris(trimethylsiloxy)silane Cyclotrisiloxane, hexamethyl-	102257 210890 102259	000541-05-9 017928-28-8 000541-05-9	46 43 43

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Data File : S678.D
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ALS Vial : 7 Sample Multiplier: 1

Search Libraries: C:\MassHunter\LIBRARY\NIST0.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
89	35.351	0.03	C:\MassHunter\LIBRARY\NIST0.L Arsenous acid, tris(trimethylsilyl)) ester	251605	055429-29-3	52
			Cyclotrisiloxane, hexamethyl-	102257	000541-05-9	50
			Ethoxy(phenyl)silanediol, 2TMS	233553	1000496-86-0	50
90	35.854	0.01	C:\MassHunter\LIBRARY\NIST0.L Tetrasiloxane, decamethyl-	210888	000141-62-8	59
			Cyclotrisiloxane, hexamethyl-	102257	000541-05-9	58
			Arsenous acid, tris(trimethylsilyl)) ester	251605	055429-29-3	58
91	36.045	0.00	C:\MassHunter\LIBRARY\NIST0.L Cyclotrisiloxane, hexamethyl-	102257	000541-05-9	58
			1,1,1,3,5,5,5-Heptamethyltrisiloxa ne	102314	001873-88-7	50
			Arsenous acid, tris(trimethylsilyl)) ester	251605	055429-29-3	50
92	36.251	0.01	C:\MassHunter\LIBRARY\NIST0.L Tetrasiloxane, decamethyl-	210888	000141-62-8	47
			Cyclotrisiloxane, hexamethyl-	102257	000541-05-9	46
			Arsenous acid, tris(trimethylsilyl)) ester	251605	055429-29-3	46
93	36.481	0.00	C:\MassHunter\LIBRARY\NIST0.L Cyclotrisiloxane, hexamethyl-	102257	000541-05-9	52
			Arsenous acid, tris(trimethylsilyl)) ester	251605	055429-29-3	52
			Tris(tert-butyl dimethylsilyloxy)ar sane	330994	1000366-57-5	50
94	37.047	0.02	C:\MassHunter\LIBRARY\NIST0.L .gamma.-Sitosterol	310597	000083-47-6	91
			.beta.-Sitosterol	310596	000083-46-5	53
			.gamma.-Sitosterol	310598	000083-47-6	53
95	37.446	0.01	C:\MassHunter\LIBRARY\NIST0.L 2-Methyl-7-phenylindole	84013	001140-08-5	46
			Benzo[h]quinoline, 2,4-dimethyl-	84038	000605-67-4	43
			Tris(tert-butyl dimethylsilyloxy)ar sane	330994	1000366-57-5	43
96	37.944	0.01	C:\MassHunter\LIBRARY\NIST0.L 5-Ethyl 11a-methyl (5S,11aS)-6,11- dihydro-3H-indolizino[6,7-b]indole -5,11a(5H)-dicarboxylate	248337	1000484-03-0	56
			1-(3,5-Di-tert-butyl-2,6-dihydroxy phenyl)ethanone	153209	1000443-79-6	47
			4-tert-Octylphenol, TMS derivative	171116	078721-87-6	43
97	38.406	0.01	C:\MassHunter\LIBRARY\NIST0.L Tris(tert-butyl dimethylsilyloxy)ar sane	330994	1000366-57-5	46

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Tetrasiloxane, decamethyl-	210888	000141-62-8	43
			Octylsilanetriol, 3TMS	306483	1000496-84-7	43
98	38.695	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			Arsenous acid, tris(trimethylsilyl	251605	055429-29-3	49
			) ester			
			4-Methyl-2-trimethylsilyloxy-aceto	101293	097389-70-3	49
			phenone			
			1H-Indole, 1-methyl-2-phenyl-	84028	003558-24-5	47
99	38.949	0.01	C:\MassHunter\LIBRARY\NIST0.L			
			Tris(tert-butyldimethylsilyloxy)ar	330994	1000366-57-5	53
			sane			
			Arsenous acid, tris(trimethylsilyl	251605	055429-29-3	52
			) ester			
			Cyclotrisiloxane, hexamethyl-	102259	000541-05-9	50
100	39.659	0.00	C:\MassHunter\LIBRARY\NIST0.L			
			Tetrasiloxane, decamethyl-	210888	000141-62-8	50
			Arsenous acid, tris(trimethylsilyl	251605	055429-29-3	49
			) ester			
			Cyclotrisiloxane, hexamethyl-	102257	000541-05-9	49