

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111715\
 Data File : BF082982.D
 Acq On : 17 Nov 2015 23:01
 Operator : UM/IZ
 Sample : G4407-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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	4.899	241	246	249	rBV	780150	990719	16.79%	2.654%
2	5.356	284	286	288	rBV	2407166	2264951	38.38%	6.069%
3	6.396	375	377	379	rBV	1709498	1390046	23.55%	3.724%
4	6.522	385	388	391	rBV	3851707	3653169	61.90%	9.788%
5	6.750	406	408	411	rBV	1206026	986335	16.71%	2.643%
6	6.910	419	422	424	rBV	4117922	3550908	60.17%	9.514%
7	7.322	455	458	460	rBV	3243467	3551122	60.17%	9.515%
8	8.042	518	521	523	rBV	1231600	1238154	20.98%	3.317%
9	9.116	612	615	618	rBV	4391071	5163947	87.50%	13.836%
10	9.516	648	650	651	rBV	116486	110939	1.88%	0.297%
11	9.791	671	674	676	rBV	1672789	1420806	24.07%	3.807%
12	10.579	740	743	746	rBV	3480863	3342631	56.64%	8.956%
13	11.265	801	803	806	rBV	1247035	1349838	22.87%	3.617%
14	12.065	871	873	876	rVB	67218	66881	1.13%	0.179%
15	12.865	940	943	945	rBV	5407619	5901788	100.00%	15.813%
16	13.780	1021	1023	1031	rBV6	25024	65392	1.11%	0.175%
17	13.894	1031	1033	1036	rBV	918434	1251942	21.21%	3.354%
18	14.762	1106	1109	1111	rBV	106397	138377	2.34%	0.371%
19	15.300	1153	1156	1158	rBV	597988	884855	14.99%	2.371%

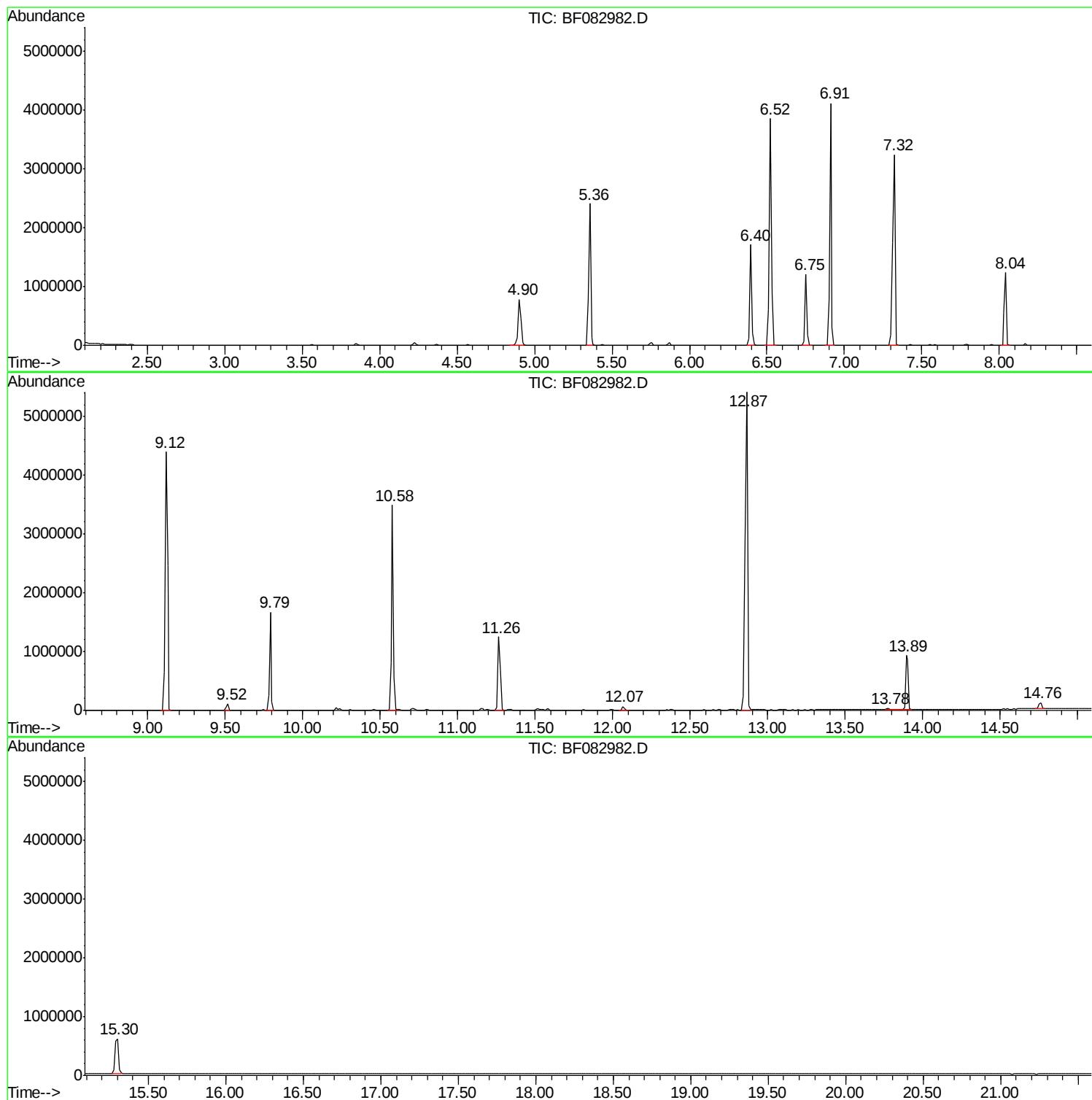
Sum of corrected areas: 37322800

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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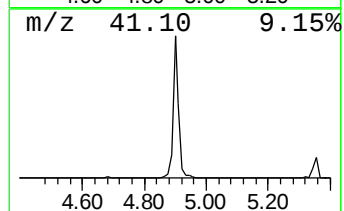
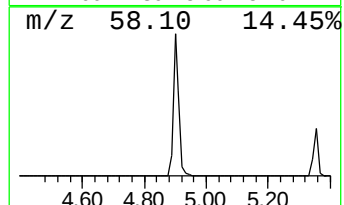
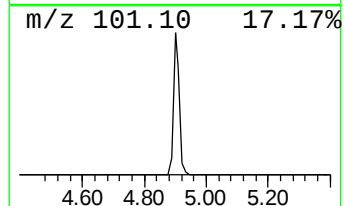
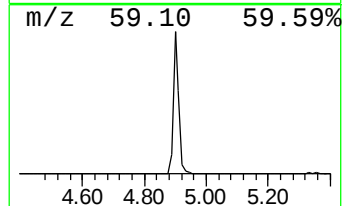
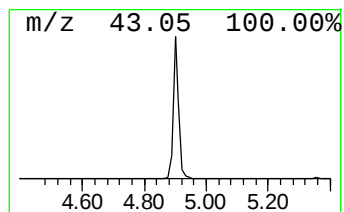
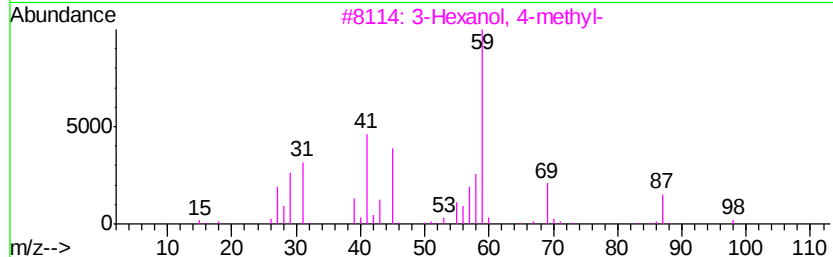
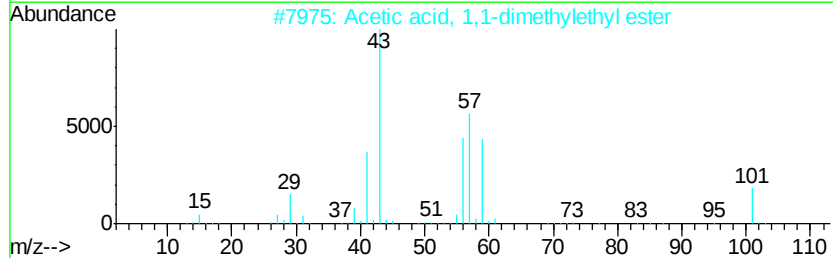
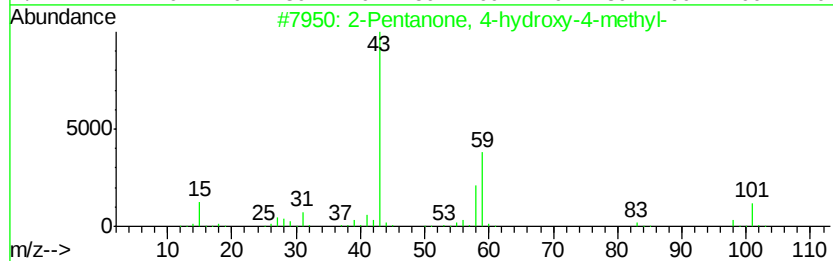
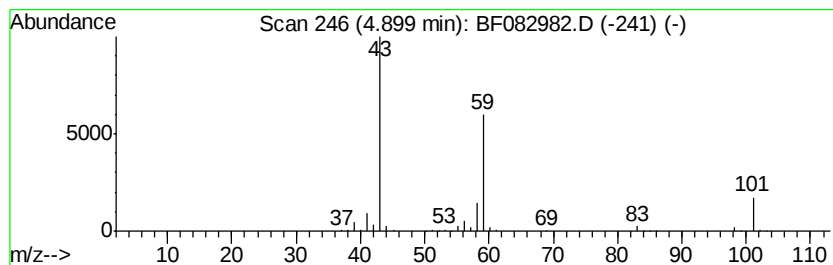
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	20.09 ng	990719	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33



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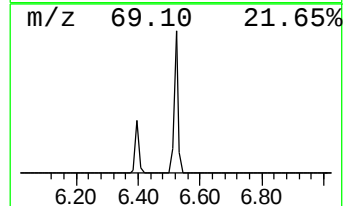
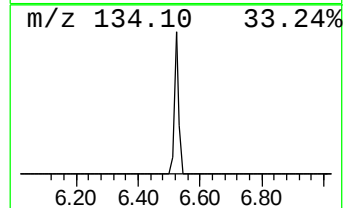
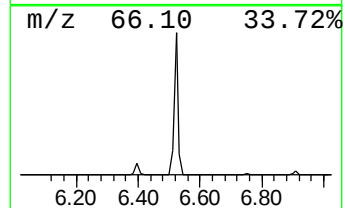
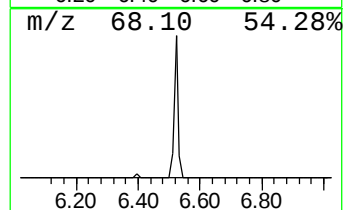
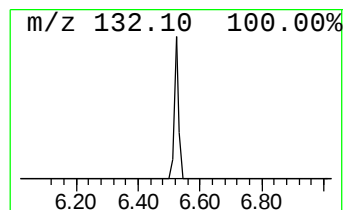
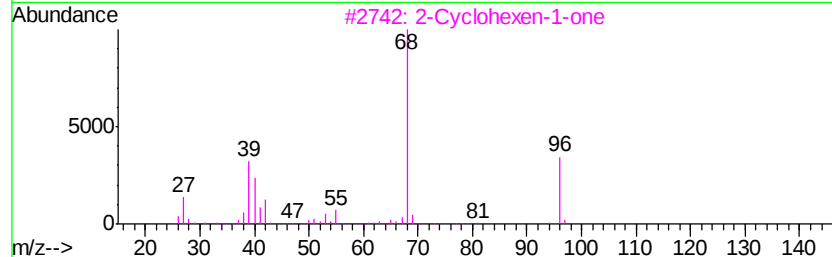
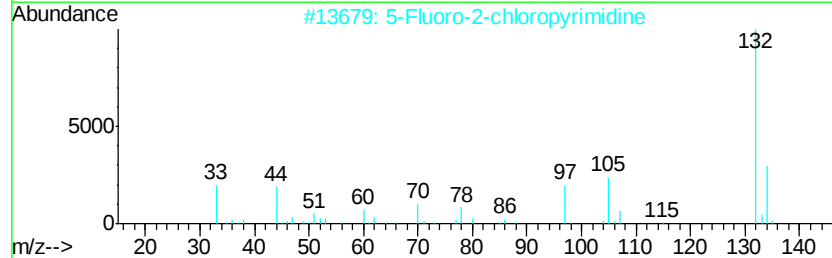
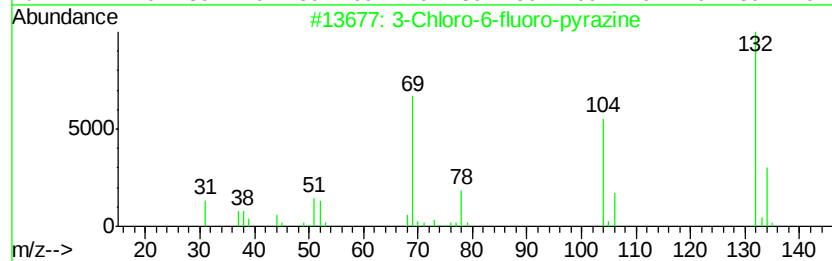
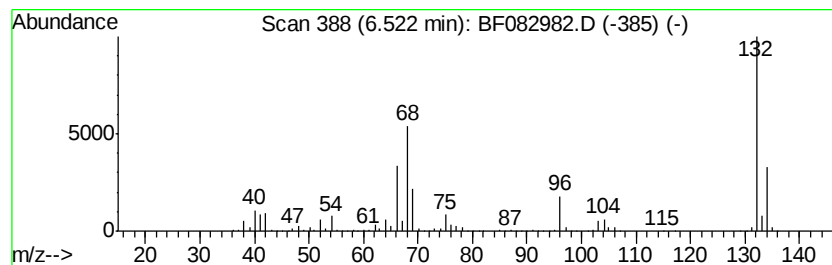
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Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	74.08 ng	3653170	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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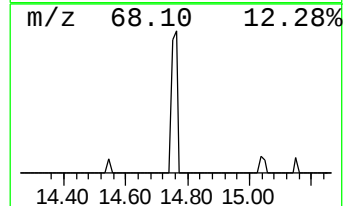
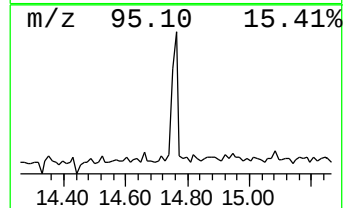
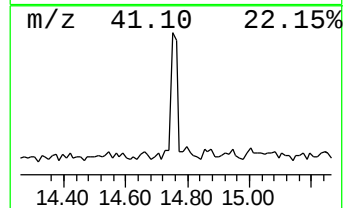
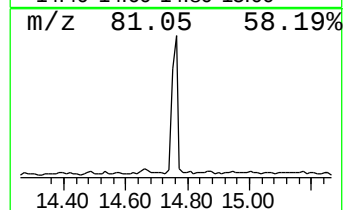
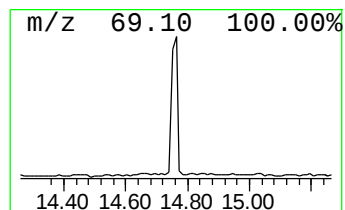
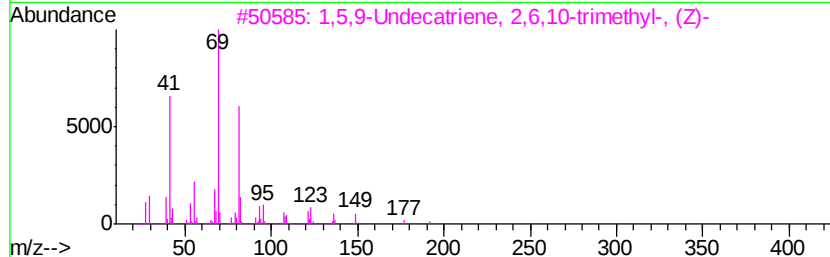
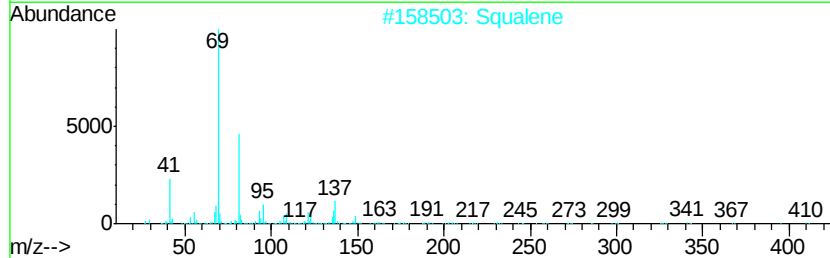
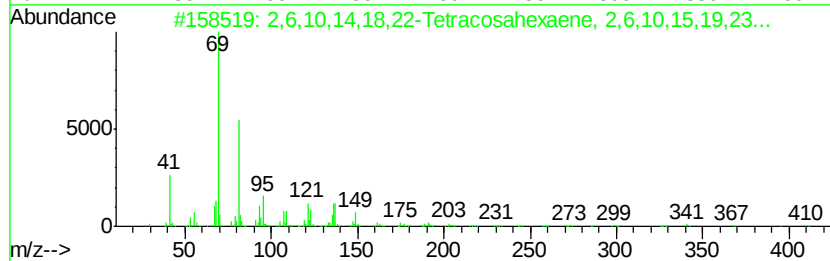
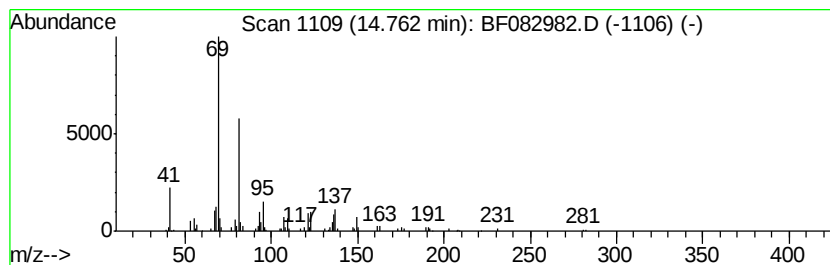
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Peak Number 4 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	3.13 ng	138377	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91		
2	Squalene	410	C30H50	007683-64-9	91		
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90		
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83		
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	20.1	ng	990719	1	6.75	986335	20.0
unknown6.52	6.52	74.1	ng	3653170	1	6.75	986335	20.0
2,6,10,14,18,22-T...	14.76	3.1	ng	138377	6	15.30	884855	20.0