

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
 Data File : BF129998.D
 Acq On : 25 Aug 2022 14:26
 Operator : CG\JU
 Sample : N4353-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3-4-COMP-2

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_F\Methods\8270-BF081422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.992	456	460	482	rBV	432436	726361	13.53%	2.209%
2	5.404	526	530	554	rBV	4477759	4254424	79.23%	12.940%
3	5.775	590	593	601	rBV	56172	55458	1.03%	0.169%
4	6.416	698	702	705	rBV	3917922	4136504	77.03%	12.581%
5	6.751	756	759	769	rVB	902070	806251	15.01%	2.452%
6	7.328	852	857	860	rBV	2834113	2753033	51.27%	8.373%
7	8.033	973	977	983	rBV	1188524	1091999	20.34%	3.321%
8	9.110	1154	1160	1163	rBV	5516402	5138997	95.70%	15.630%
9	9.786	1271	1275	1279	rBV	1430429	1241714	23.12%	3.777%
10	10.586	1407	1411	1414	rBV	3830416	3374992	62.85%	10.265%
11	11.280	1525	1529	1533	rBV	1478751	1255616	23.38%	3.819%
12	11.798	1611	1617	1629	rBV2	94860	124966	2.33%	0.380%
13	12.863	1794	1798	1802	rBV	5288838	5369833	100.00%	16.332%
14	13.745	1945	1948	1952	rBV	65519	57104	1.06%	0.174%
15	13.827	1954	1962	1970	rBV7	37610	142549	2.65%	0.434%
16	13.927	1975	1979	1988	rVV	1155970	1079051	20.09%	3.282%
17	14.010	1988	1993	1998	rVV	79539	89986	1.68%	0.274%
18	14.062	1998	2002	2005	rVB	78606	72746	1.35%	0.221%
19	14.362	2050	2053	2058	rVB	84404	74463	1.39%	0.226%
20	14.662	2100	2104	2107	rBV	66434	64408	1.20%	0.196%
21	14.733	2112	2116	2119	rVB	107952	97754	1.82%	0.297%
22	14.980	2154	2158	2162	rBV	51025	57837	1.08%	0.176%
23	15.374	2221	2225	2234	rVB	623068	812751	15.14%	2.472%

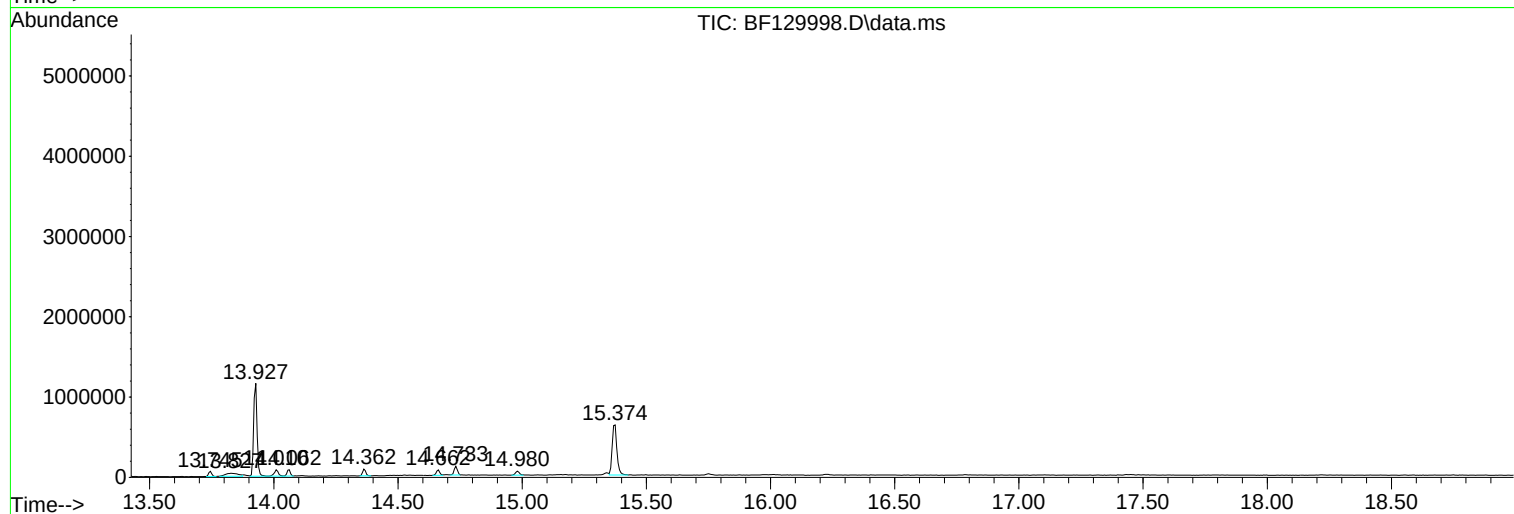
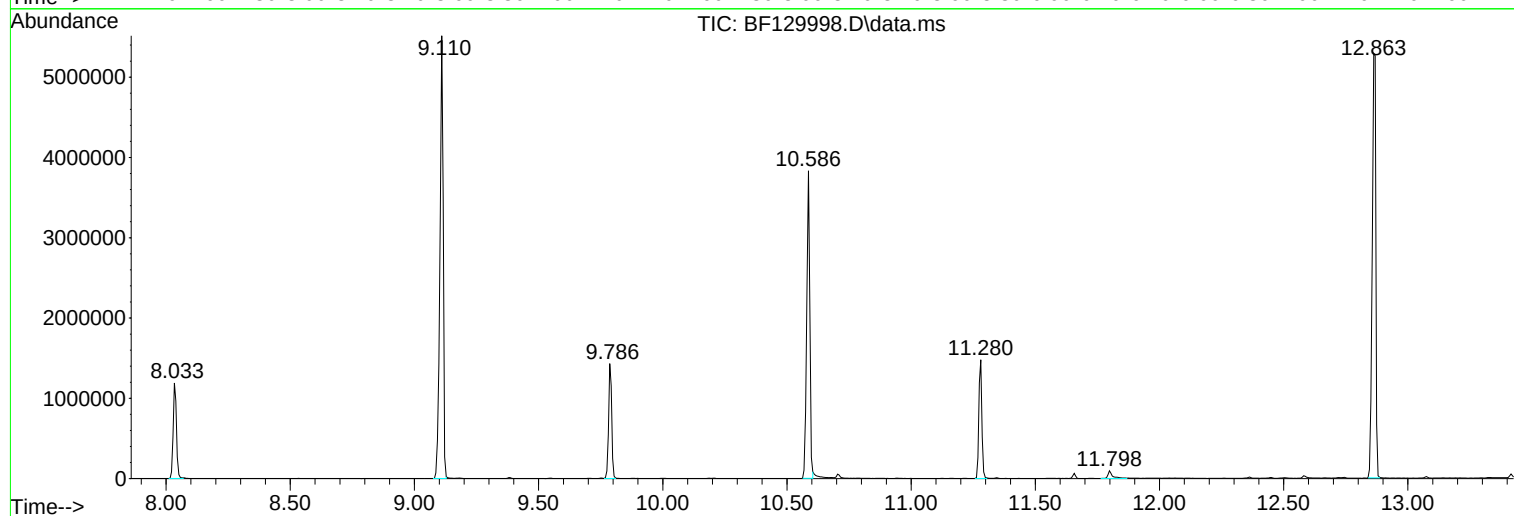
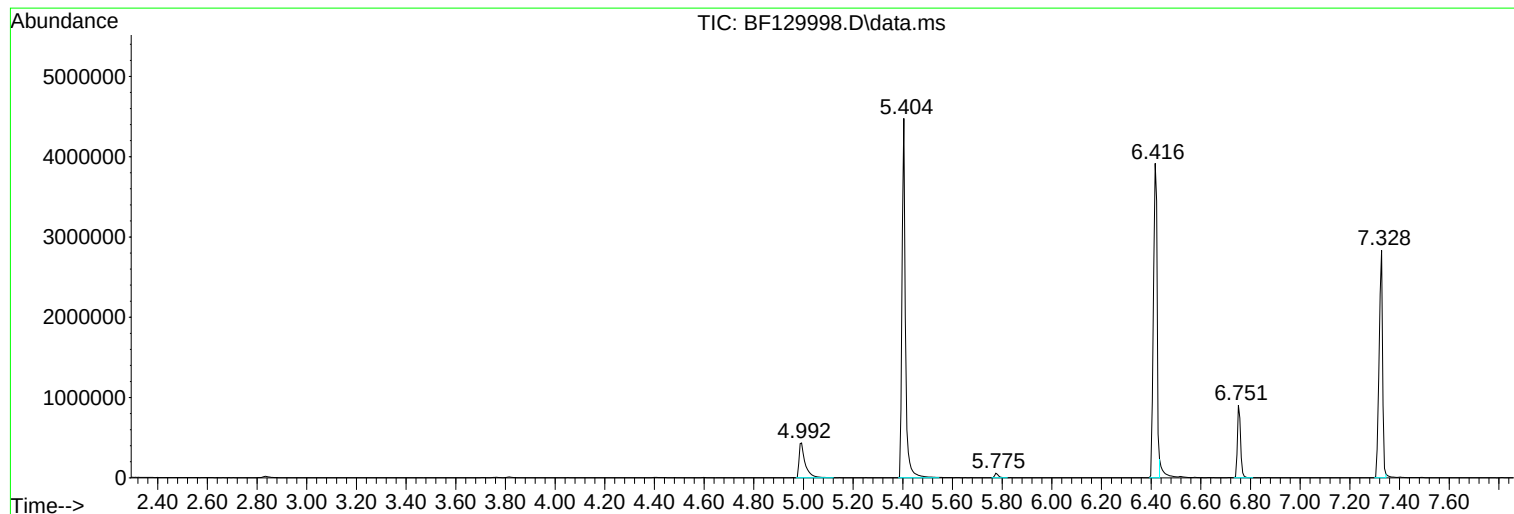
Sum of corrected areas: 32878797

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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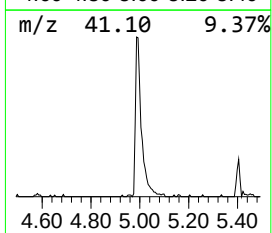
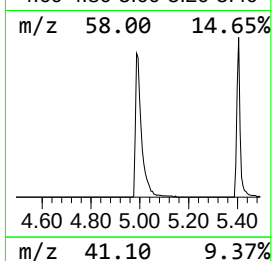
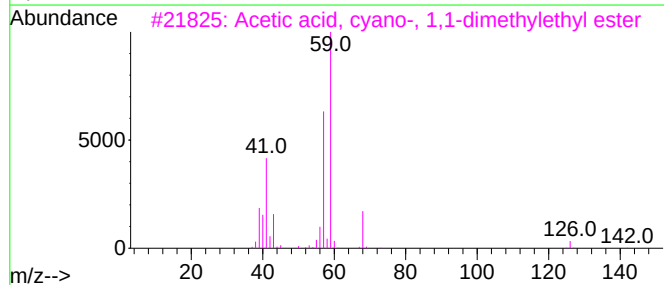
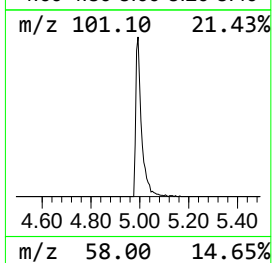
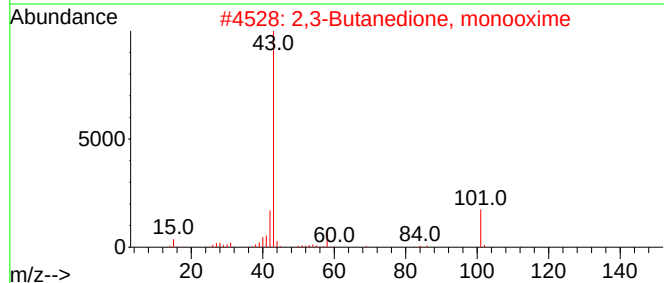
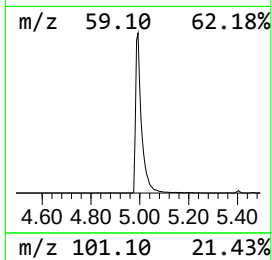
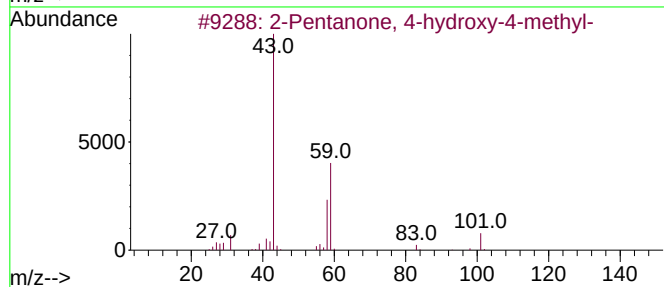
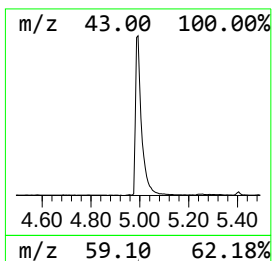
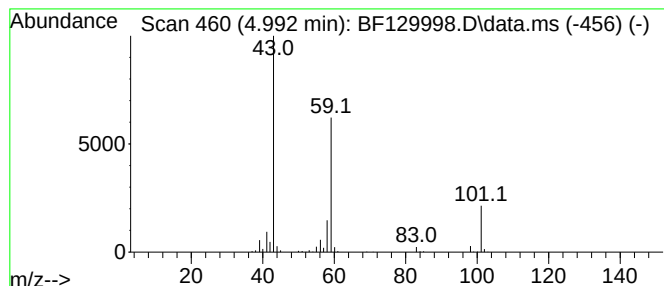
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	18.02 ng	726361	1,4-Dichlorobenzene-d4	6.751

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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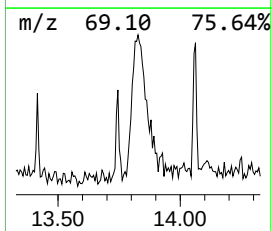
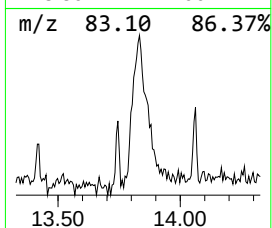
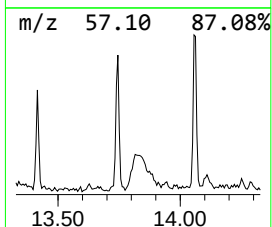
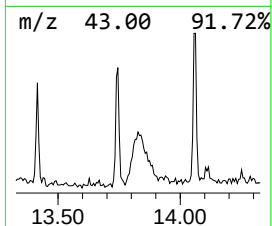
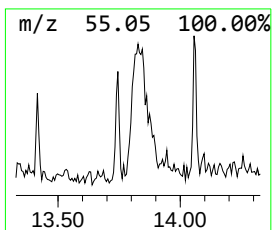
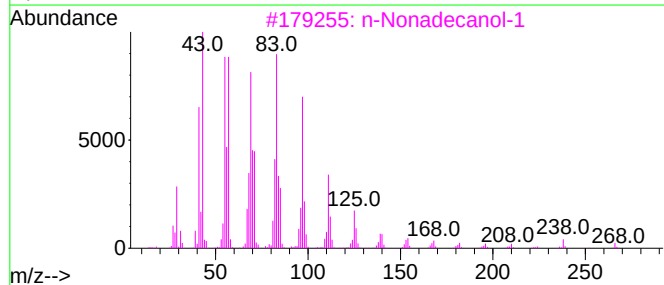
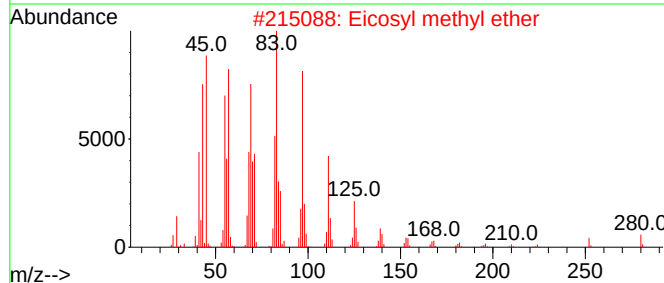
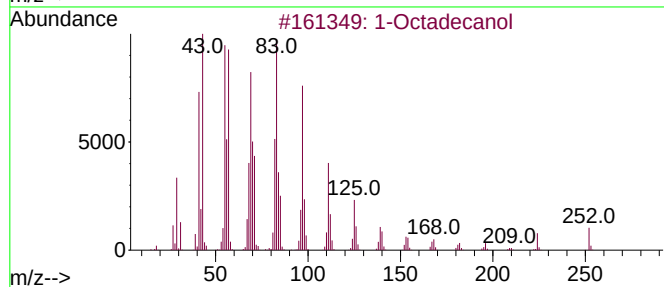
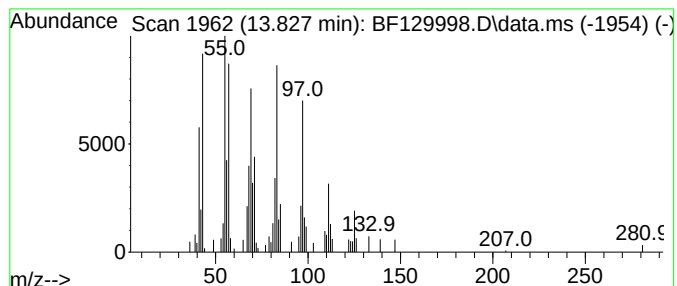
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Peak Number 2 1-Octadecanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	2.64 ng	142549	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	91
2			Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87



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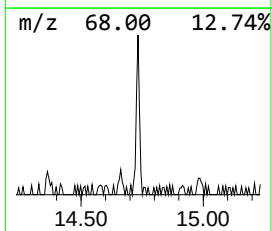
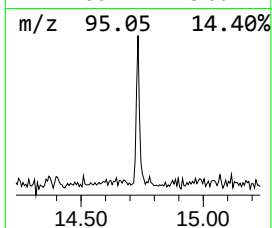
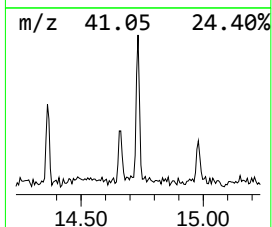
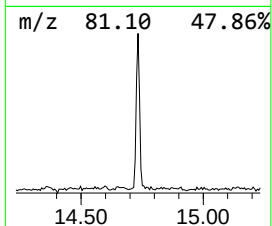
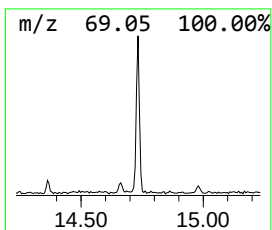
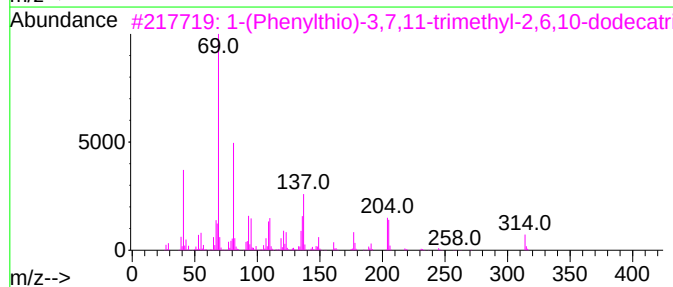
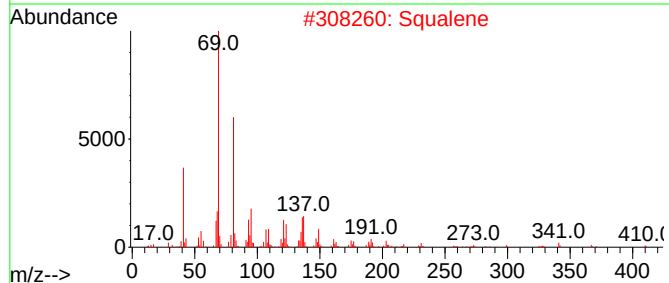
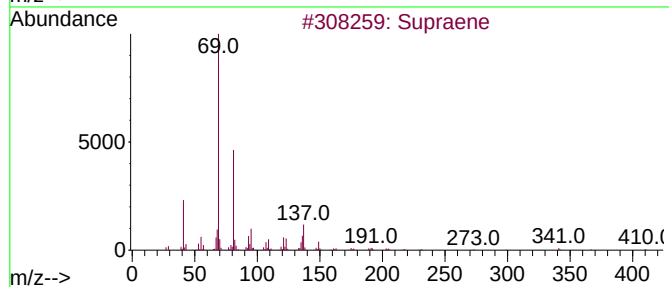
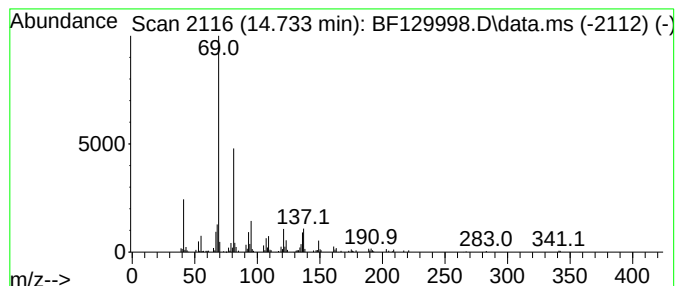
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Peak Number 3 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	2.41 ng	97754	Perylene-d12	15.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	83
3			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.992	18.0	ng	726361	1	6.751	806251	20.0
1-Octadecanol	13.827	2.6	ng	142549	5	13.927	1079050	20.0
Supraene	14.733	2.4	ng	97754	6	15.374	812751	20.0