

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
 Data File : BF092303.D
 Acq On : 16 Jan 2017 23:46
 Operator : UM/SJ
 Sample : I1162-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-47-COMP

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-BF122116.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	4.679	250	253	272	rVB	1431400	2328549	41.55%	4.668%
2	5.147	292	294	315	rBV	3039145	4918761	87.77%	9.862%
3	6.233	386	389	391	rBV	4872167	5604145	100.00%	11.236%
4	6.336	396	398	400	rBV	5167300	4799555	85.64%	9.623%
5	6.564	415	418	420	rBV	1162728	1206153	21.52%	2.418%
6	6.713	429	431	434	rBV	3053616	3433086	61.26%	6.883%
7	7.136	465	468	470	rBV	3167327	2975712	53.10%	5.966%
8	7.845	528	530	533	rBV	1273705	1496313	26.70%	3.000%
9	8.930	622	625	627	rBV	5641653	5485382	97.88%	10.998%
10	9.330	658	660	662	rBV	514311	443488	7.91%	0.889%
11	9.548	677	679	681	rBV	76456	70847	1.26%	0.142%
12	9.593	681	683	685	rBV	2438084	2043410	36.46%	4.097%
13	10.039	721	722	724	rVB	105480	118850	2.12%	0.238%
14	10.268	739	742	745	rBV	40645	72967	1.30%	0.146%
15	10.382	750	752	755	rBV	3223063	3363979	60.03%	6.744%
16	10.519	762	764	768	rBV	129023	198251	3.54%	0.397%
17	10.965	801	803	804	rBV	75598	103198	1.84%	0.207%
18	11.068	810	812	815	rBV	2122650	1968394	35.12%	3.946%
19	11.628	859	861	866	rBV2	103751	152662	2.72%	0.306%
20	12.496	934	937	939	rBV	130691	122841	2.19%	0.246%
21	12.576	939	944	946	rVB2	31361	63029	1.12%	0.126%
22	12.656	948	951	953	rBV	5097873	5050569	90.12%	10.126%
23	13.194	996	998	1000	rBV	97360	104175	1.86%	0.209%
24	13.571	1028	1031	1039	rBV	152105	327193	5.84%	0.656%
25	13.697	1039	1042	1045	rBV	1966062	1904912	33.99%	3.819%
26	14.485	1106	1111	1114	rBV2	38122	75603	1.35%	0.152%
27	14.542	1114	1116	1119	rVV	64570	65813	1.17%	0.132%
28	15.045	1157	1160	1163	rBV	1019545	1250819	22.32%	2.508%
29	15.445	1192	1195	1198	rBV	41165	60535	1.08%	0.121%
30	15.857	1227	1231	1234	rBV	33658	68952	1.23%	0.138%

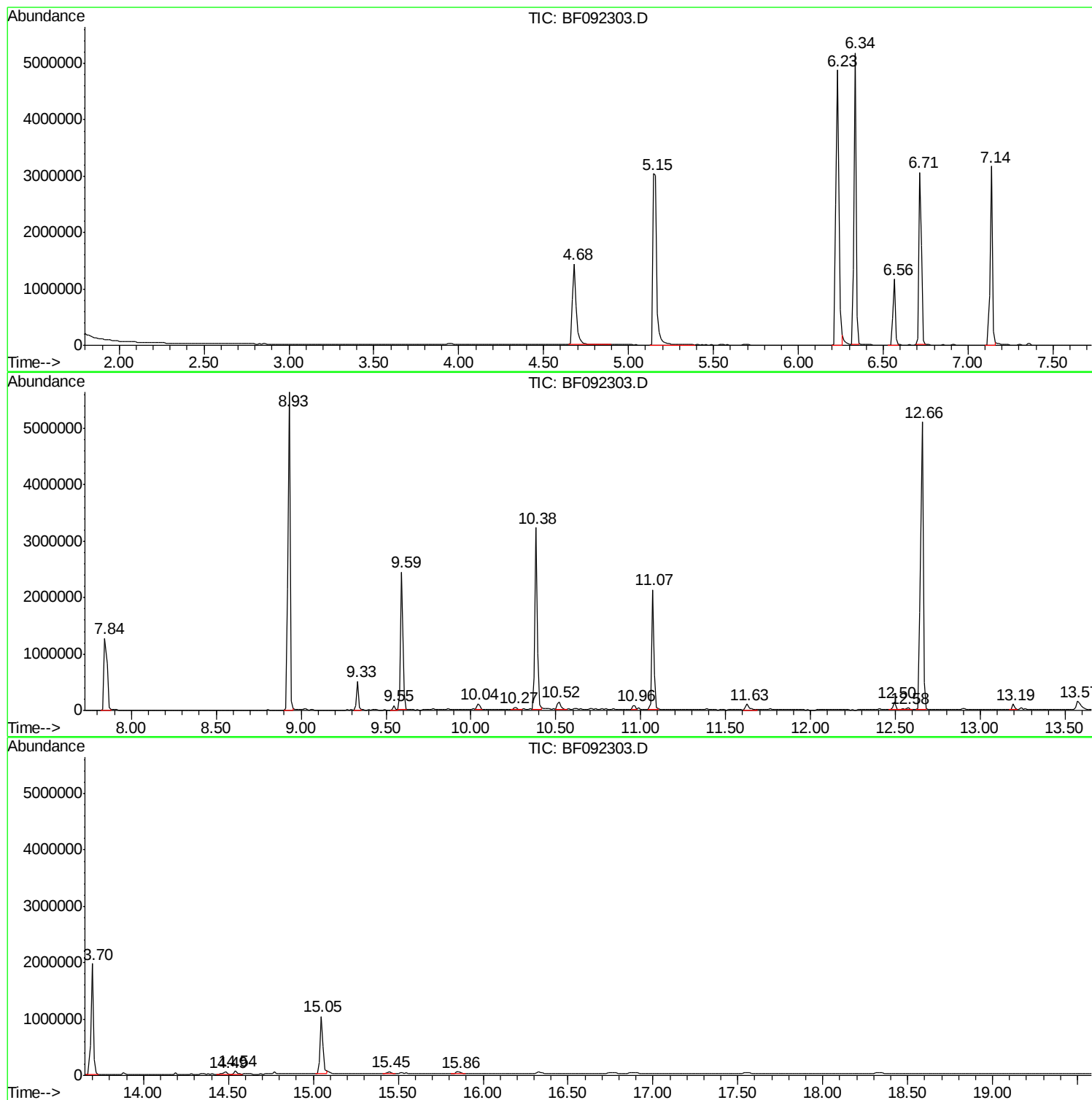
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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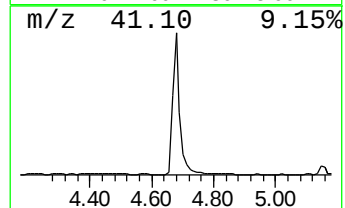
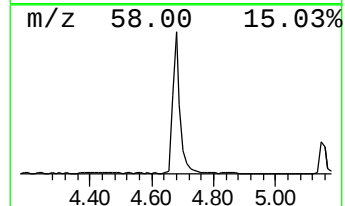
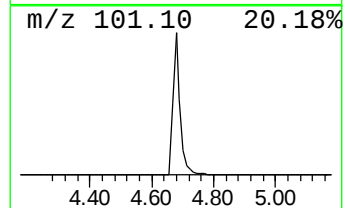
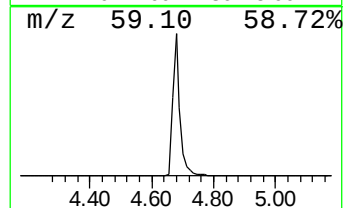
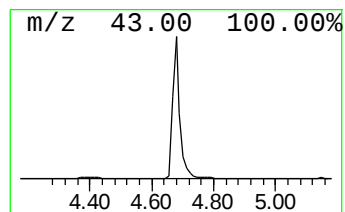
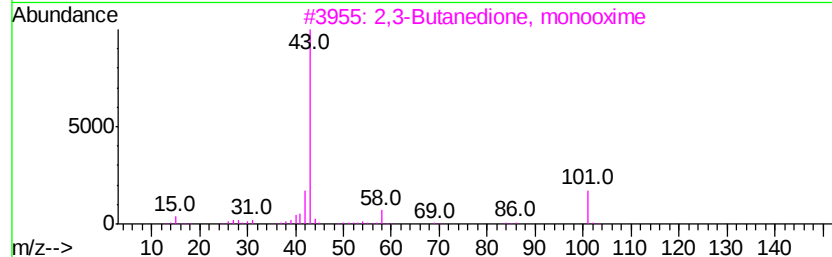
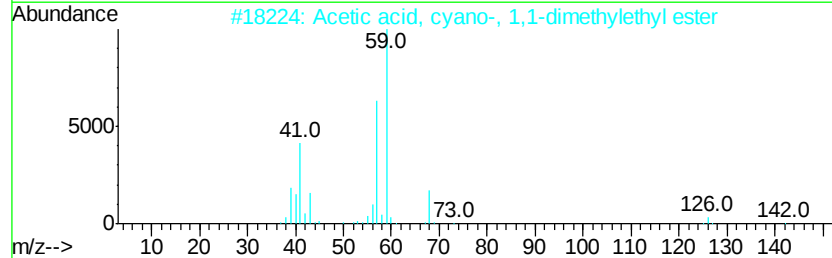
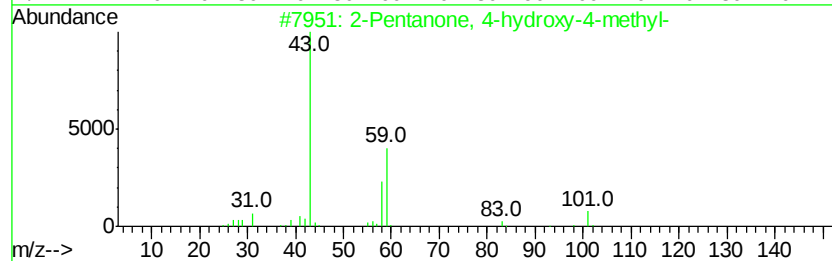
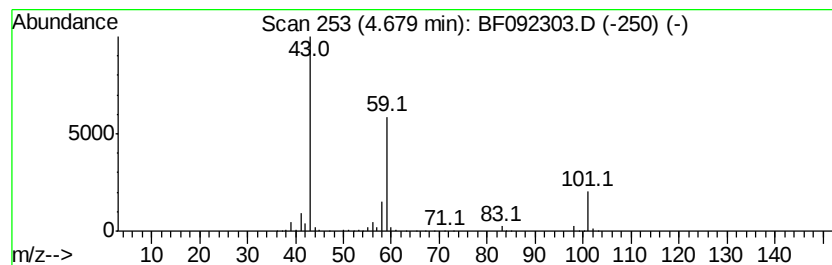
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	38.61 ng	2328550	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9	



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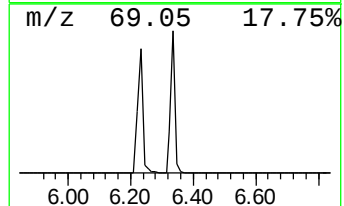
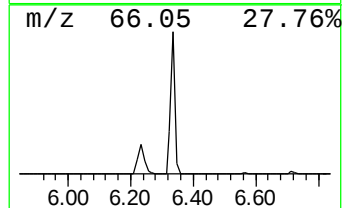
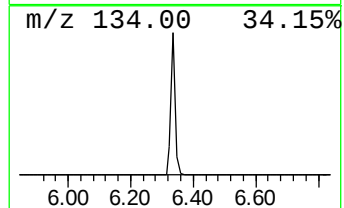
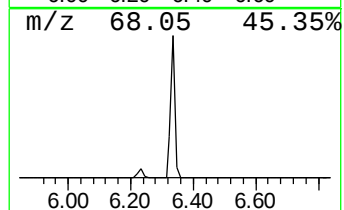
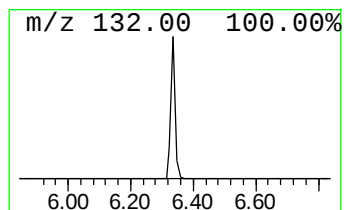
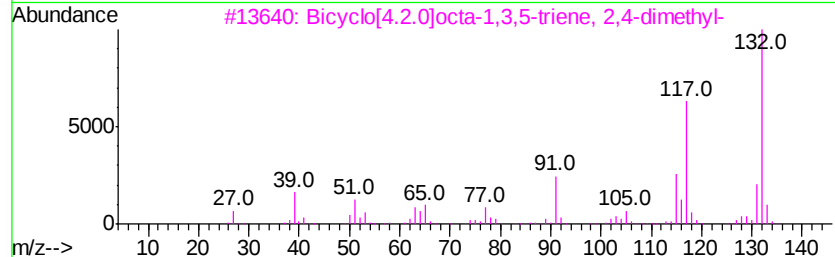
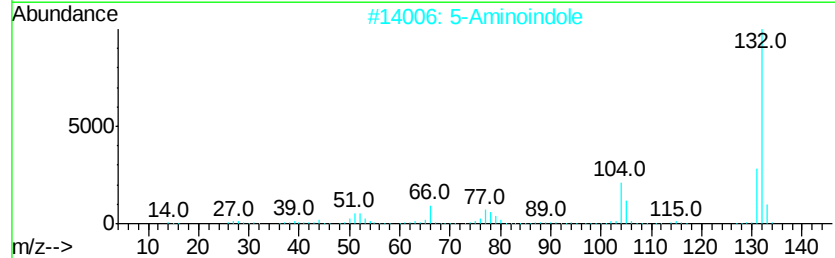
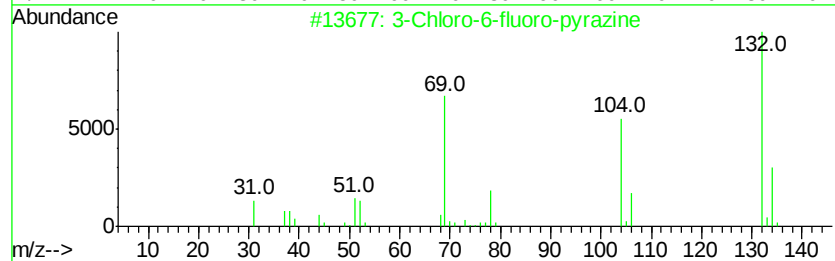
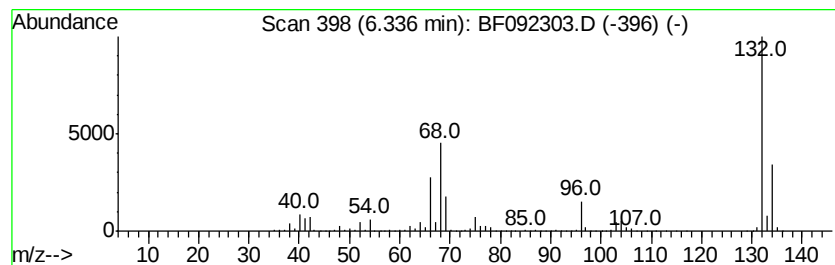
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Peak Number 2 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	79.58 ng	4799560	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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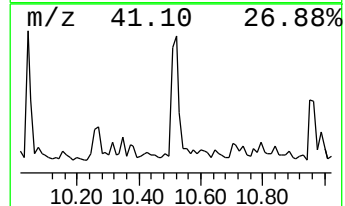
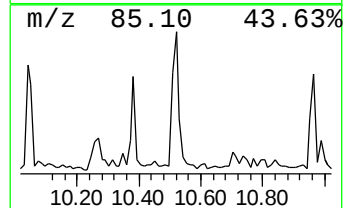
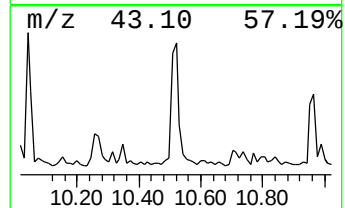
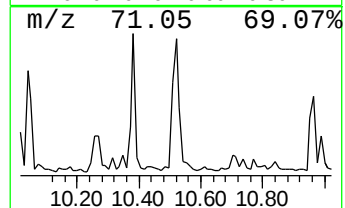
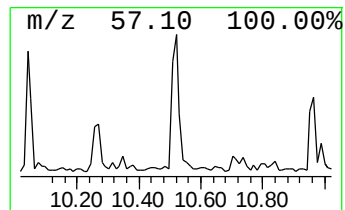
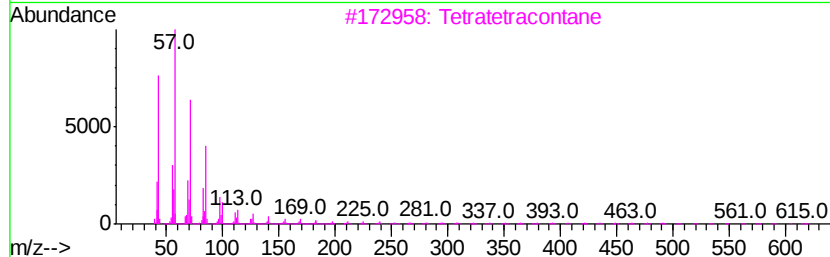
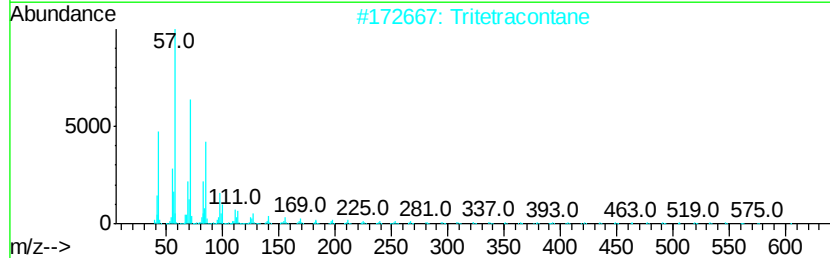
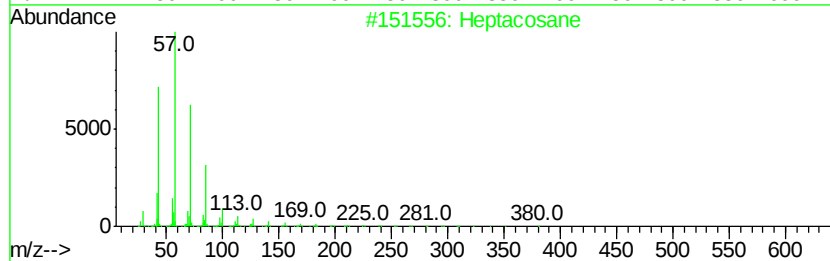
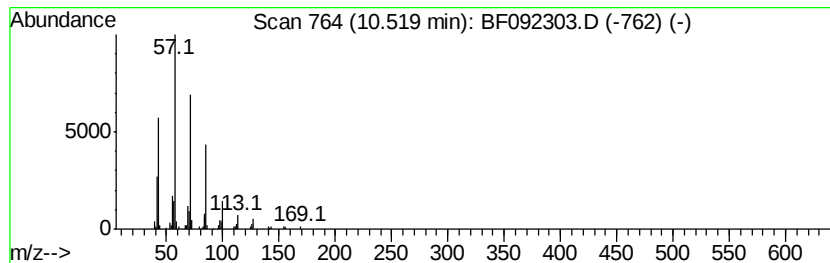
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Peak Number 4 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	2.01 ng	198251	Phenanthrene-d10	11.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Tritetracontane		605	C43H88	007098-21-7	90
3	Tetratetracontane		619	C44H90	007098-22-8	90
4	Tetracosane		338	C24H50	000646-31-1	90
5	Hexadecane		226	C16H34	000544-76-3	90



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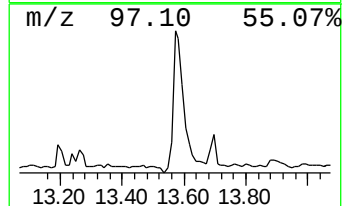
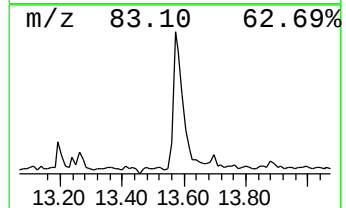
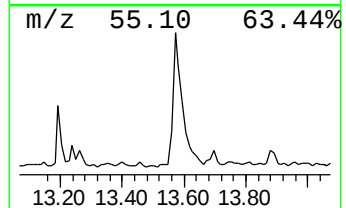
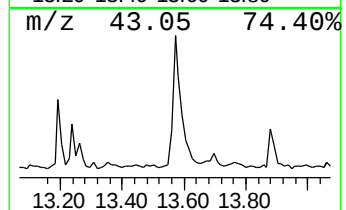
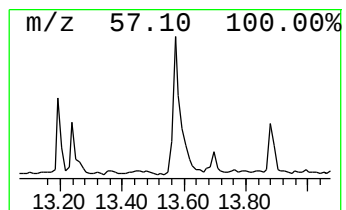
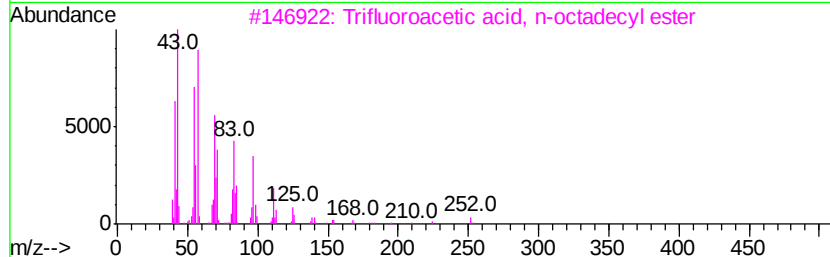
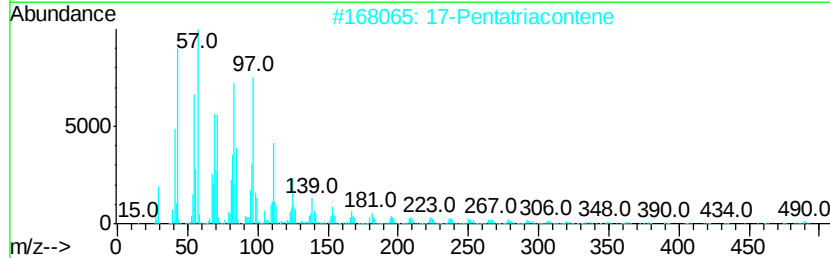
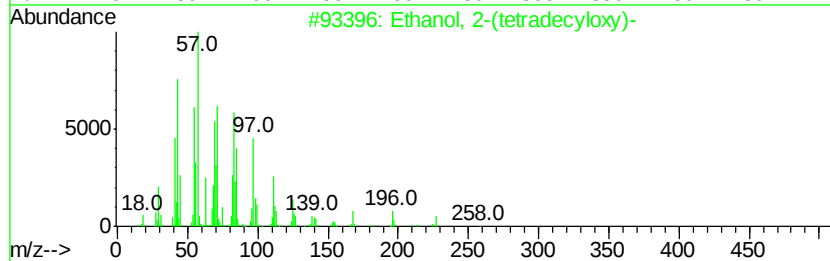
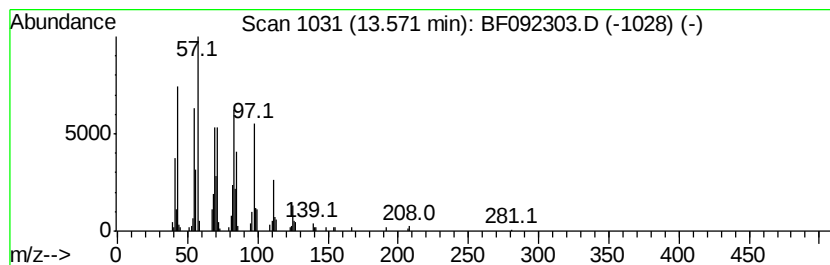
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	3.44 ng	327193	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2		17-Pentatriacontene	491	C35H70	006971-40-0	90
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	87
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	86
5		1-Octadecanol	270	C18H38O	000112-92-5	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	38.6	ng	2328550	1	6.56	1206150	20.0
unknown6.34	6.34	79.6	ng	4799560	1	6.56	1206150	20.0
Heptacosane	10.52	2.0	ng	198251	4	11.07	1968390	20.0
Ethanol, 2-(tetra...	13.57	3.4	ng	327193	5	13.70	1904910	20.0