

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
 Data File : BF086773.D
 Acq On : 7 May 2016 14:46
 Operator : UM/SJ
 Sample : H2779-01
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RODNEY-AVE-PS(0-2)KRE

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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	245	246	252	rBV	141090	283678	4.63%	0.564%
2	5.310	280	282	285	rBV	4161488	5143798	83.89%	10.223%
3	6.362	371	374	377	rBV	4143790	5781995	94.30%	11.491%
4	6.476	382	384	387	rBV	4879444	5195758	84.74%	10.326%
5	6.704	402	404	406	rBV	1135302	1205873	19.67%	2.397%
6	6.853	415	417	420	rBV	3089584	4264778	69.55%	8.476%
7	7.276	451	454	456	rBV	3380390	3751244	61.18%	7.455%
8	7.985	514	516	527	rBV	1314562	1619632	26.41%	3.219%
9	9.070	607	611	613	rBV	5283547	6131754	100.00%	12.186%
10	9.470	643	646	648	rBV	477889	498007	8.12%	0.990%
11	9.676	662	664	666	rBV	142387	134364	2.19%	0.267%
12	9.733	666	669	672	rBV	1408313	1719020	28.03%	3.416%
13	10.179	704	708	709	rBV	198052	211901	3.46%	0.421%
14	10.396	724	727	730	rBV	65494	113799	1.86%	0.226%
15	10.533	736	739	741	rBV2	2709243	3822925	62.35%	7.598%
16	10.648	747	749	754	rVB	213887	240295	3.92%	0.478%
17	11.093	786	788	790	rBV	66934	66732	1.09%	0.133%
18	11.219	797	799	801	rBV	1684183	1651621	26.94%	3.282%
19	11.756	844	846	857	rBV	254296	357307	5.83%	0.710%
20	12.545	913	915	918	rBV	53037	96242	1.57%	0.191%
21	12.625	921	922	925	rVB	81762	103781	1.69%	0.206%
22	12.808	935	938	940	rBV	4351714	5460345	89.05%	10.852%
23	13.334	982	984	986	rBV	88835	73406	1.20%	0.146%
24	13.711	1014	1017	1026	rBV	118819	203813	3.32%	0.405%
25	13.848	1026	1029	1031	rBV	954448	1222805	19.94%	2.430%
26	15.220	1147	1149	1156	rBV	678580	961938	15.69%	1.912%

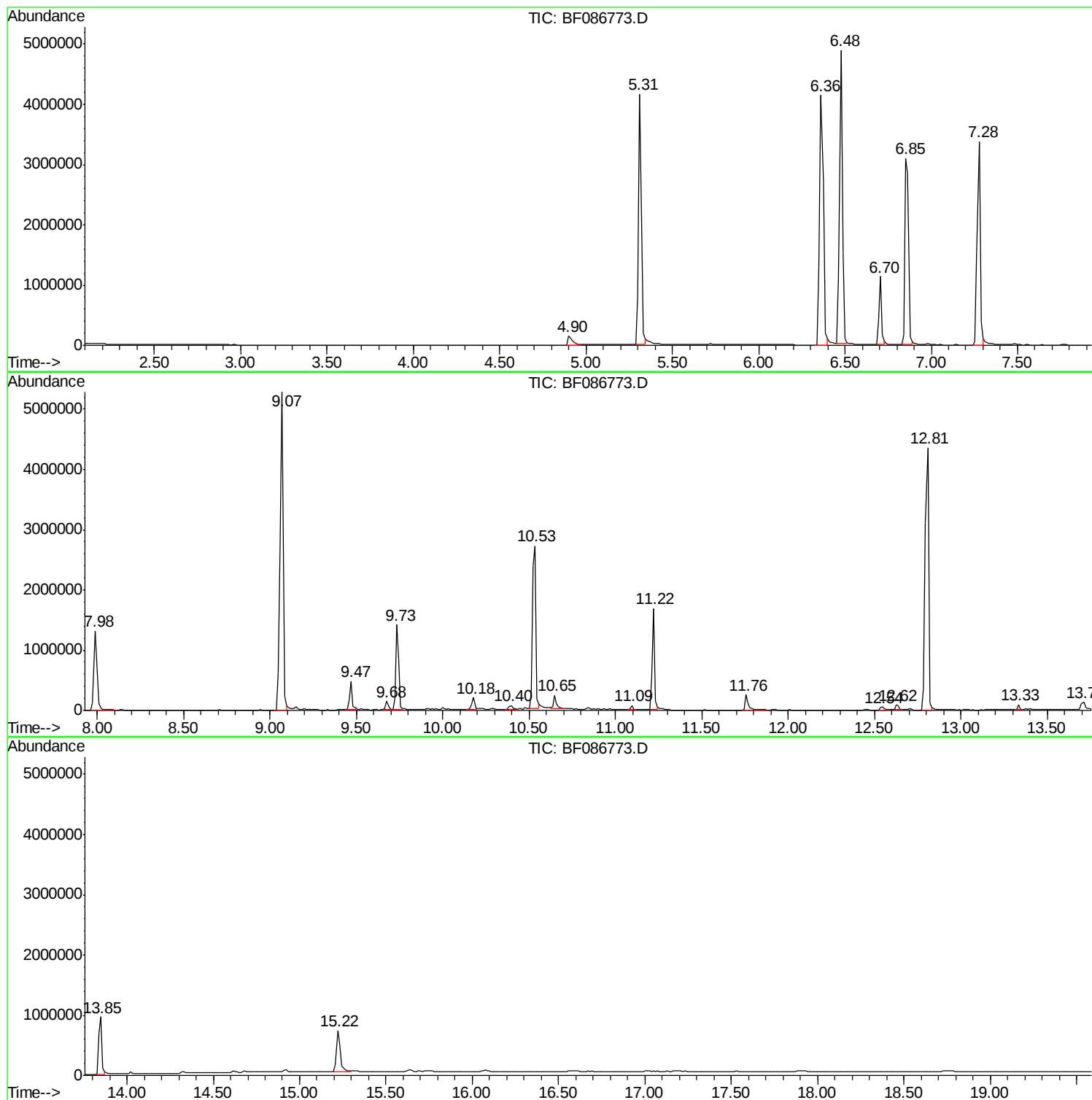
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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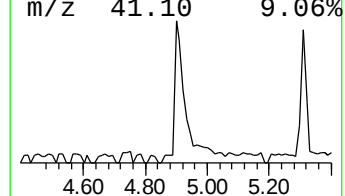
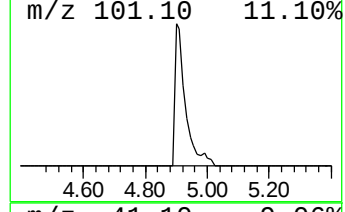
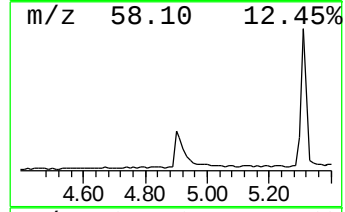
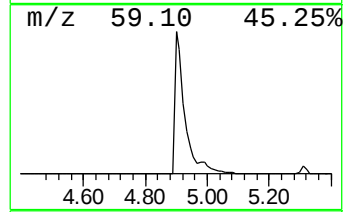
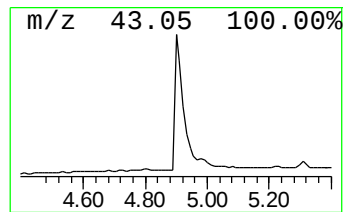
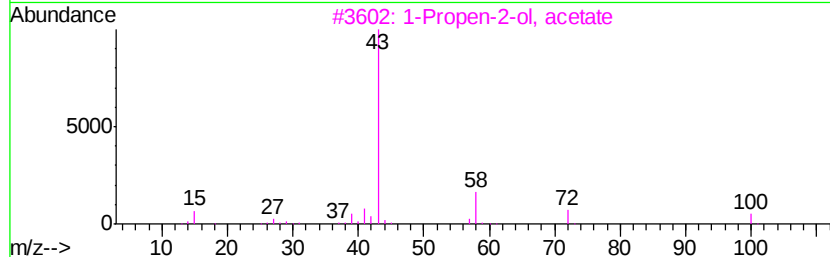
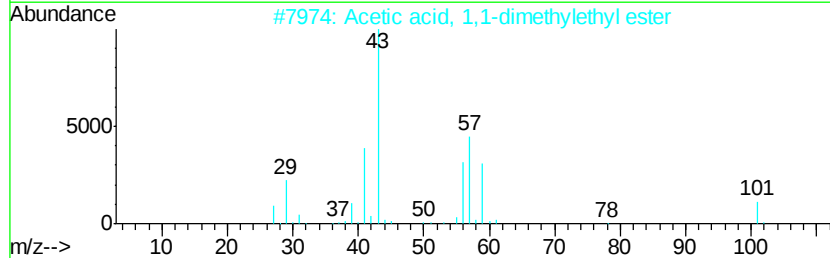
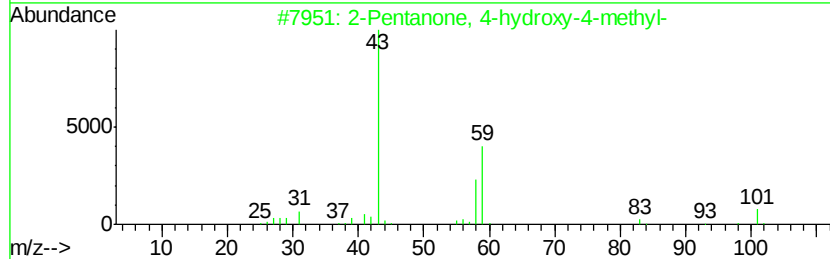
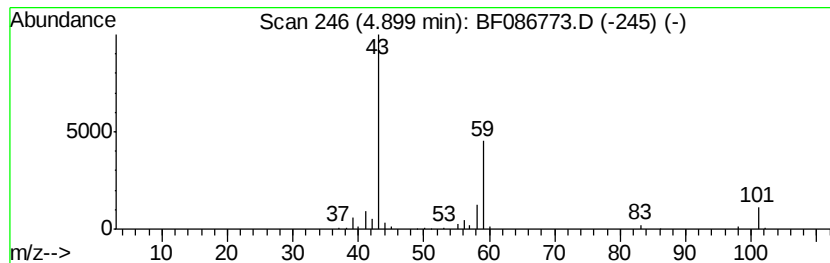
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	9.41 ng	283678	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane	58	C4H10	000106-97-8	9
5		Propylamine	59	C3H9N	000107-10-8	9



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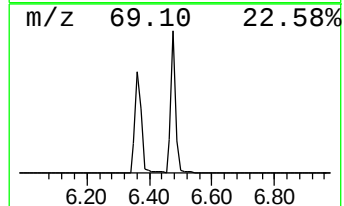
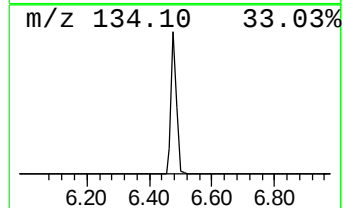
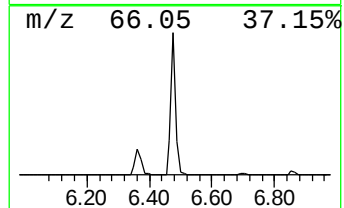
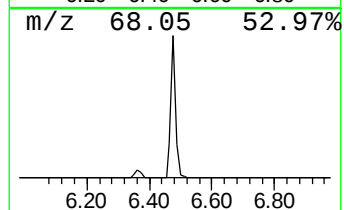
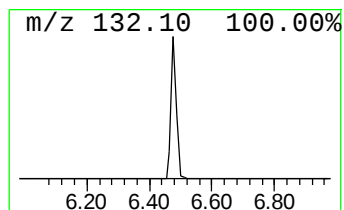
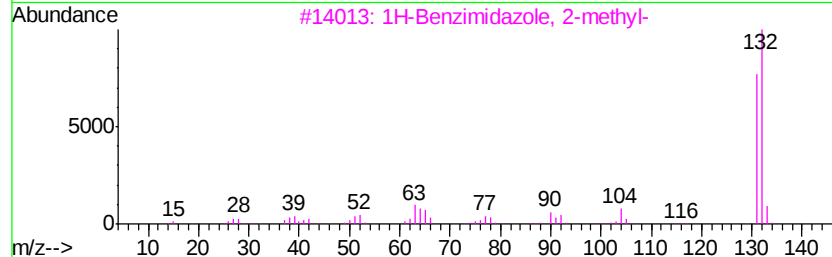
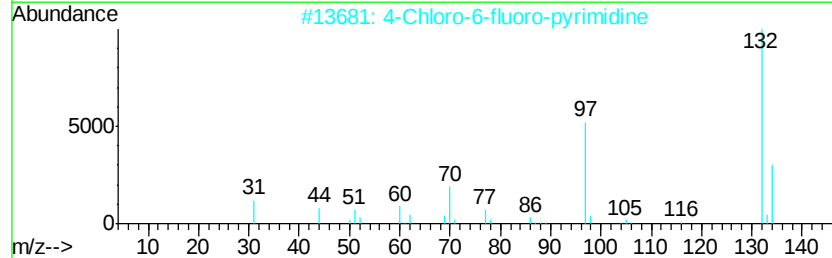
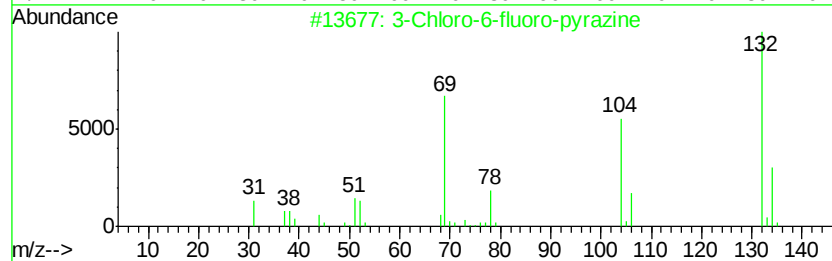
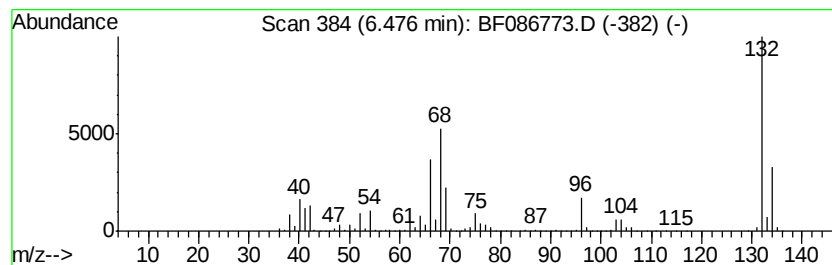
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	172.35 ng	5195760	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4			Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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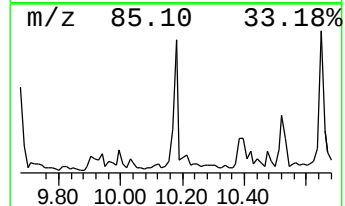
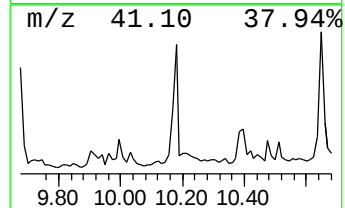
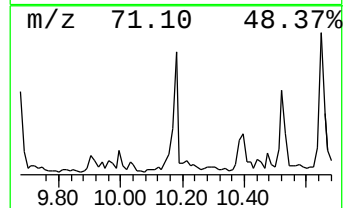
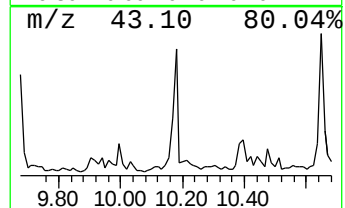
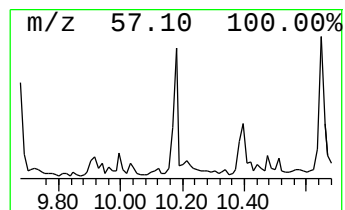
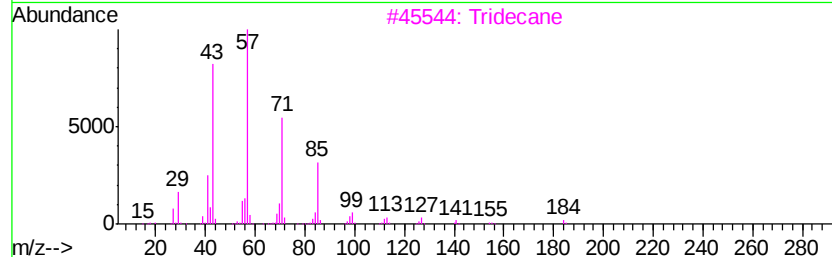
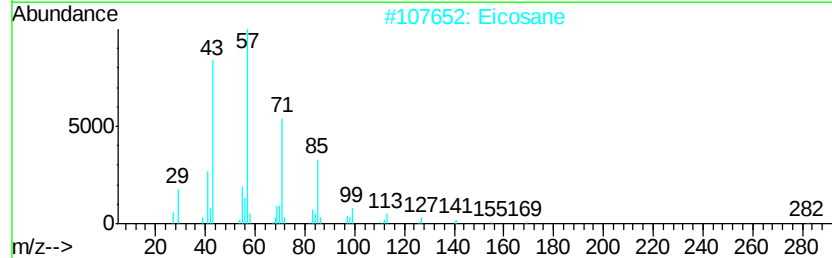
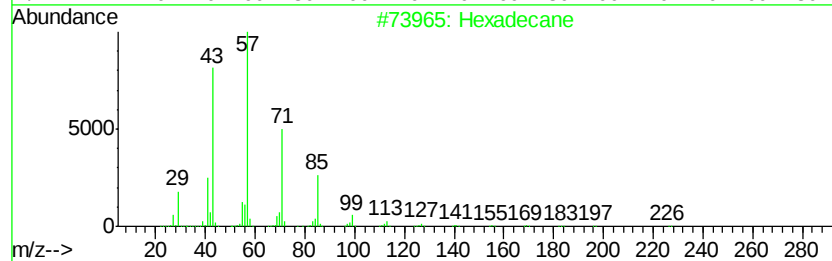
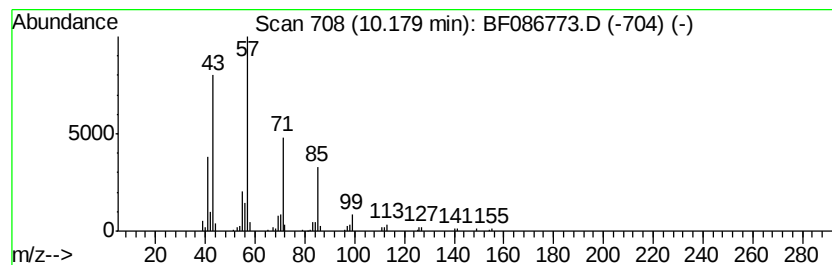
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.18	4.93 ng	211901	Acenaphthene-d10		9.73	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Eicosane		282	C20H42	000112-95-8	87
3	Tridecane		184	C13H28	000629-50-5	86
4	Tetradecane		198	C14H30	000629-59-4	80
5	Decane, 3-bromo-		220	C10H21Br	030571-71-2	80



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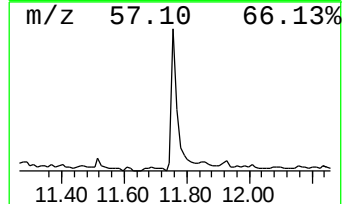
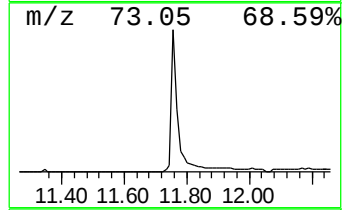
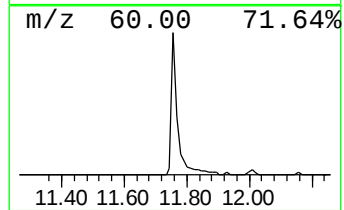
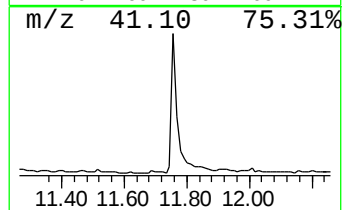
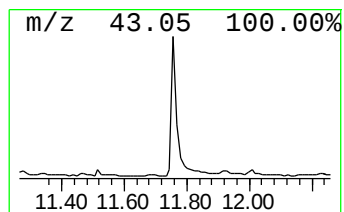
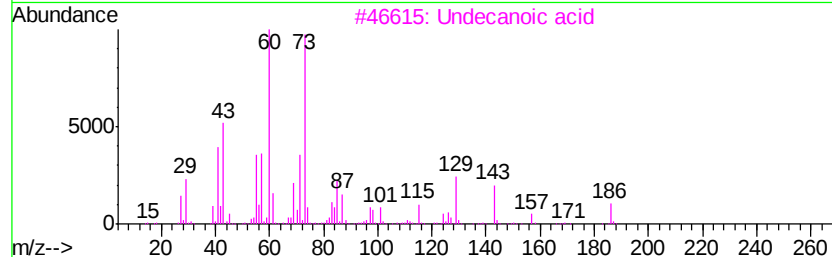
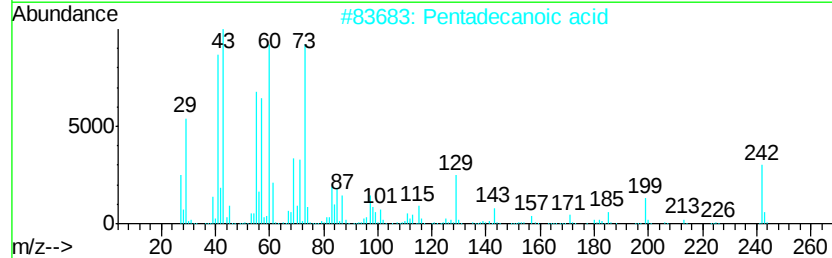
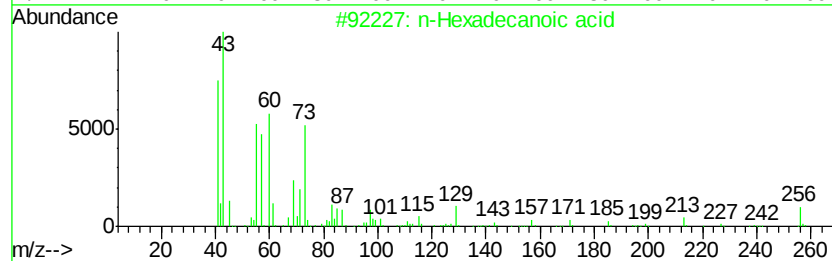
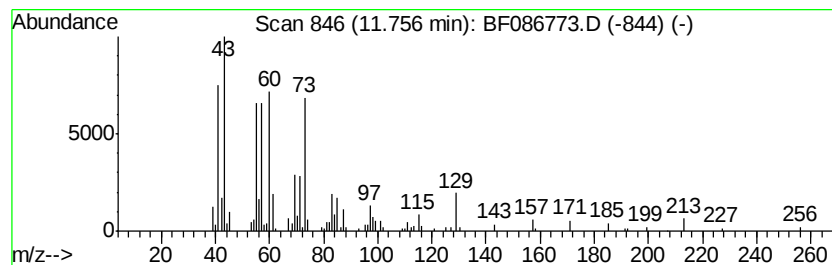
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	8.65 ng	357307	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Undecanoic acid	186	C11H22O2	000112-37-8	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Tridecanoic acid	214	C13H26O2	000638-53-9	72



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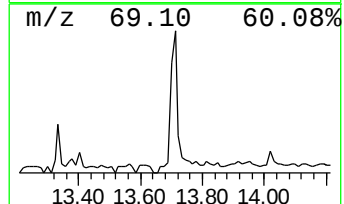
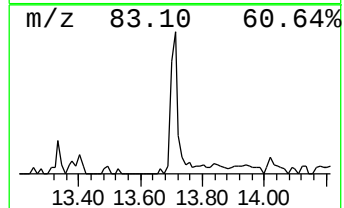
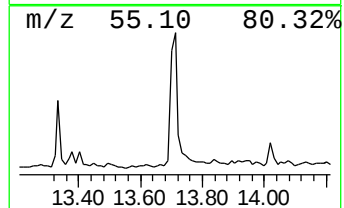
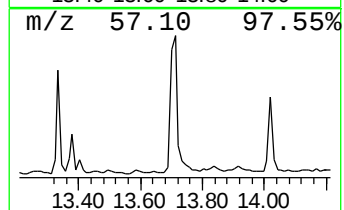
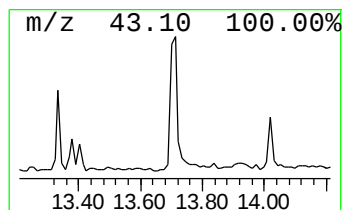
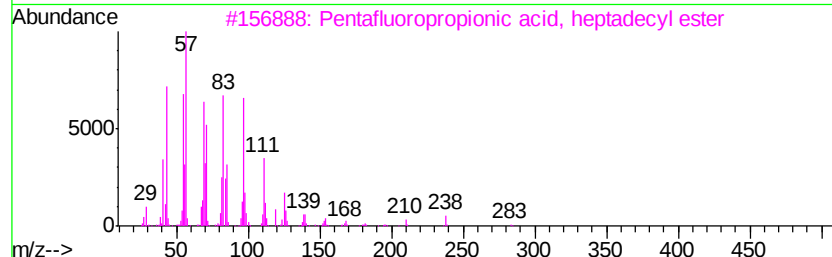
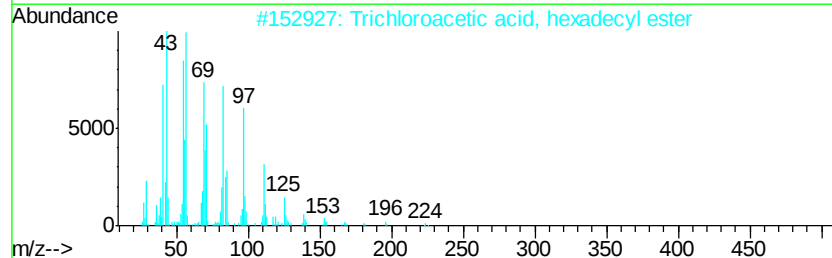
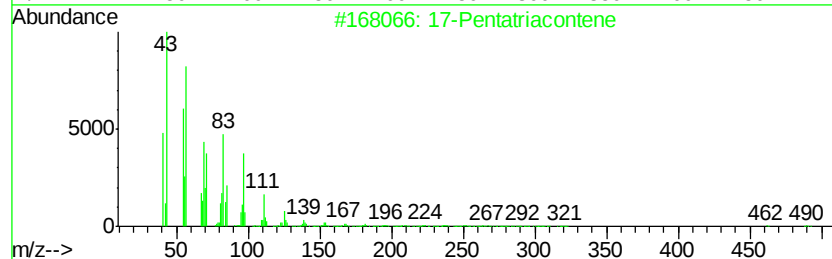
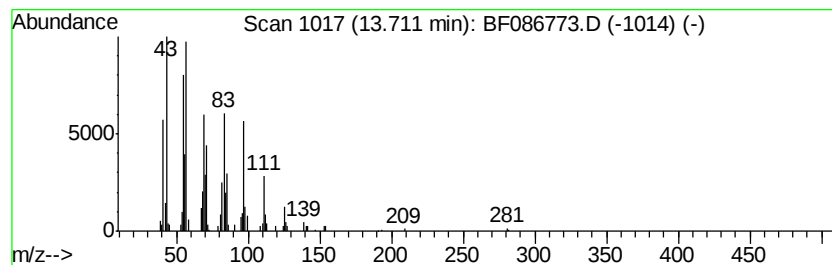
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Peak Number 7 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	6.67 ng	203813	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	9.4	ng	283678	1	6.70	1205870	40.0
unknown6.48	6.48	172.3	ng	5195760	1	6.70	1205870	40.0
Hexadecane	10.18	4.9	ng	211901	3	9.73	1719020	40.0
n-Hexadecanoic acid	11.76	8.7	ng	357307	4	11.22	1651620	40.0
17-Pentatriacontene	13.71	6.7	ng	203813	5	13.85	1222810	40.0