

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101218\
 Data File : BF109867.D
 Acq On : 13 Oct 2018 6:53
 Operator : JU/SJ
 Sample : J5444-10
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101018-DBRI-F-U-S

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-BF100818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	473	476	490	rBV	66672	94751	2.62%	0.517%
2	5.310	545	548	567	rBV	506056	720452	19.90%	3.933%
3	6.339	720	723	740	rBV	282072	537944	14.86%	2.936%
4	6.463	740	744	769	rVV	1609665	1757646	48.55%	9.594%
5	6.692	780	783	805	rBV	420467	583258	16.11%	3.184%
6	6.851	805	810	831	rBV	2382603	2530475	69.90%	13.812%
7	7.263	875	880	913	rBV	1570399	2147799	59.33%	11.724%
8	7.975	997	1001	1028	rBV	534231	727698	20.10%	3.972%
9	9.051	1179	1184	1203	rBV	3431842	3619931	100.00%	19.759%
10	9.722	1294	1298	1312	rBV	699388	727151	20.09%	3.969%
11	10.504	1428	1431	1451	rBV	789507	1091943	30.16%	5.960%
12	11.198	1546	1549	1571	rBV	367561	562792	15.55%	3.072%
13	12.780	1814	1818	1839	rBV	2185576	2233021	61.69%	12.189%
14	13.827	1992	1996	2014	rBV	391395	506491	13.99%	2.765%
15	14.657	2134	2137	2141	rBV	57729	60411	1.67%	0.330%
16	15.227	2230	2234	2251	rBV	222768	418483	11.56%	2.284%

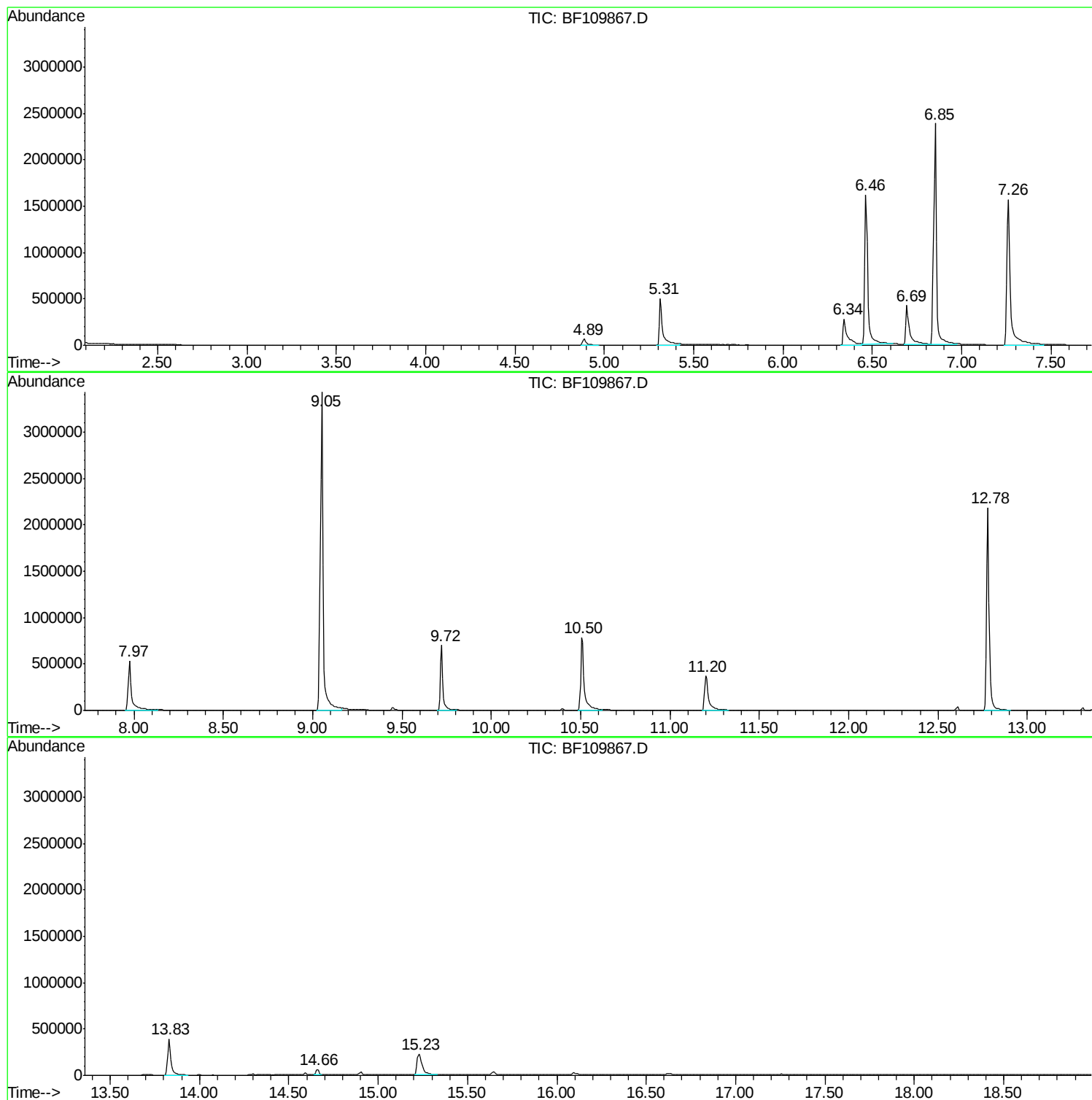
Sum of corrected areas: 18320246

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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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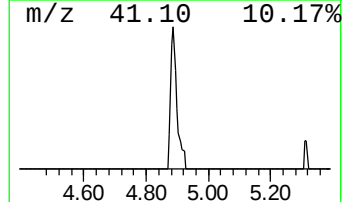
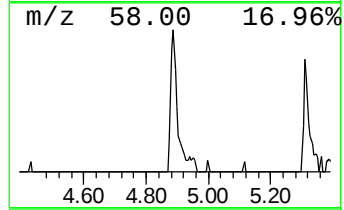
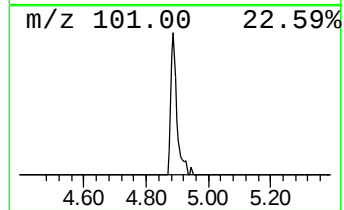
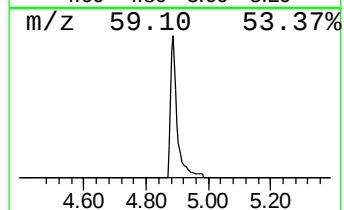
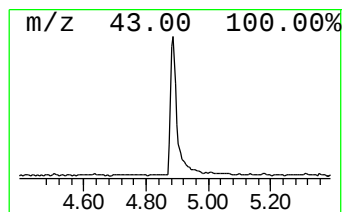
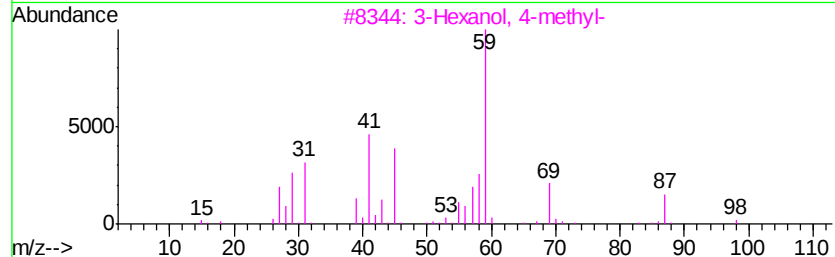
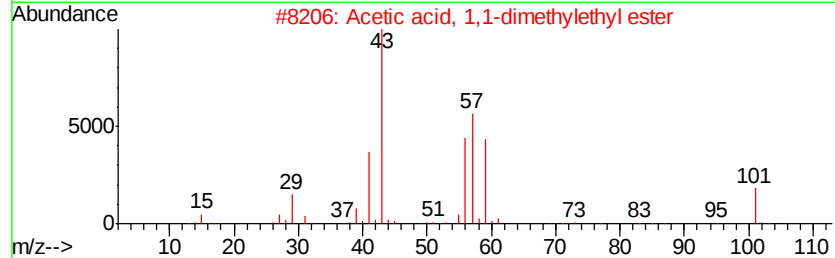
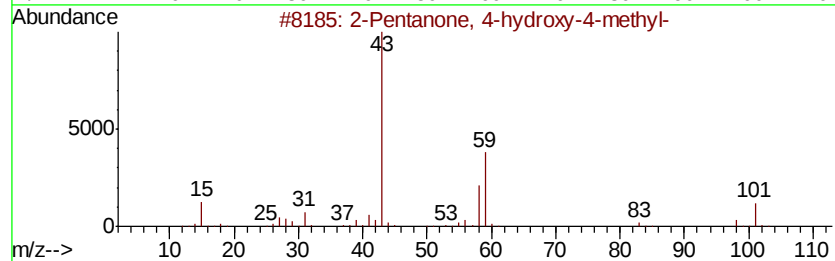
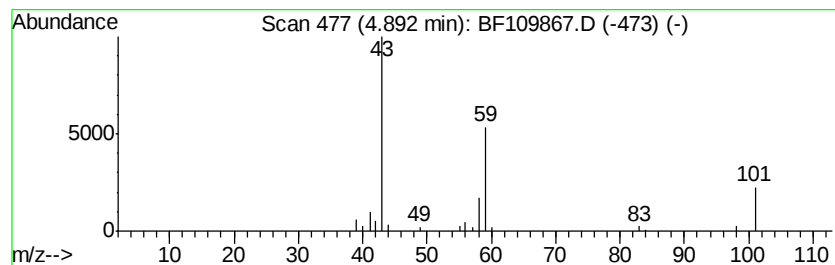
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.25 ng	94751	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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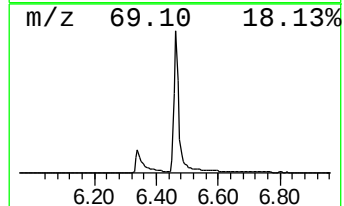
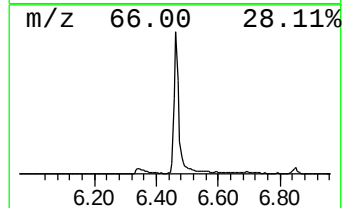
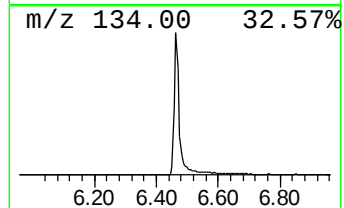
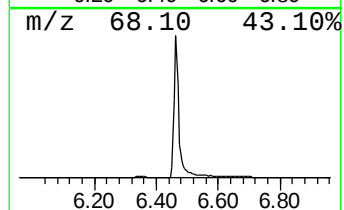
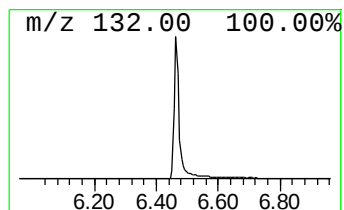
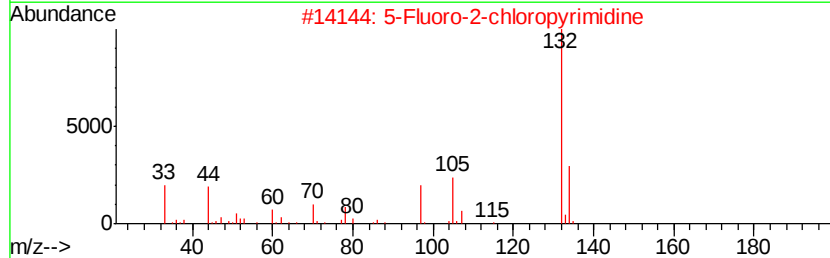
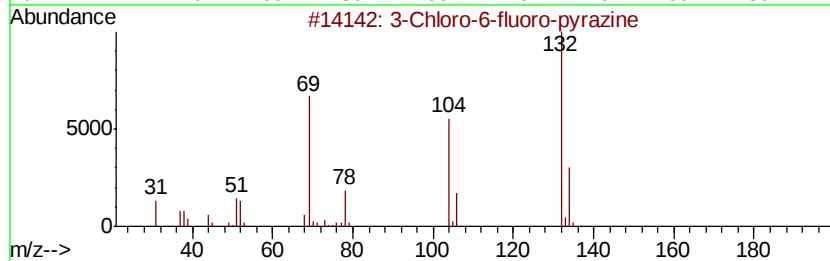
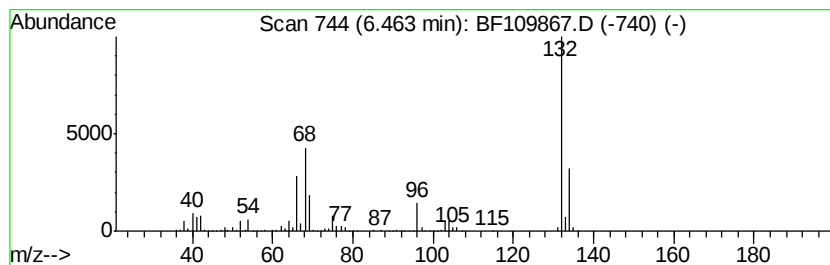
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Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	60.27 ng	1757650	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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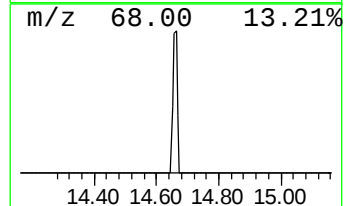
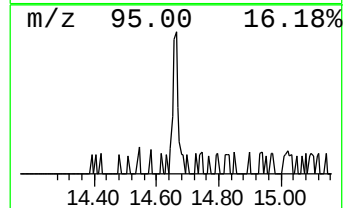
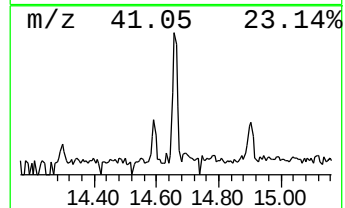
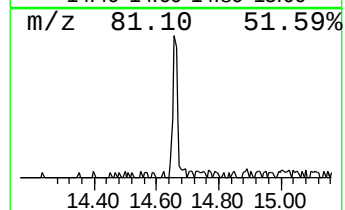
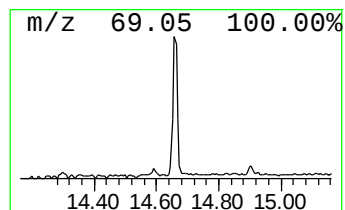
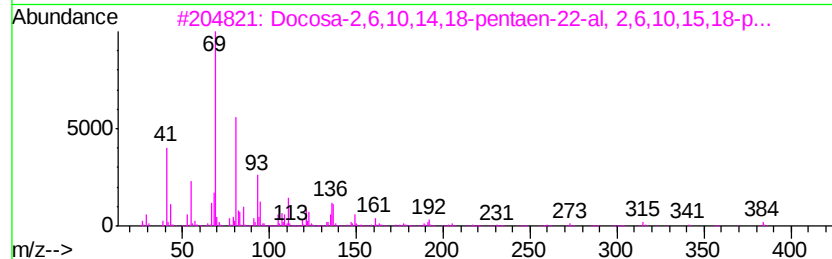
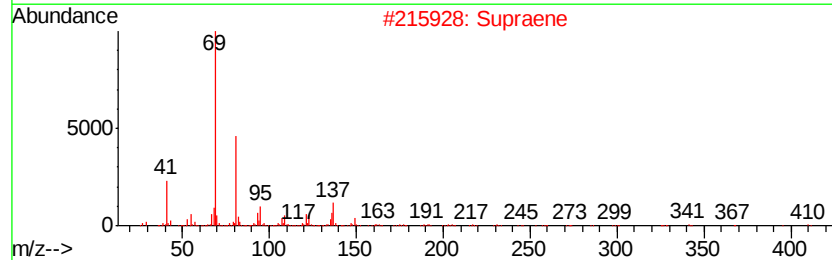
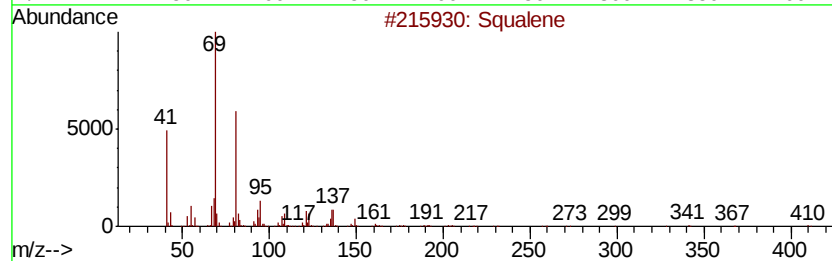
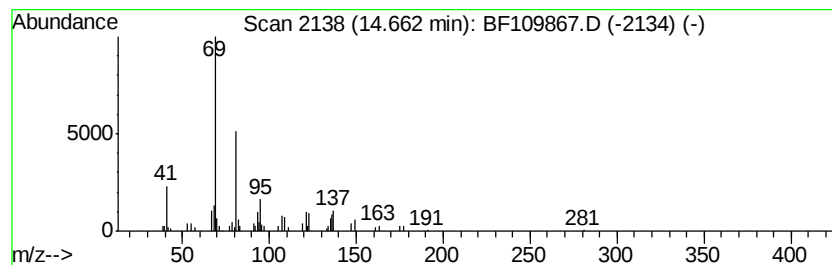
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Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.89 ng	60411	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	3.3	ng	94751	1	6.69	583258	20.0
unknown6.46	6.46	60.3	ng	1757650	1	6.69	583258	20.0
Squalene	14.66	2.9	ng	60411	6	15.23	418483	20.0