

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041321\
 Data File : BG048687.D
 Acq On : 13 Apr 2021 23:44
 Operator : CG/JU
 Sample : M2020-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 105-SB-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.630	384	390	397	rBV	222985	340120	29.31%	6.931%
2	7.240	657	664	676	rVB2	223263	389060	33.53%	7.928%
3	8.080	801	807	814	rVB2	58535	97896	8.44%	1.995%
4	9.250	998	1006	1013	rBV	136030	247469	21.32%	5.043%
5	10.907	1280	1288	1295	rBV	74519	131058	11.29%	2.671%
6	13.357	1696	1705	1712	rBV	379148	561510	48.39%	11.442%
7	14.179	1838	1845	1852	rBV2	11655	17993	1.55%	0.367%
8	14.737	1934	1940	1948	rVB	129334	197111	16.99%	4.017%
9	16.230	2187	2194	2202	rBV	384531	586078	50.50%	11.943%
10	17.493	2403	2409	2415	rBV	190399	287878	24.81%	5.866%
11	18.374	2554	2559	2565	rBV3	23947	34597	2.98%	0.705%
12	20.102	2847	2853	2858	rBV	914236	1160468	100.00%	23.648%
13	20.742	2957	2962	2966	rBV5	12823	19554	1.69%	0.398%
14	21.406	3071	3075	3085	rBV4	48290	86271	7.43%	1.758%
15	21.788	3131	3140	3150	rBV	209194	361756	31.17%	7.372%
16	23.515	3429	3434	3442	rVB5	21102	42615	3.67%	0.868%
17	25.125	3698	3708	3719	rVB2	113555	334082	28.79%	6.808%
18	26.335	3908	3914	3919	rBV6	5857	11723	1.01%	0.239%

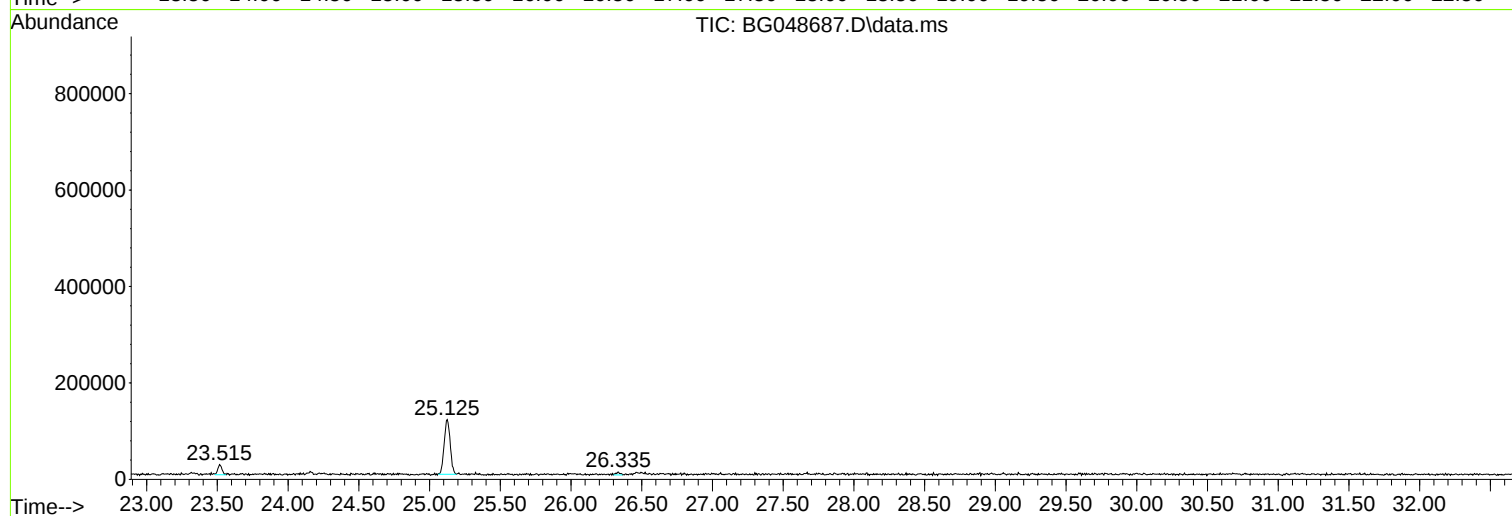
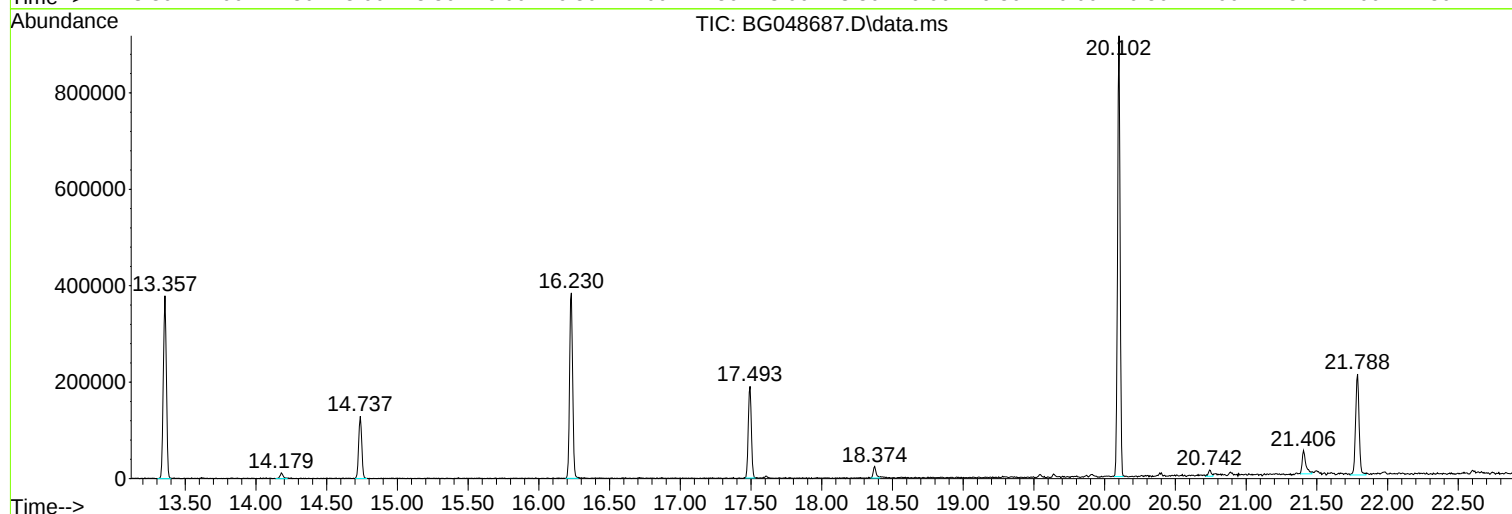
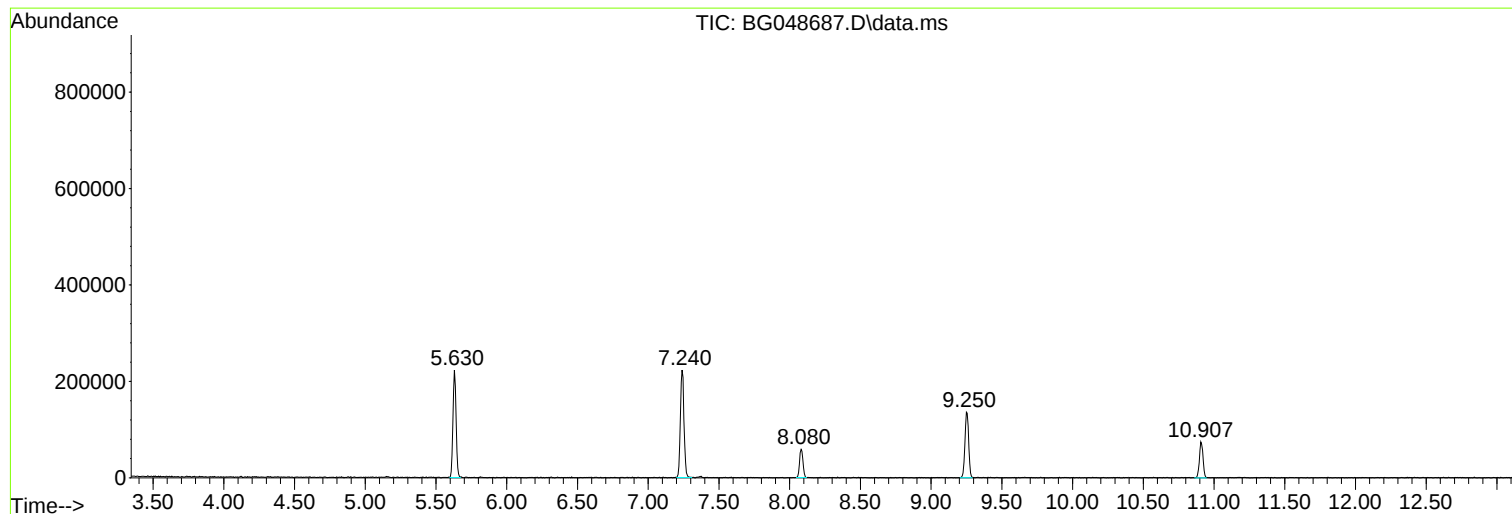
Sum of corrected areas: 4907239

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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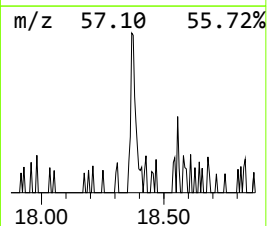
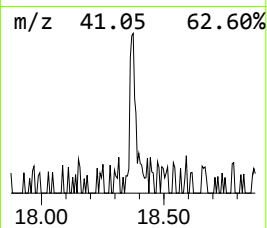
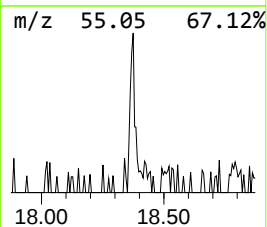
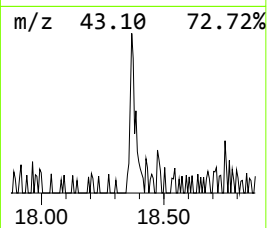
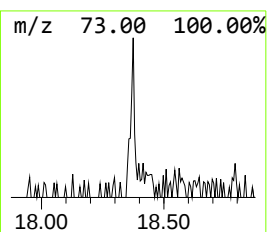
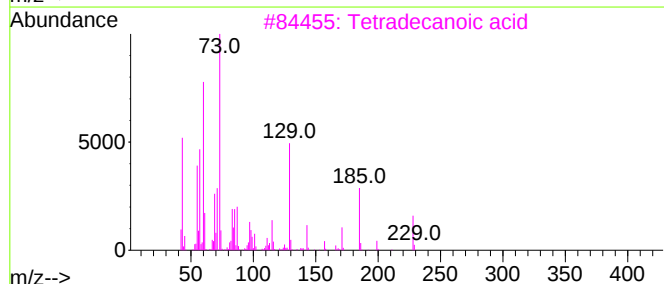
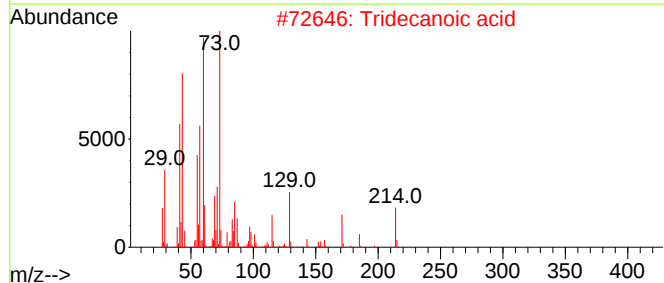
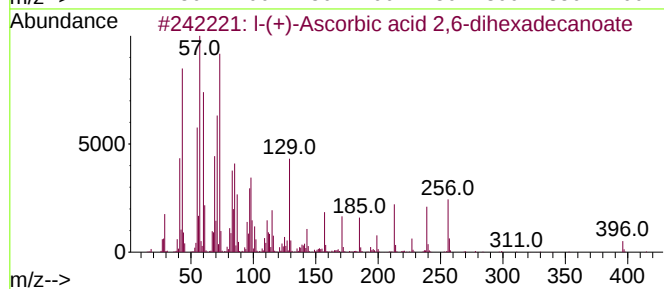
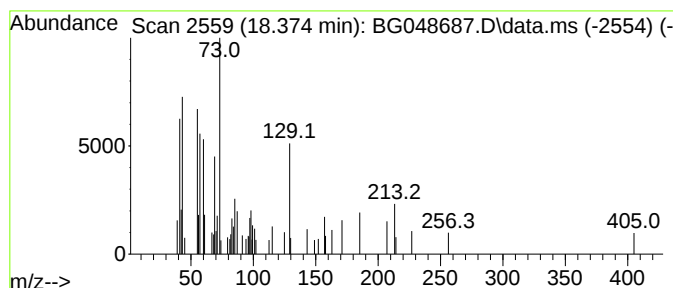
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-(+)-Ascorbic acid 2,6-dih... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.374	2.40 ng	34597	Phenanthrene-d10	17.493	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	58
2	Tridecanoic acid	214	C13H26O2	000638-53-9	52
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	35
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	27



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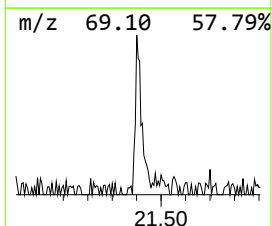
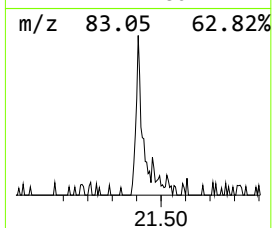
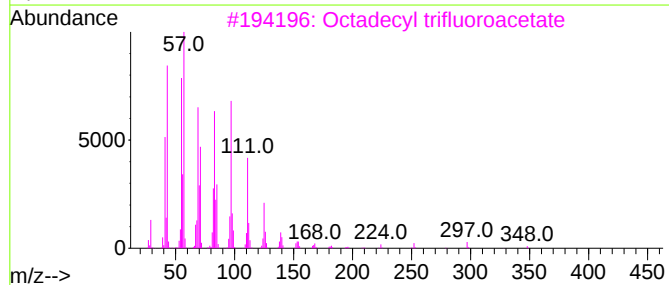
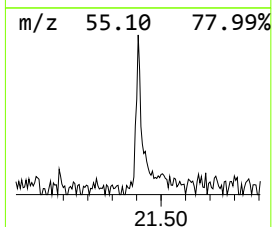
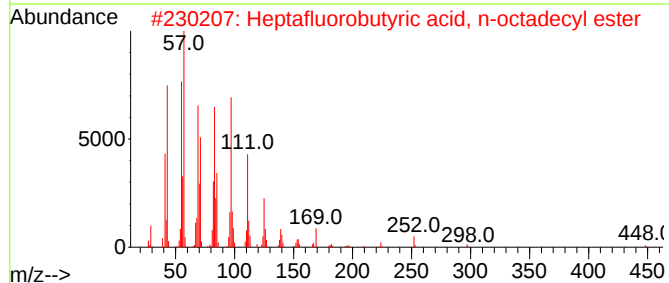
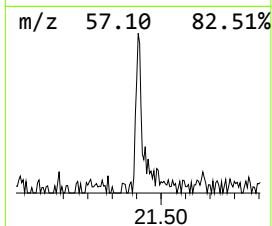
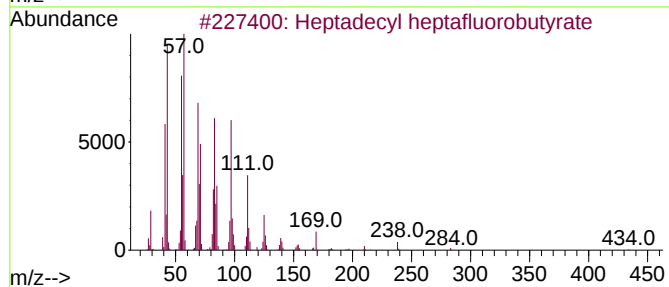
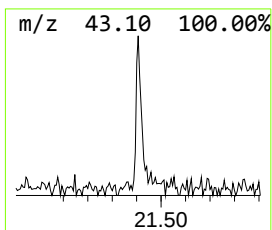
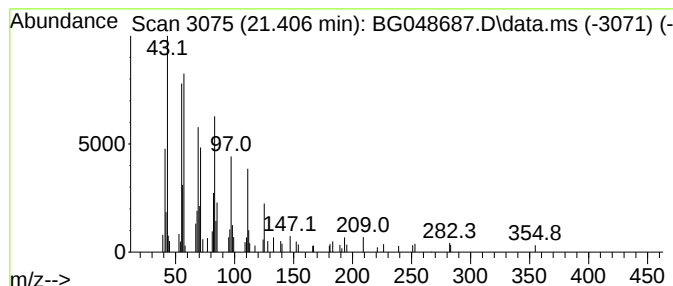
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Peak Number 2 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.406	4.77 ng	86271	Chrysene-d12	21.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	83
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83
4			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	83
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	80



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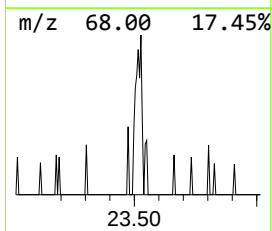
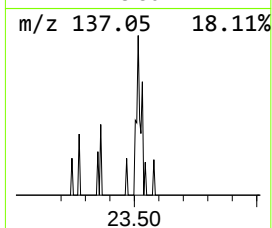
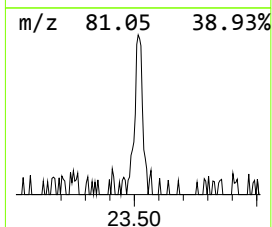
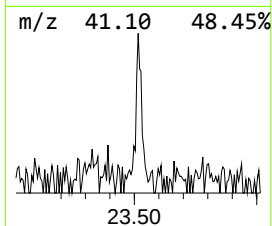
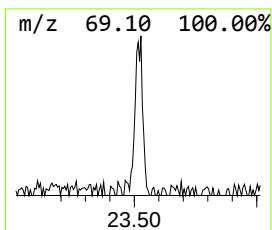
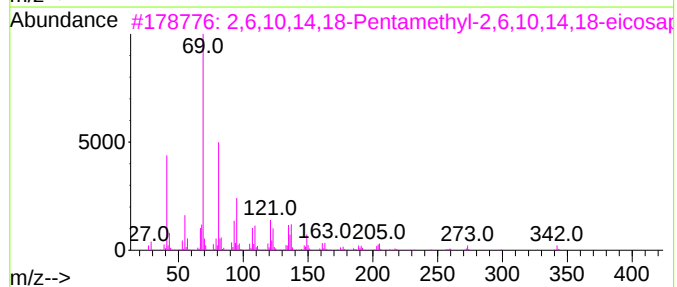
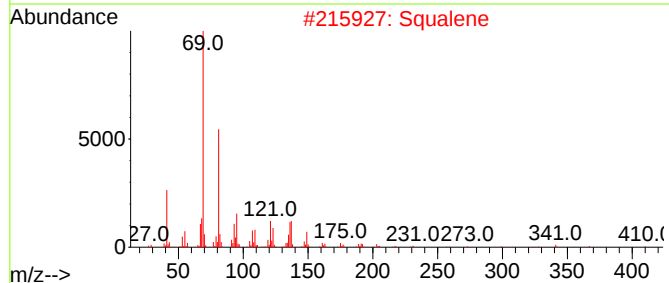
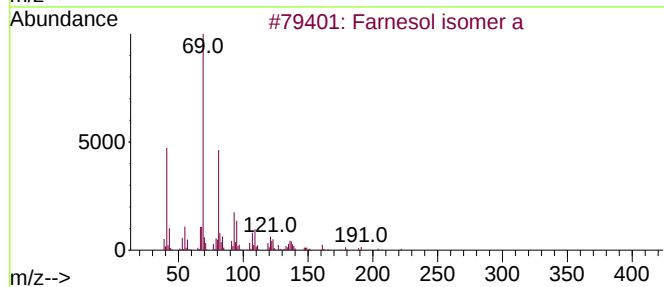
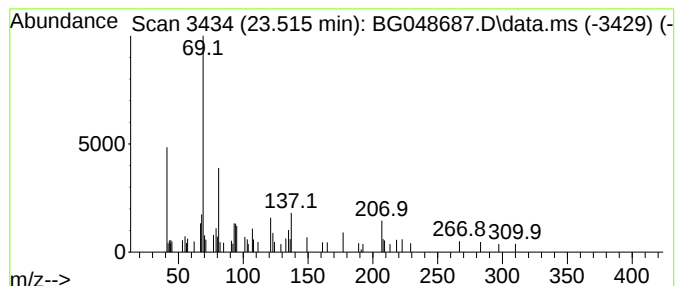
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Peak Number 3 Farnesol isomer a Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.515	2.55 ng	42615	Perylene-d12	25.125

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesol isomer a	222	C15H26O	1000108-92-4	60
2			Squalene	410	C30H50	000111-02-4	53
3			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	50
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	50
5			trans-Farnesol	222	C15H26O	000106-28-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-(+)-Ascorbic ...	18.374	2.4	ng	34597	4	17.493	287878	20.0
Heptadecyl hept...	21.406	4.8	ng	86271	5	21.788	361756	20.0
Farnesol isomer a	23.515	2.5	ng	42615	6	25.125	334082	20.0