

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090716\
 Data File : BF090006.D
 Acq On : 7 Sep 2016 15:49
 Operator : UM/SJ
 Sample : H4676-09
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEMP-AB-(0-2)-10

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-BF083116.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	1.735	11	13	47	rVB	1998286	4612942	86.14%	9.156%
2	3.313	148	151	158	rVB	21947	54630	1.02%	0.108%
3	4.741	274	276	290	rBV	622127	1246633	23.28%	2.474%
4	5.199	313	316	318	rBV	3705501	4448312	83.07%	8.829%
5	6.262	406	409	417	rBV	3144890	5046019	94.23%	10.016%
6	6.387	417	420	422	rBV	3734884	5027939	93.89%	9.980%
7	6.616	438	440	446	rBV	916400	1028541	19.21%	2.042%
8	6.764	451	453	456	rBV	2470003	3678066	68.68%	7.300%
9	7.187	487	490	492	rBV	2575838	3320174	62.00%	6.590%
10	7.896	550	552	555	rBV	1147695	1311323	24.49%	2.603%
11	8.982	644	647	649	rBV	5092254	5355086	100.00%	10.629%
12	9.382	679	682	684	rBV	631050	876858	16.37%	1.740%
13	9.645	702	705	713	rVB	1730833	1656875	30.94%	3.289%
14	10.102	737	745	746	rBV2	74227	135557	2.53%	0.269%
15	10.319	761	764	767	rBV	35369	62366	1.16%	0.124%
16	10.433	771	774	776	rBV	2517770	3340843	62.39%	6.631%
17	10.571	784	786	790	rBV	98222	145759	2.72%	0.289%
18	11.016	820	825	826	rBV	58710	77722	1.45%	0.154%
19	11.119	831	834	836	rBV	1455064	1739264	32.48%	3.452%
20	12.696	969	972	975	rBV	3943005	4296833	80.24%	8.529%
21	13.611	1049	1052	1060	rBV	209936	351531	6.56%	0.698%
22	13.725	1060	1062	1065	rBV	1443441	1443757	26.96%	2.866%
23	14.239	1104	1107	1113	rBV	24991	55353	1.03%	0.110%
24	15.074	1177	1180	1182	rBV	794689	1068723	19.96%	2.121%

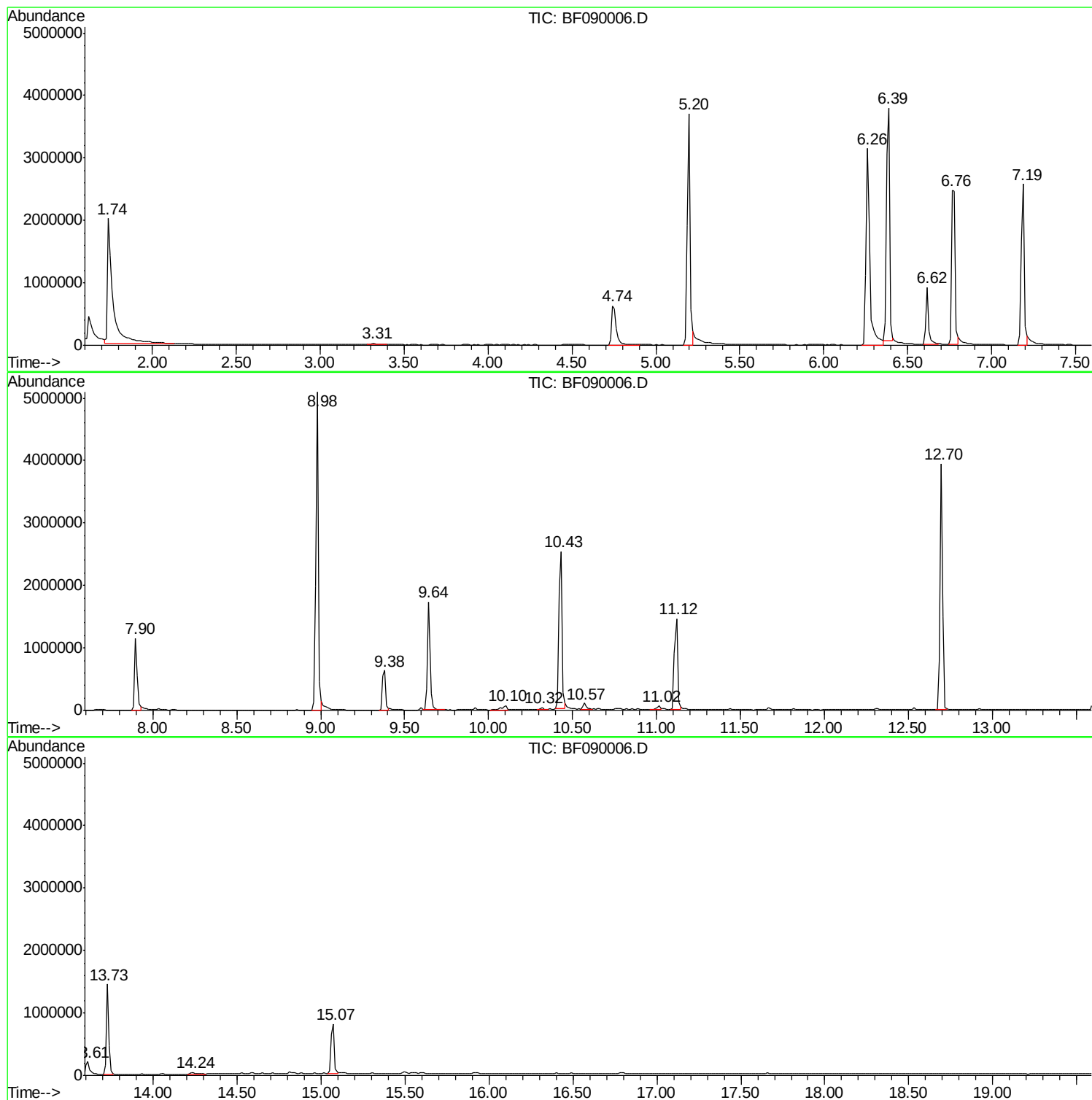
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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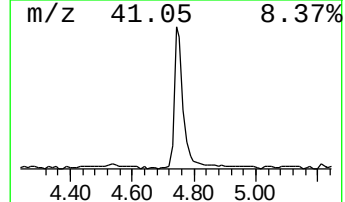
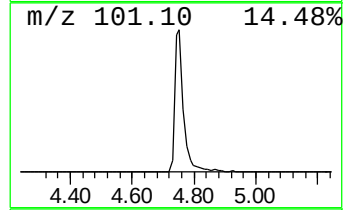
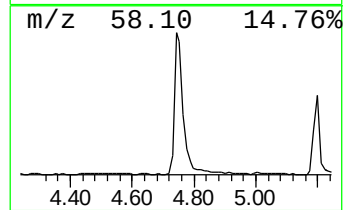
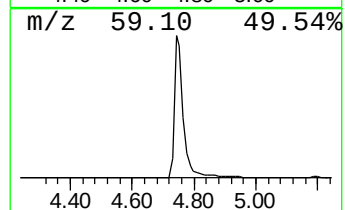
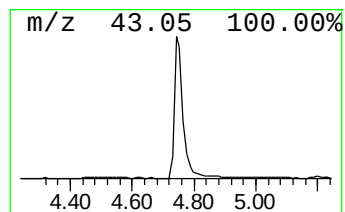
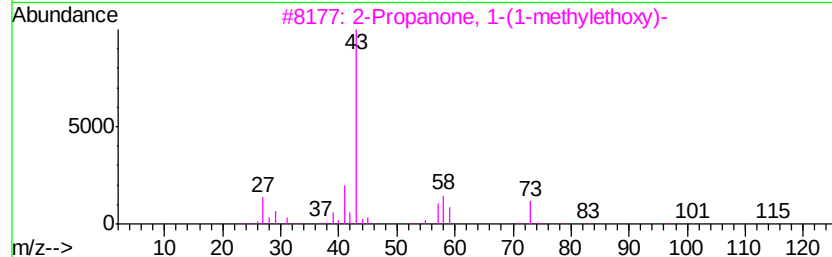
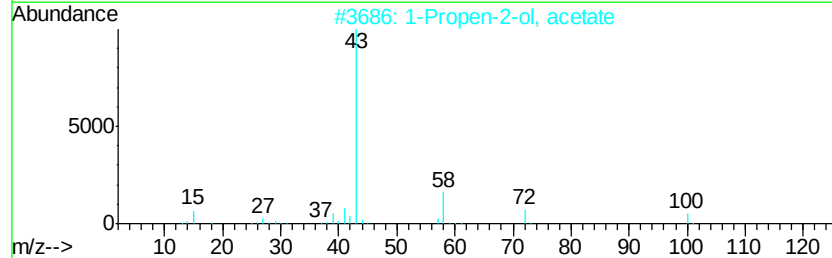
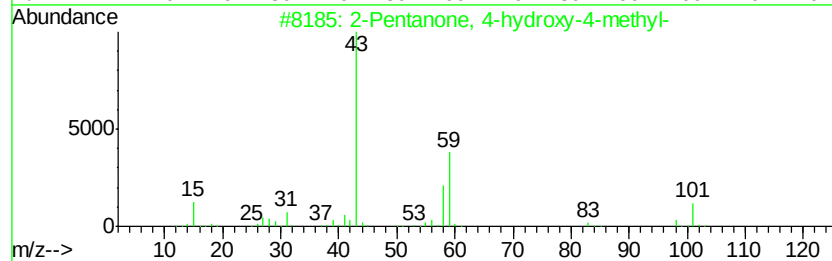
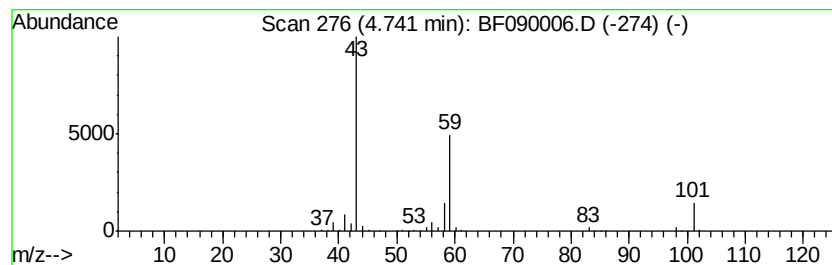
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	24.24 ng	1246630	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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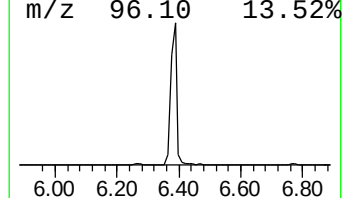
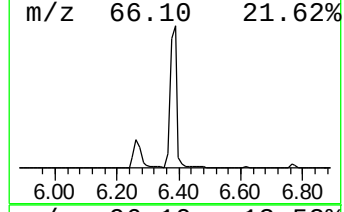
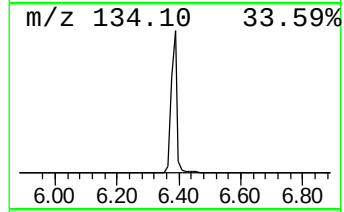
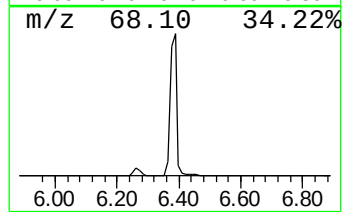
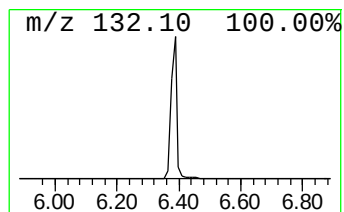
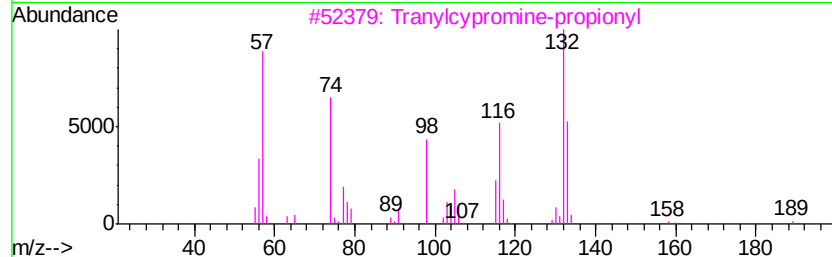
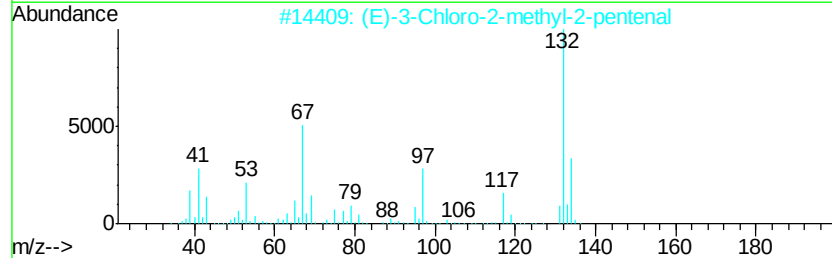
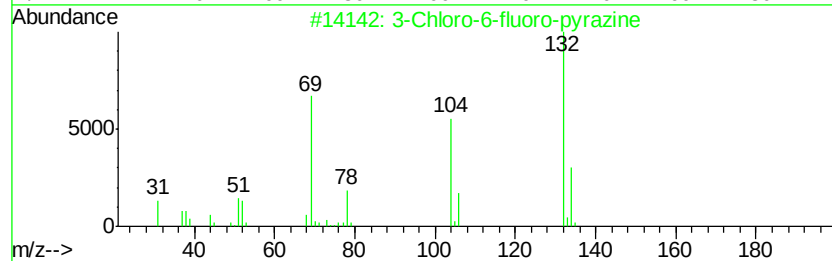
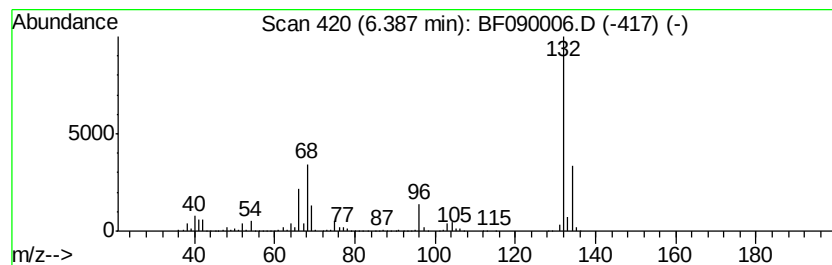
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Peak Number 3 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	97.77 ng	5027940	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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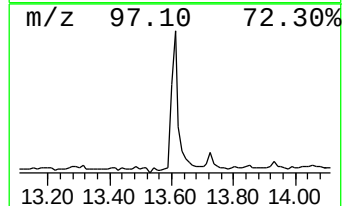
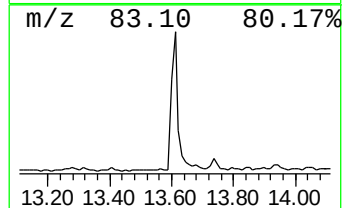
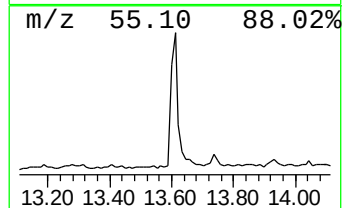
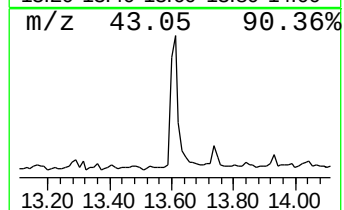
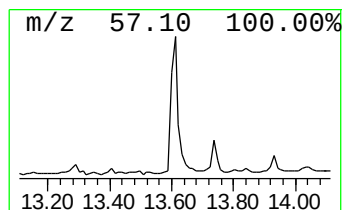
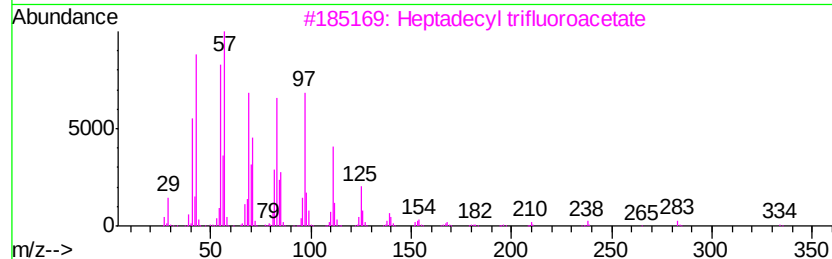
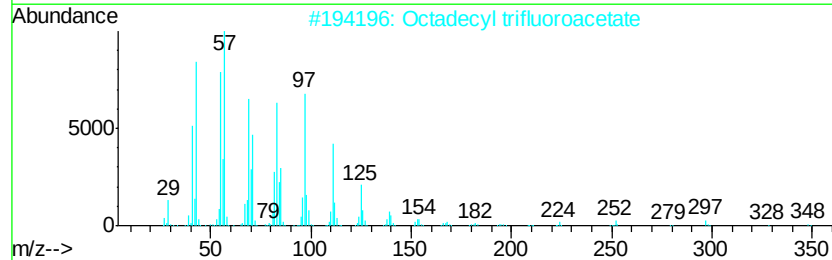
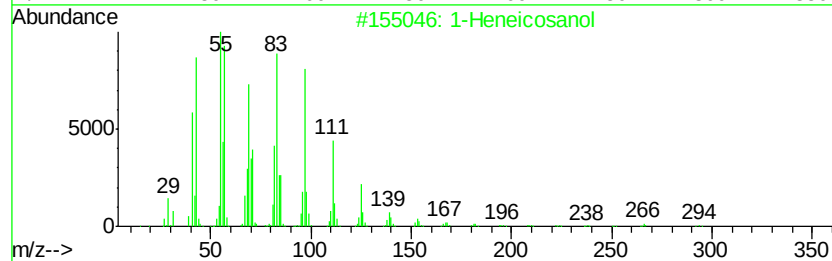
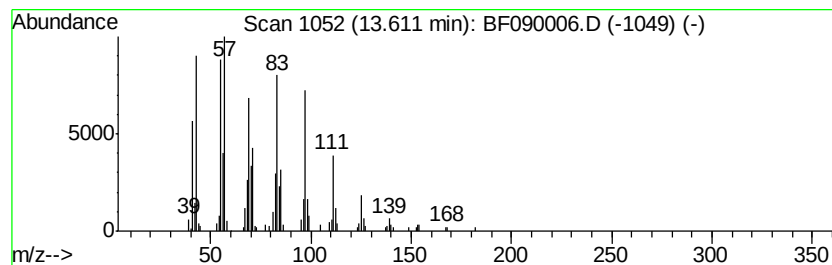
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	4.87 ng	351531	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.74	24.2	ng	1246630	1	6.62	1028540	20.0
unknown6.39	6.39	97.8	ng	5027940	1	6.62	1028540	20.0
1-Heneicosanol	13.61	4.9	ng	351531	5	13.73	1443760	20.0