

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
 Data File : BF088748.D
 Acq On : 6 Jul 2016 21:59
 Operator : UM/SJ
 Sample : H3878-16
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C2.1-08

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-BF063016.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	1.701	8	10	19	rVB	197518	317922	9.61%	1.625%
2	1.827	19	21	70	rVB	1576930	3306941	100.00%	16.901%
3	4.901	288	290	294	rBB	56185	72421	2.19%	0.370%
4	5.336	325	328	330	rBV	1460802	1362174	41.19%	6.962%
5	6.376	416	419	422	rBV	1155925	1364634	41.27%	6.975%
6	6.513	428	431	433	rBV	1660977	1559758	47.17%	7.972%
7	6.742	449	451	453	rBB	476533	476620	14.41%	2.436%
8	6.902	462	465	467	rBB	1369759	1139632	34.46%	5.825%
9	7.313	498	501	503	rBV	861810	1016357	30.73%	5.195%
10	8.033	561	564	566	rBV	740352	717380	21.69%	3.666%
11	9.108	655	658	660	rBV	2155739	1868763	56.51%	9.551%
12	9.496	690	692	695	rVB	247838	276026	8.35%	1.411%
13	9.782	714	717	719	rVB	812207	819869	24.79%	4.190%
14	10.559	783	785	788	rBV	973163	880363	26.62%	4.499%
15	10.696	795	797	800	rBV	37628	43146	1.30%	0.221%
16	11.142	834	836	837	rBV	54109	51051	1.54%	0.261%
17	11.256	843	846	848	rVB	941190	885963	26.79%	4.528%
18	11.496	864	867	871	rBV2	21643	40169	1.21%	0.205%
19	11.565	871	873	876	rVB	39659	35529	1.07%	0.182%
20	12.834	982	984	987	rBV	1601180	1778663	53.79%	9.091%
21	13.748	1061	1064	1072	rBV	88707	161042	4.87%	0.823%
22	13.874	1072	1075	1078	rVB	863514	775515	23.45%	3.964%
23	14.731	1147	1150	1152	rBV	37135	48112	1.45%	0.246%
24	15.257	1193	1196	1198	rBV	483916	567956	17.17%	2.903%

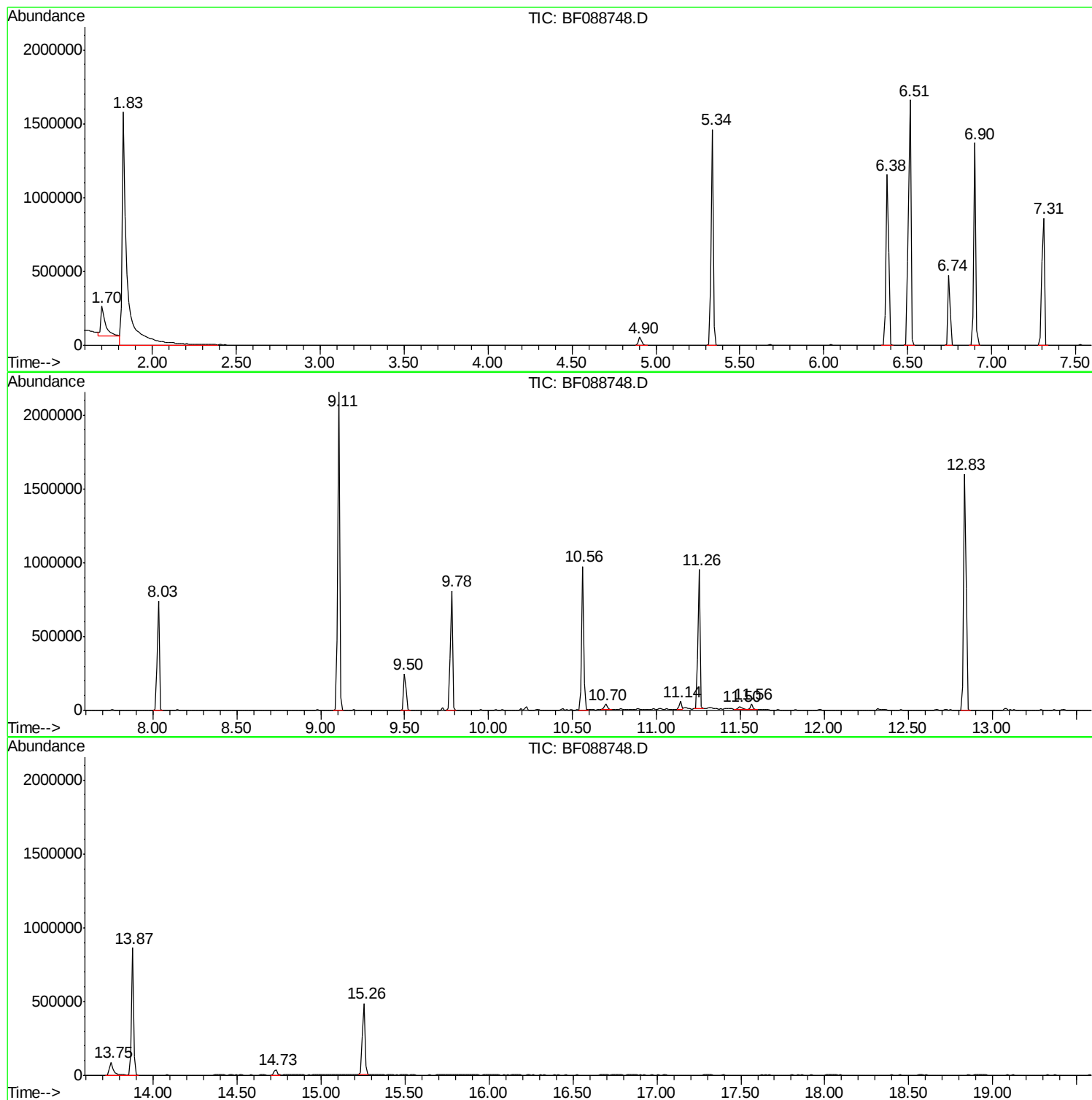
Sum of corrected areas: 19566006

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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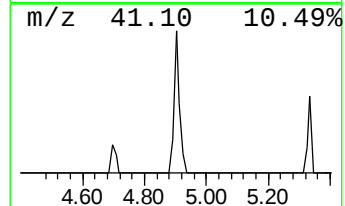
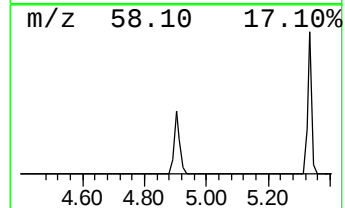
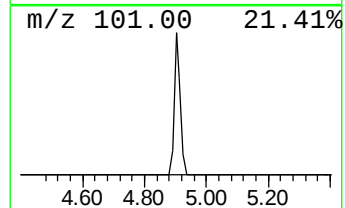
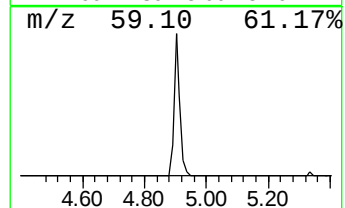
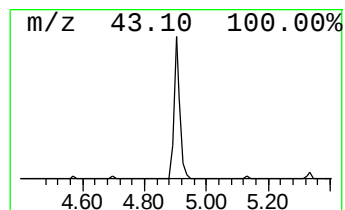
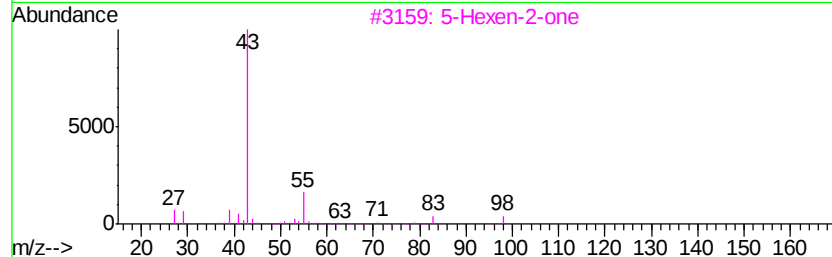
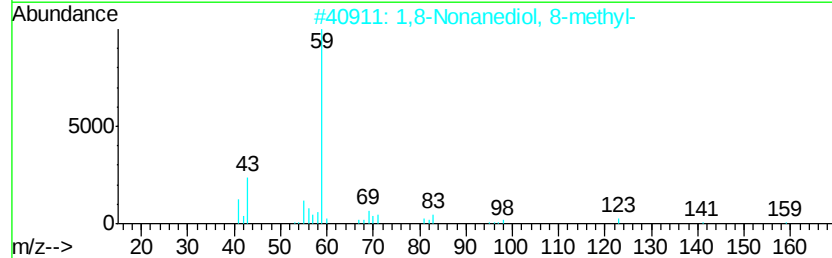
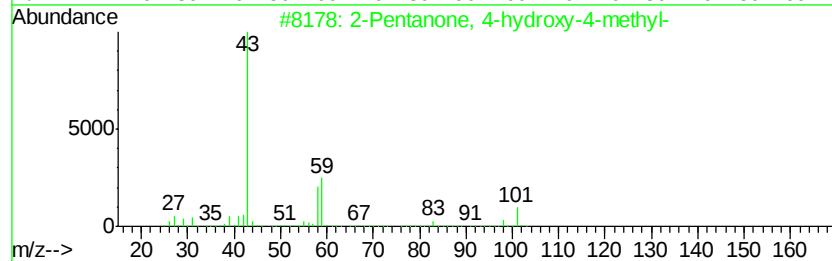
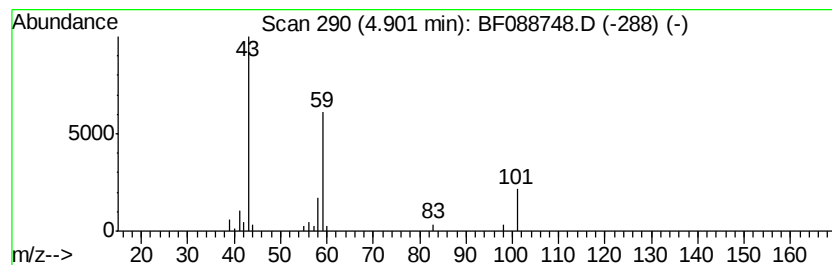
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.04 ng	72421	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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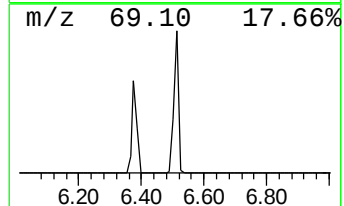
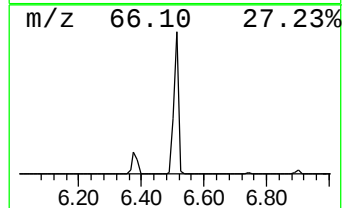
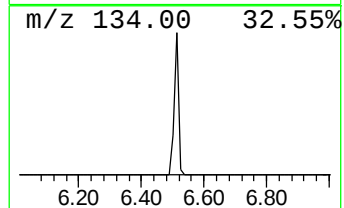
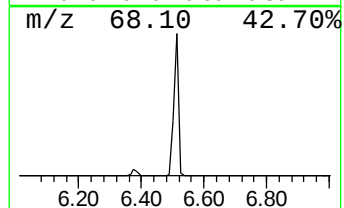
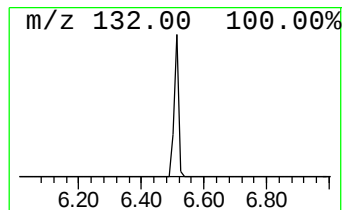
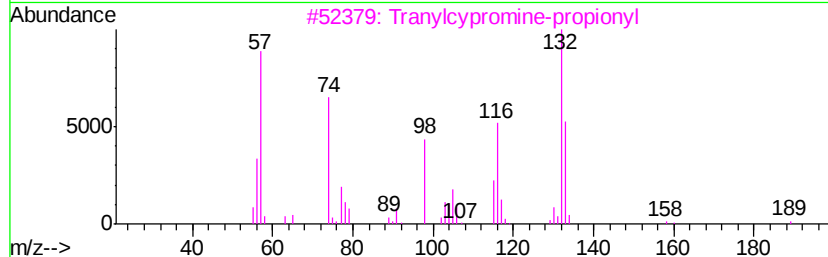
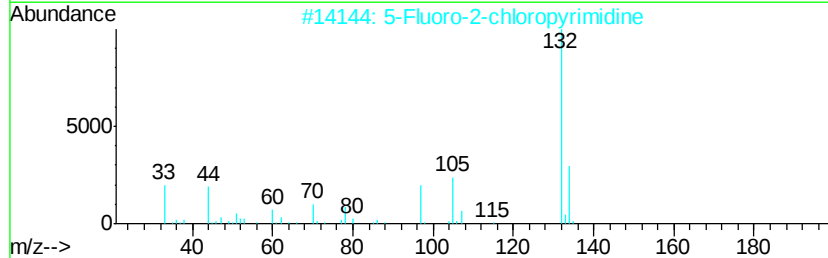
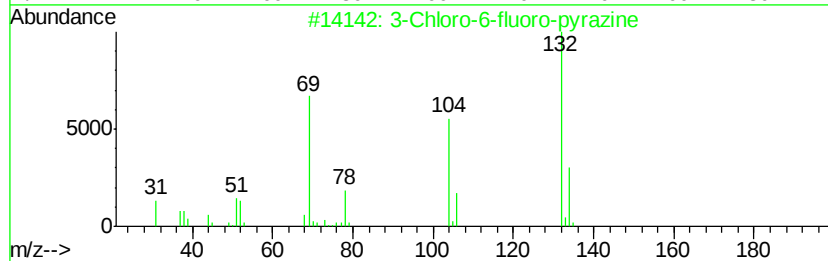
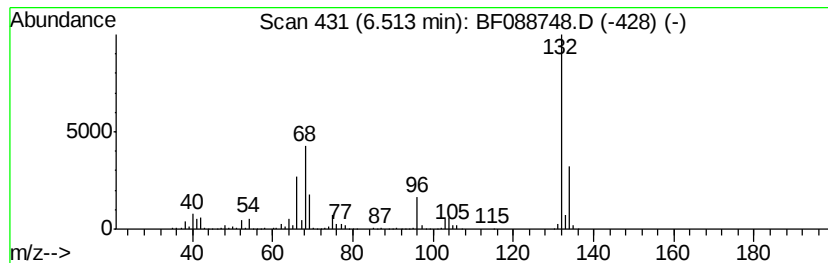
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Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	65.45 ng	1559760	1,4-Dichlorobenzene-d4	6.74

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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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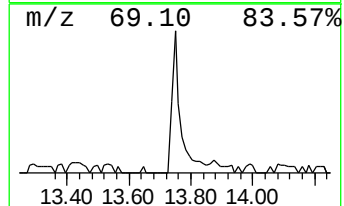
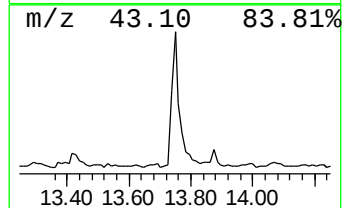
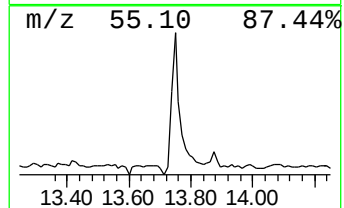
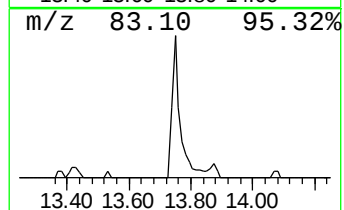
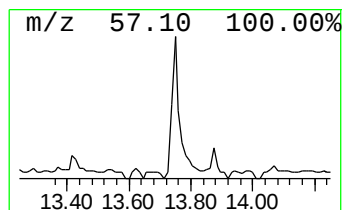
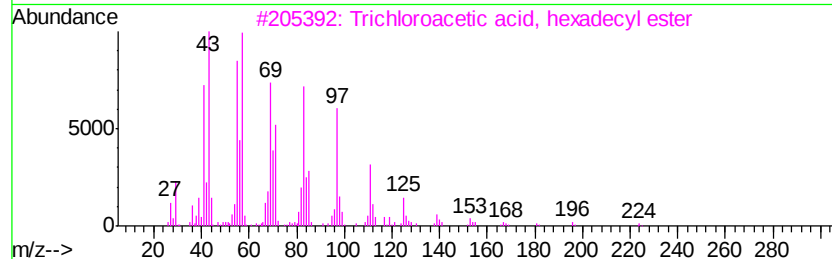
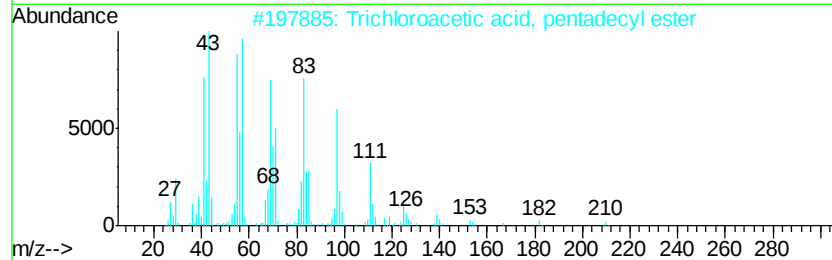
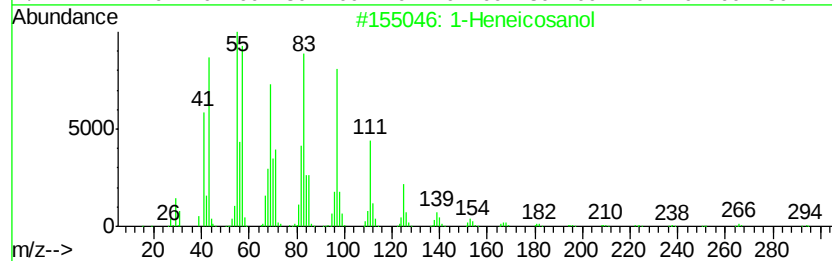
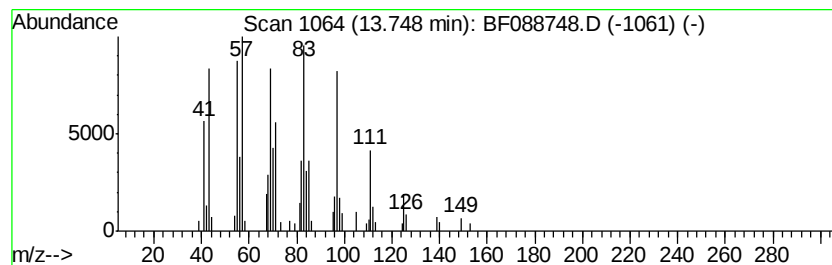
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	4.15 ng	161042	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	3.0	ng	72421	1	6.74	476620	20.0
unknown6.51	6.51	65.5	ng	1559760	1	6.74	476620	20.0
1-Heneicosanol	13.75	4.2	ng	161042	5	13.87	775515	20.0