

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091917\
 Data File : BF098648.D
 Acq On : 19 Sep 2017 18:28
 Operator : SJ/JU
 Sample : I5276-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-117-4(0-5)

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-BF091117.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	3.569	235	252	255	rBV	7225333	19720537	100.00%	38.588%
2	4.804	459	462	481	rBV	376832	611918	3.10%	1.197%
3	5.240	531	536	557	rBV	3109716	3176341	16.11%	6.215%
4	6.287	709	714	729	rBV	3078013	3355849	17.02%	6.567%
5	6.398	729	733	736	rBV	3631802	3255230	16.51%	6.370%
6	6.622	768	771	780	rVB	739705	694677	3.52%	1.359%
7	6.781	794	798	811	rBV	2149936	1802404	9.14%	3.527%
8	7.198	864	869	872	rBV	1884339	1782985	9.04%	3.489%
9	7.910	986	990	1001	rBV	1147115	947895	4.81%	1.855%
10	8.986	1168	1173	1176	rBV	3478042	3007241	15.25%	5.884%
11	9.386	1237	1241	1249	rVB	335349	280367	1.42%	0.549%
12	9.657	1283	1287	1296	rVB	1209585	1149064	5.83%	2.248%
13	10.451	1418	1422	1435	rBV	2342093	2352397	11.93%	4.603%
14	11.145	1536	1540	1543	rBV	1616281	1535712	7.79%	3.005%
15	12.733	1804	1810	1813	rBV	4163195	4137777	20.98%	8.097%
16	13.621	1957	1961	1974	rBV	302870	392535	1.99%	0.768%
17	13.780	1983	1988	1991	rBV	1677230	1492547	7.57%	2.921%
18	15.180	2220	2226	2233	rBV	1119780	1409476	7.15%	2.758%

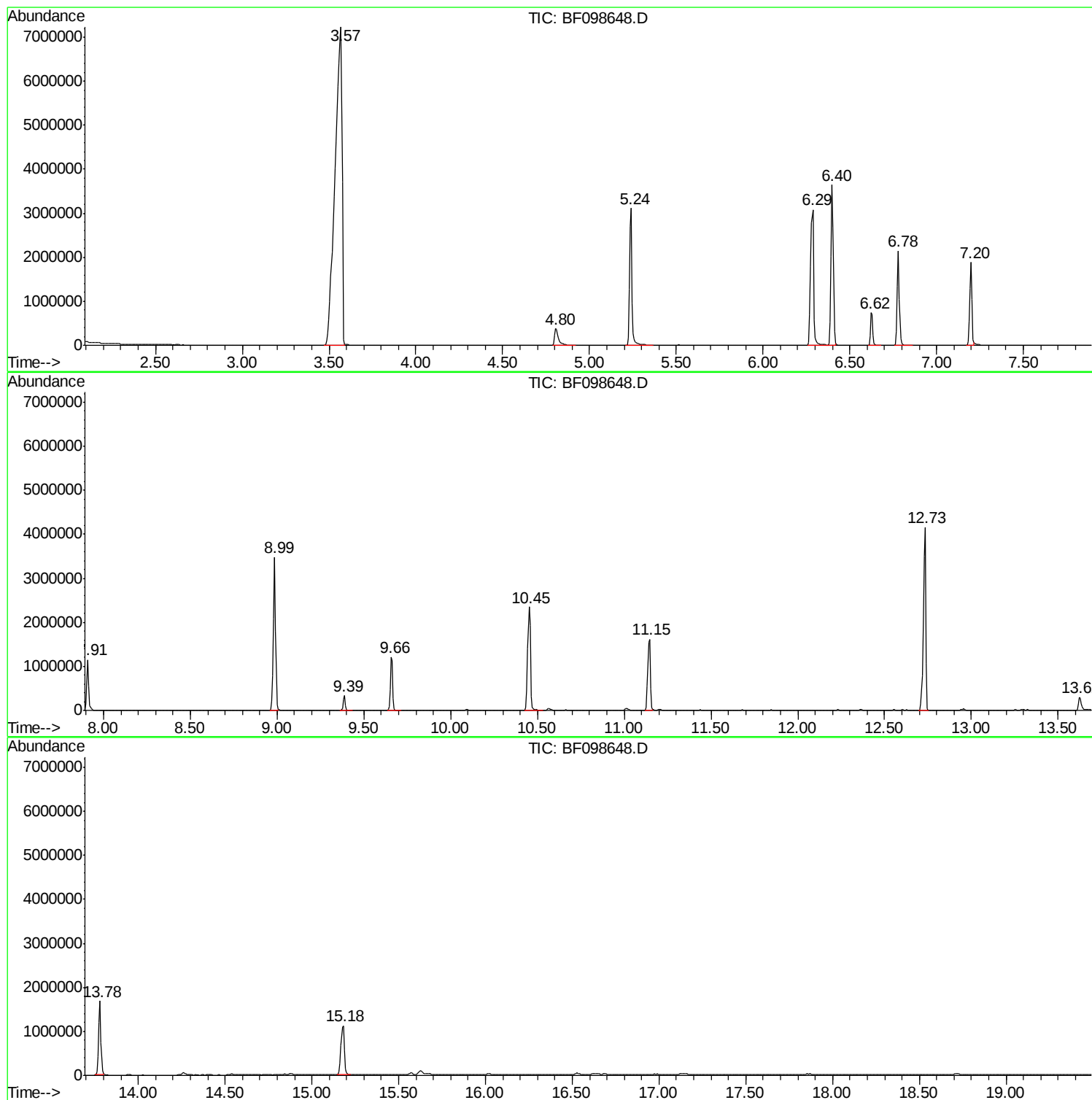
Sum of corrected areas: 51104952

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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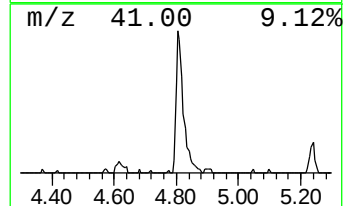
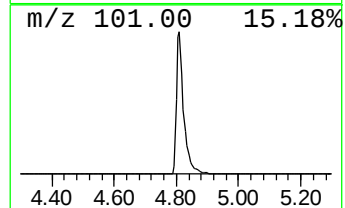
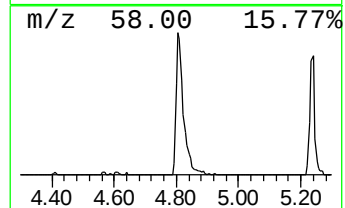
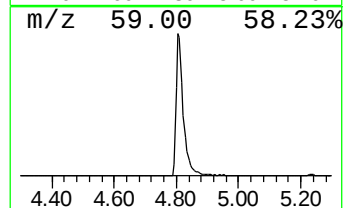
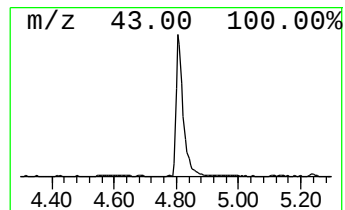
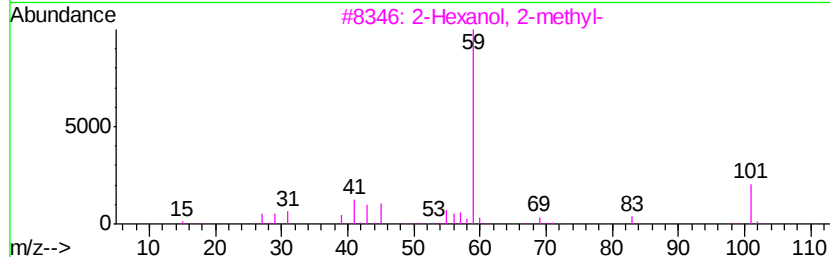
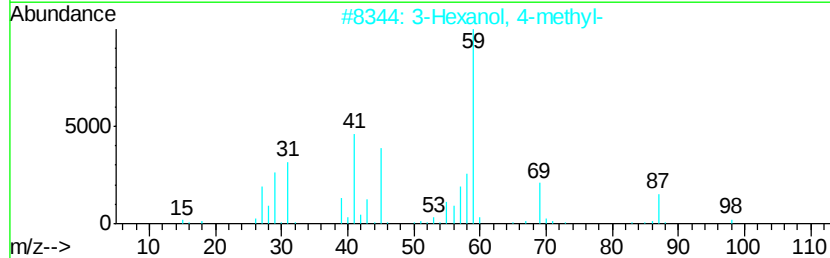
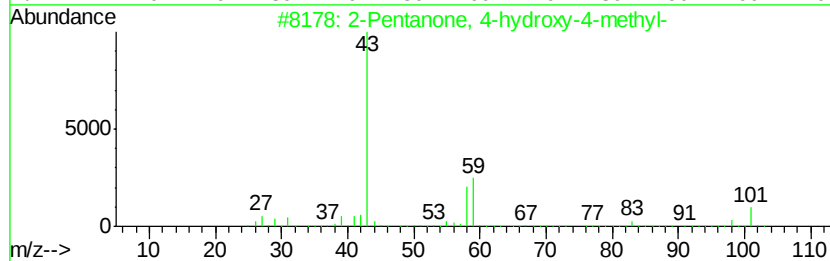
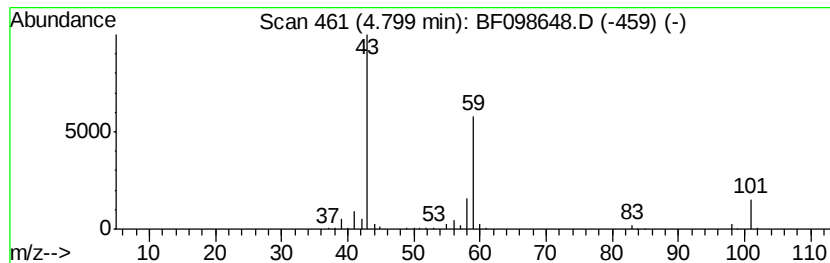
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	17.62 ng	611918	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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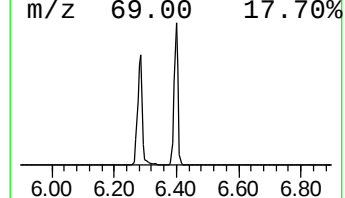
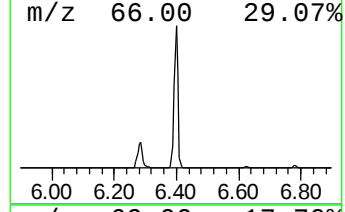
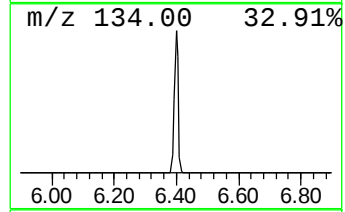
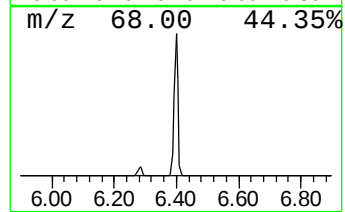
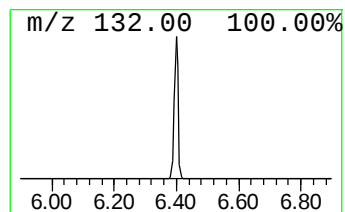
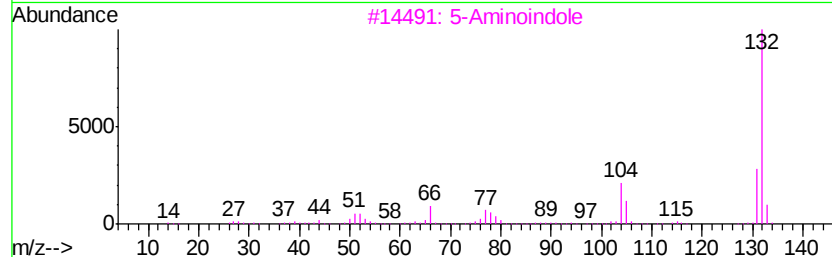
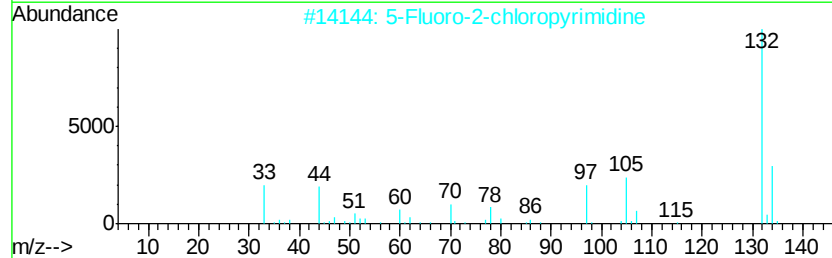
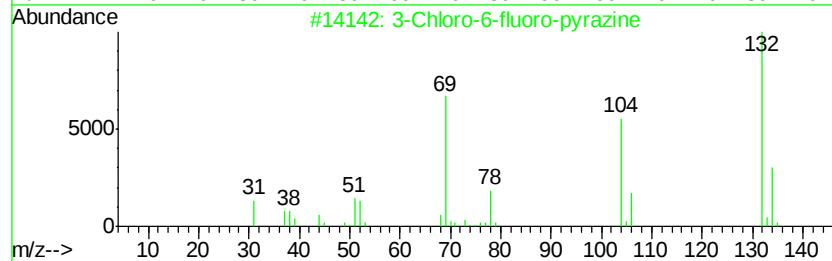
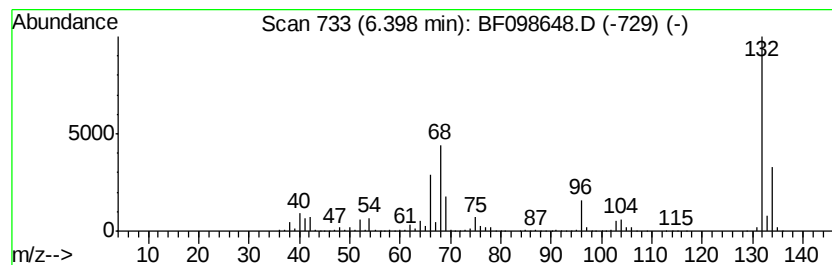
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Peak Number 3 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	93.72 ng	3255230	1,4-Dichlorobenzene-d4	6.63

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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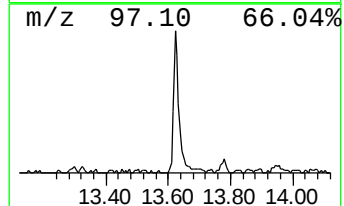
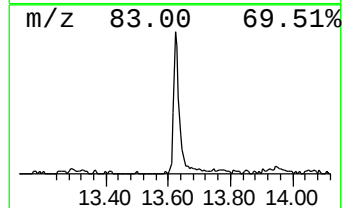
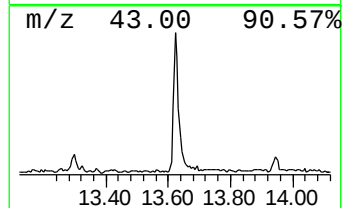
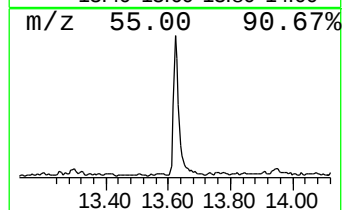
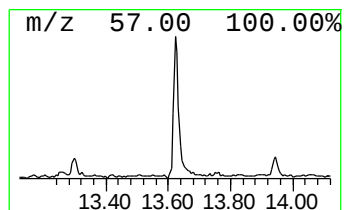
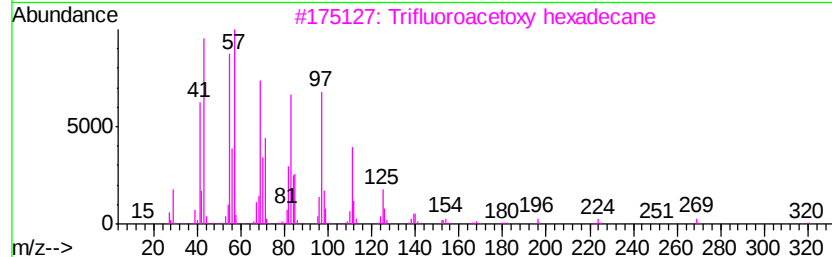
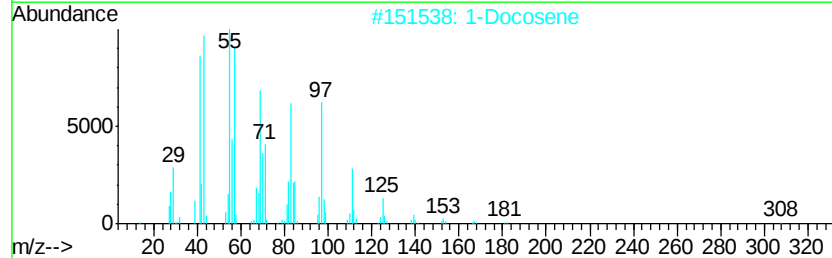
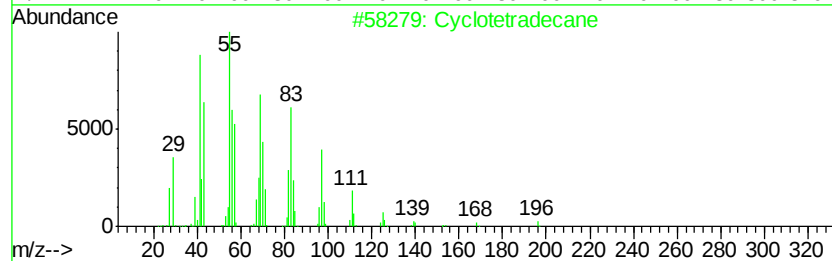
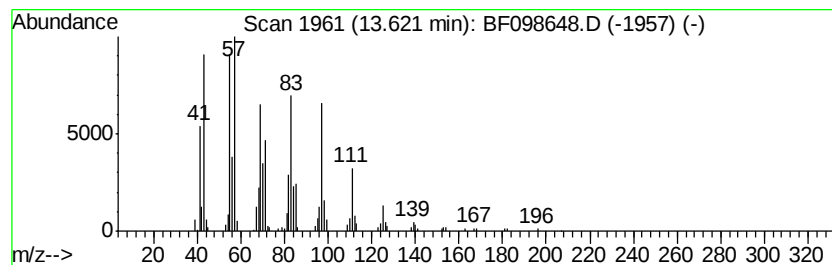
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Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	5.26 ng	392535	Chrysene-d12	13.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	95
2		1-Docosene	308	C22H44	001599-67-3	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Octacosanol	410	C28H58O	000557-61-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	17.6	ng	611918	1	6.63	694677	20.0
unknown6.40	6.40	93.7	ng	3255230	1	6.63	694677	20.0
Cyclotetradecane	13.62	5.3	ng	392535	5	13.78	1492550	20.0