

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070317\
 Data File : BF096457.D
 Acq On : 4 Jul 2017 00:02
 Operator : SJ/MA
 Sample : I3997-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW12-14.5-15-GRAB

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-BF070117.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	3.769	271	286	289	rBV	6541185	17527877	100.00%	45.853%
2	4.922	477	482	493	rVB	340186	423907	2.42%	1.109%
3	5.346	549	554	557	rBV	2769959	2688778	15.34%	7.034%
4	6.369	718	728	734	rBV	2644498	2738041	15.62%	7.163%
5	6.498	745	750	753	rBV	2601145	2329087	13.29%	6.093%
6	6.728	785	789	792	rBV	782733	640709	3.66%	1.676%
7	6.887	811	816	819	rBV	2109562	1926800	10.99%	5.040%
8	7.287	879	884	887	rBV	1607033	1447451	8.26%	3.786%
9	8.010	1003	1007	1010	rBV	836685	703142	4.01%	1.839%
10	9.086	1185	1190	1193	rBV	2559780	2222683	12.68%	5.814%
11	9.475	1252	1256	1260	rBV	599642	480480	2.74%	1.257%
12	9.757	1300	1304	1310	rVB	689755	658443	3.76%	1.722%
13	10.545	1434	1438	1442	rBV	1092125	951639	5.43%	2.489%
14	11.239	1553	1556	1560	rVB	729456	589428	3.36%	1.542%
15	12.827	1821	1826	1829	rBV	1925968	1737905	9.92%	4.546%
16	13.727	1975	1979	1987	rBV	187515	221799	1.27%	0.580%
17	13.868	1999	2003	2007	rBV	624590	559666	3.19%	1.464%
18	15.280	2239	2243	2249	rVB	300885	378789	2.16%	0.991%

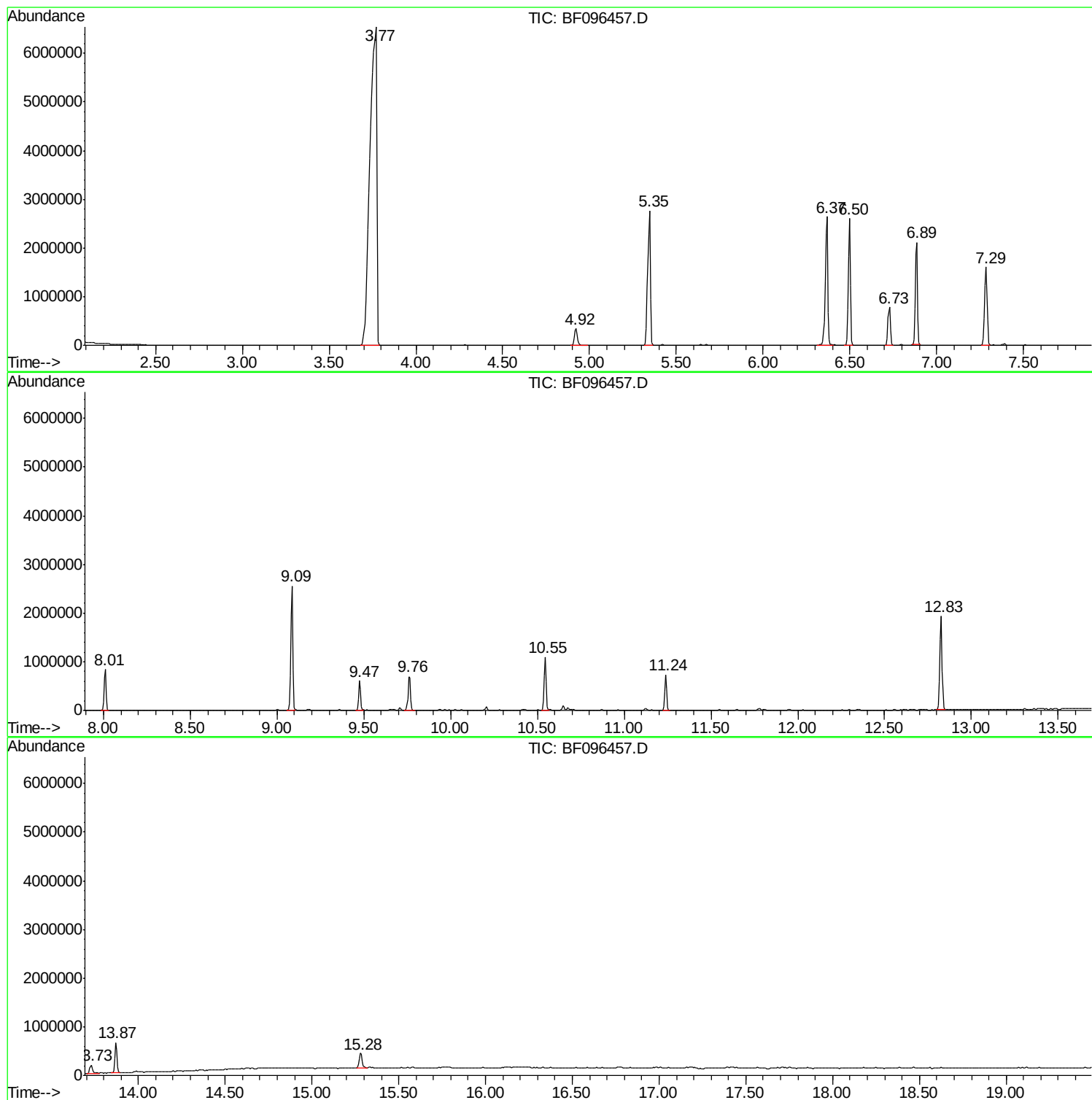
Sum of corrected areas: 38226624

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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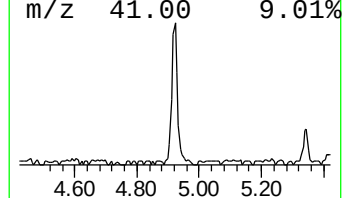
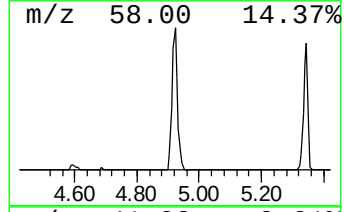
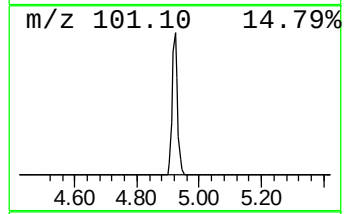
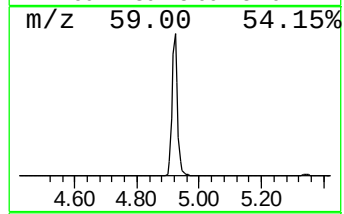
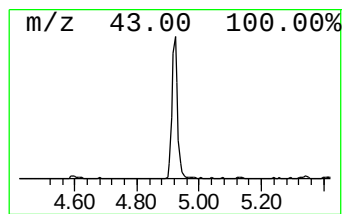
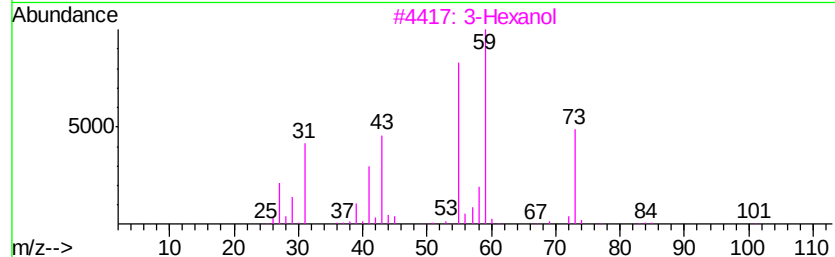
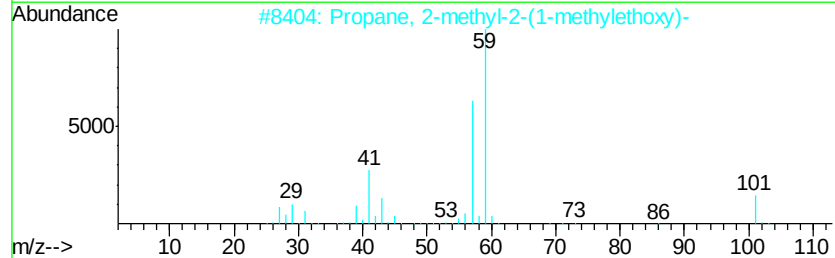
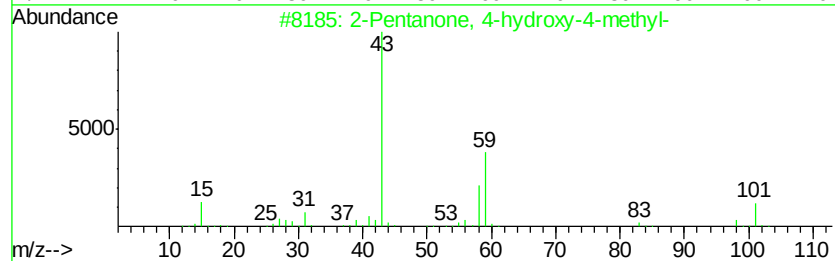
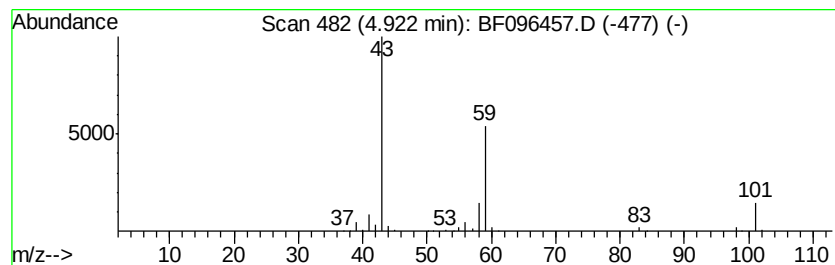
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	13.23 ng	423907	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



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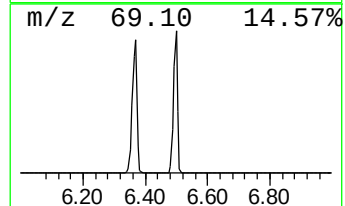
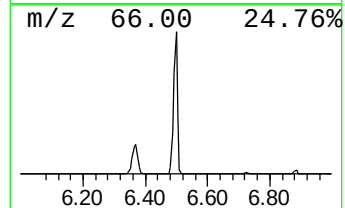
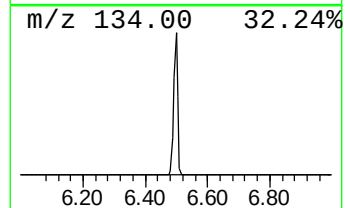
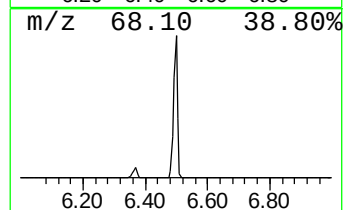
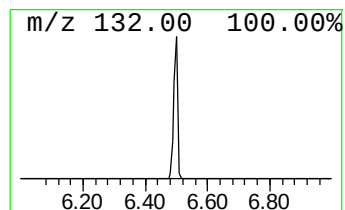
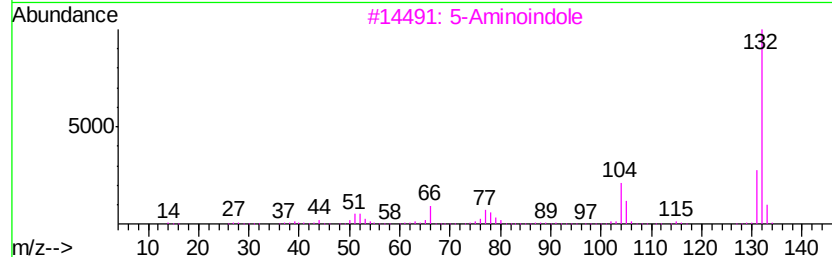
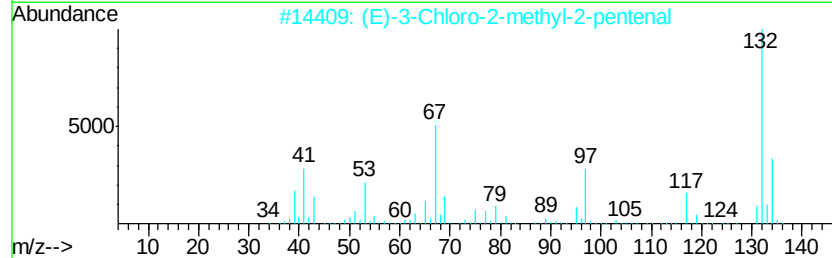
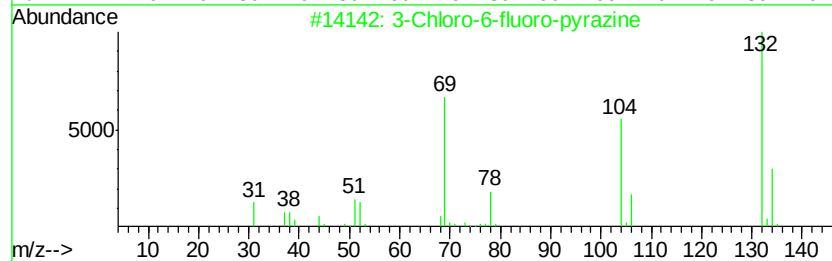
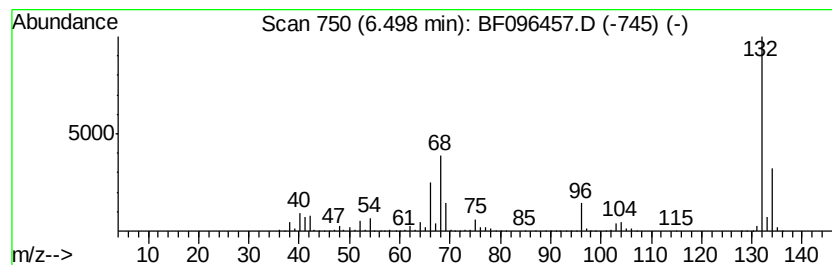
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Peak Number 3 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	72.70 ng	2329090	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Amphetaminil	250	C17H18N2	017590-01-1	10



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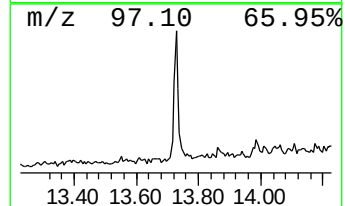
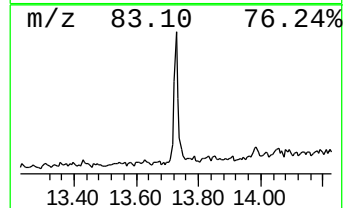
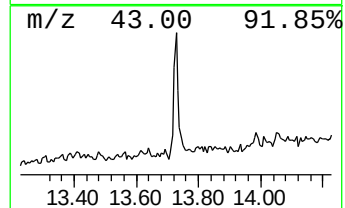
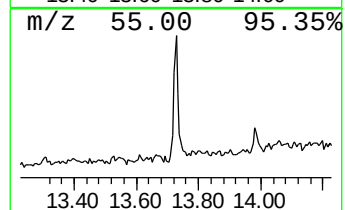
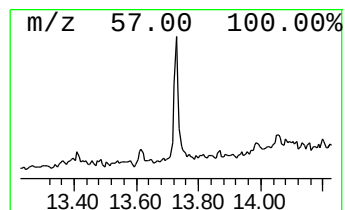
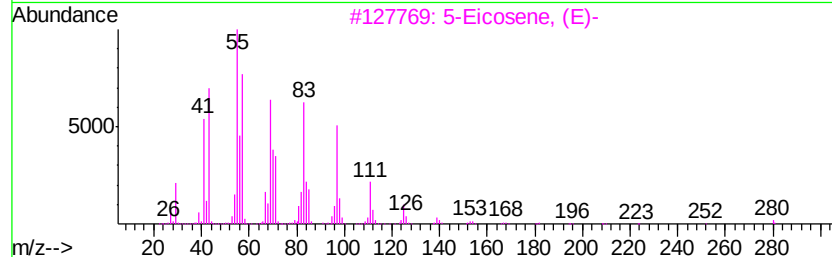
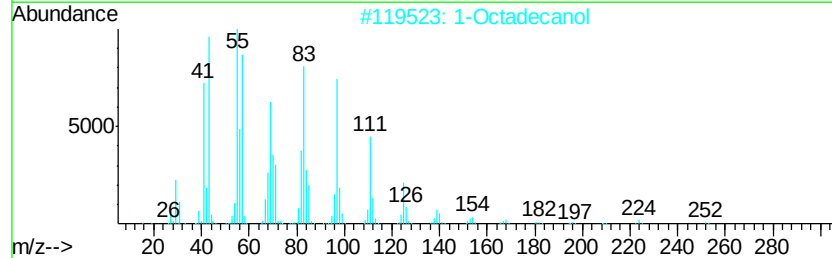
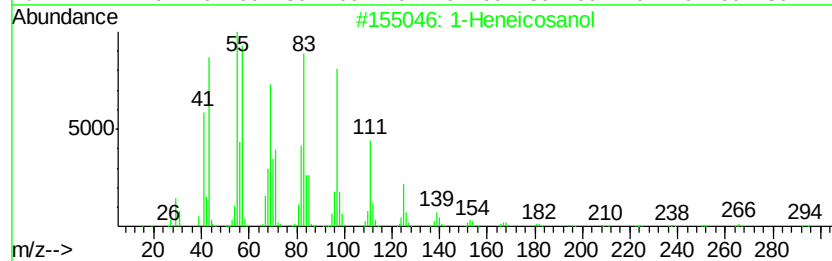
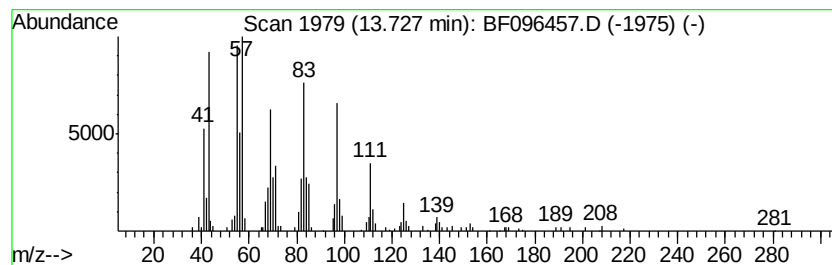
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.93 ng	221799	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	93
2	1-Octadecanol		270	C18H38O	000112-92-5	91
3	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
4	3-Chloropropionic acid, heptadec...		346	C20H39ClO2	1000283-05-1	91
5	Pentafluoropropionic acid, tride...		346	C16H27F5O2	959261-22-4	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	13.2	ng	423907	1	6.73	640709	20.0
unknown6.50	6.50	72.7	ng	2329090	1	6.73	640709	20.0
1-Heneicosanol	13.73	7.9	ng	221799	5	13.87	559666	20.0