

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
 Data File : BF092552.D
 Acq On : 27 Jan 2017 3:48
 Operator : SJ/MA
 Sample : I1452-05
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-23

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-BF012417.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	5.150	266	268	274	rBV	484507	562953	12.54%	1.601%
2	5.562	301	304	307	rBV	2083923	1857640	41.39%	5.282%
3	6.590	391	394	396	rBV	1449462	1317250	29.35%	3.745%
4	6.739	404	407	409	rBV	2502280	3460616	77.11%	9.840%
5	6.967	425	427	429	rBV	1231410	1047677	23.34%	2.979%
6	7.127	438	441	443	rBV	3292444	3193186	71.15%	9.079%
7	7.539	474	477	479	rBV	2566884	3039058	67.72%	8.641%
8	8.259	537	540	542	rBV	1382374	1328294	29.60%	3.777%
9	8.533	558	564	567	rBV	24058	56073	1.25%	0.159%
10	8.991	600	604	606	rBV	64705	98755	2.20%	0.281%
11	9.185	617	621	623	rBV3	25101	80394	1.79%	0.229%
12	9.231	623	625	630	rVB5	25108	61090	1.36%	0.174%
13	9.345	631	635	638	rBV	4044359	4487903	100.00%	12.761%
14	9.745	667	670	672	rBV	451117	504852	11.25%	1.435%
15	9.836	674	678	680	rBV4	35273	63806	1.42%	0.181%
16	10.031	692	695	697	rBV	1566536	1580843	35.22%	4.495%
17	10.225	707	712	714	rBV4	32525	86426	1.93%	0.246%
18	10.316	717	720	722	rVV4	47264	86411	1.93%	0.246%
19	10.442	729	731	734	rVB3	82648	127201	2.83%	0.362%
20	10.545	737	740	741	rBV3	31083	46989	1.05%	0.134%
21	10.671	749	751	754	rBV3	94183	102947	2.29%	0.293%
22	10.819	761	764	767	rBV	2507765	2723520	60.69%	7.744%
23	10.865	767	768	770	rVV	63550	69245	1.54%	0.197%
24	10.934	772	774	778	rVB	88576	133442	2.97%	0.379%
25	11.025	778	782	787	rBV8	25060	79543	1.77%	0.226%
26	11.379	811	813	815	rBV2	84472	92637	2.06%	0.263%
27	11.516	822	825	827	rBV	1799107	1548747	34.51%	4.404%
28	11.722	841	843	846	rBV	148880	147864	3.29%	0.420%
29	11.802	849	850	853	rVB	39236	52703	1.17%	0.150%
30	12.042	869	871	878	rVB2	83716	129284	2.88%	0.368%
31	12.877	942	944	946	rBV	127287	139318	3.10%	0.396%
32	12.922	946	948	950	rVV	97833	89223	1.99%	0.254%
33	12.991	952	954	958	rVB	74296	102801	2.29%	0.292%
34	13.105	961	964	967	rBV	3787852	3936540	87.71%	11.193%

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35	13.631	1008	1010	1011	rBV	63222	61419	1.37%	0.175%
36	13.882	1031	1032	1035	rBV	71739	69301	1.54%	0.197%
37	13.997	1040	1042	1051	rVB	113936	162158	3.61%	0.461%
38	14.157	1053	1056	1058	rBV	1362631	1326501	29.56%	3.772%
39	15.631	1182	1185	1188	rBV	681844	993526	22.14%	2.825%
40	16.111	1225	1227	1230	rVB2	30682	51097	1.14%	0.145%
41	16.637	1270	1273	1277	rVB2	29535	70883	1.58%	0.202%

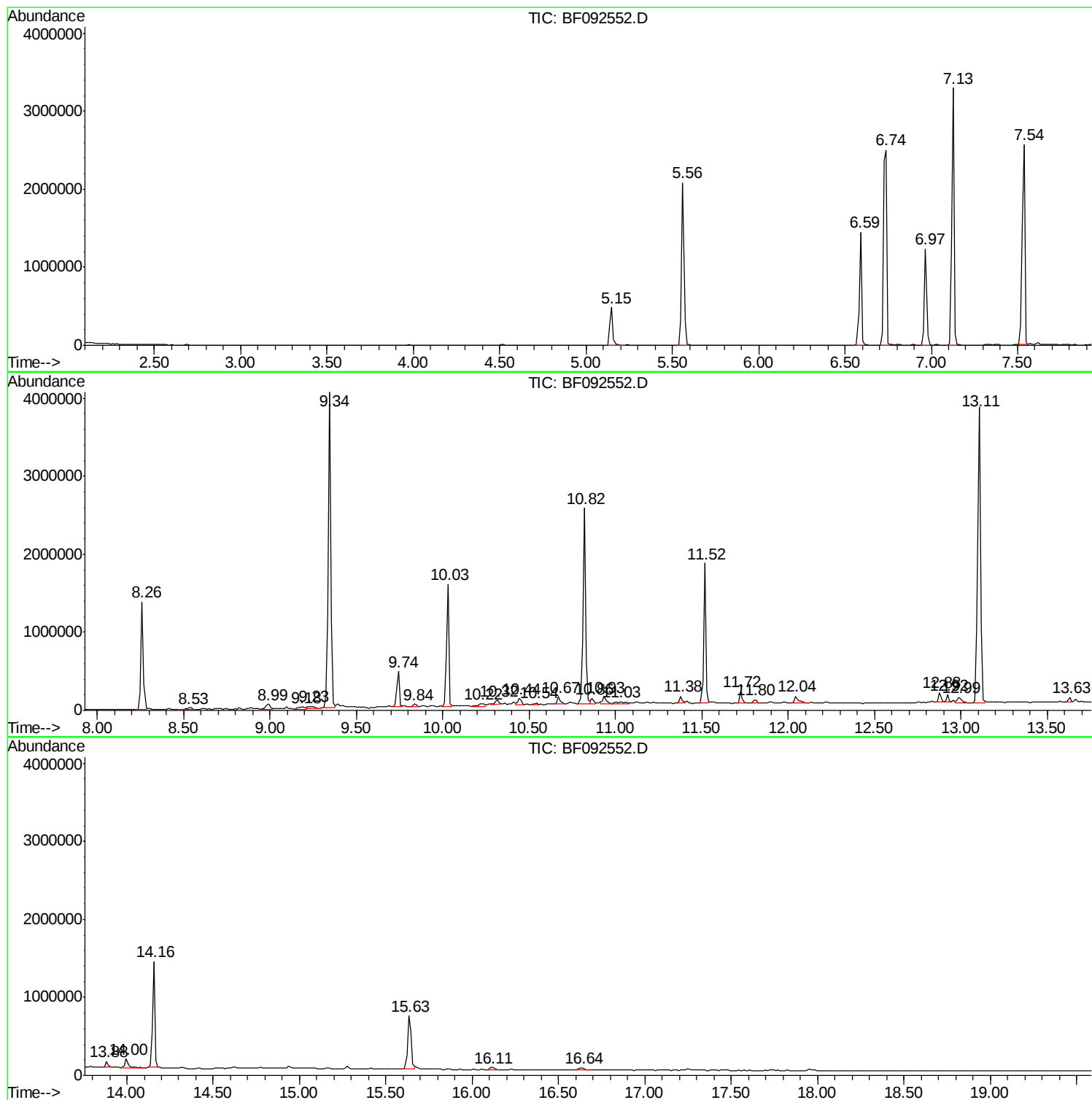
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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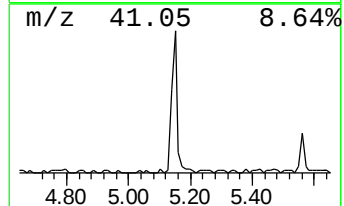
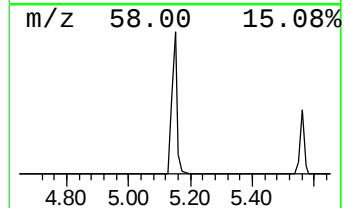
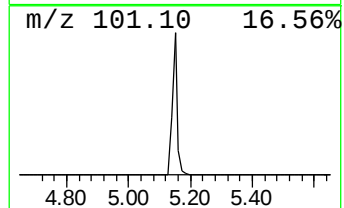
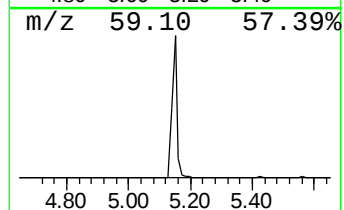
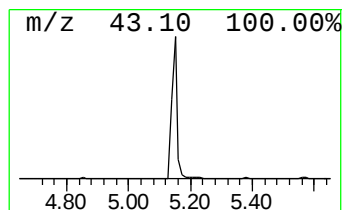
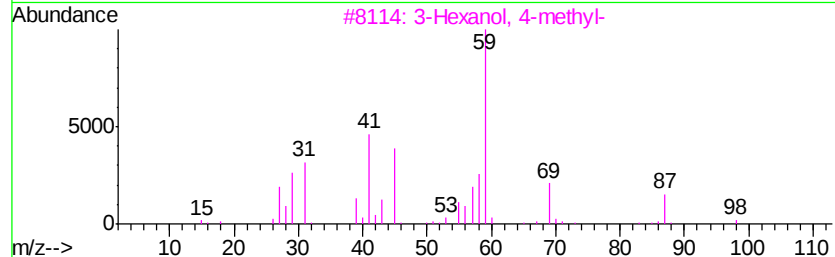
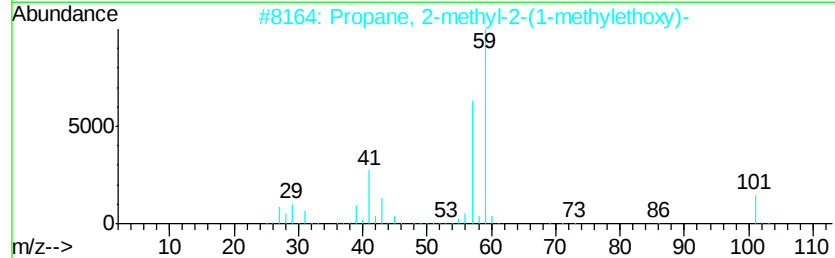
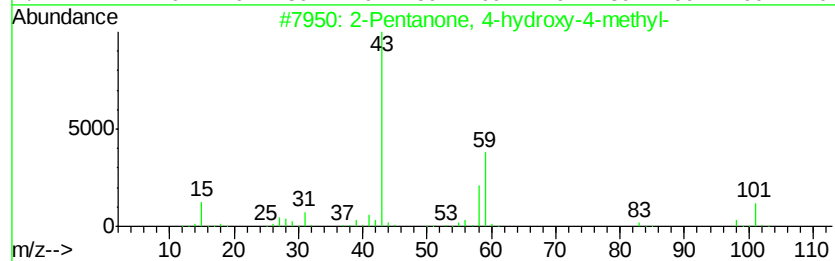
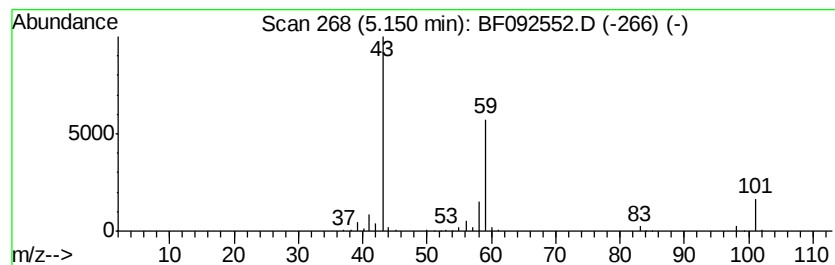
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	10.75 ng	562953	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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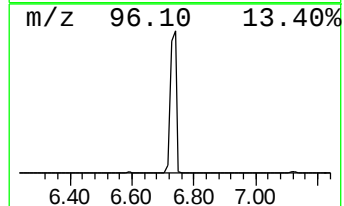
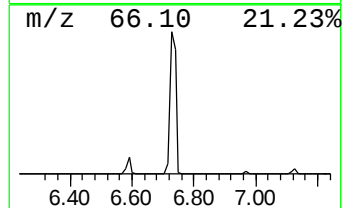
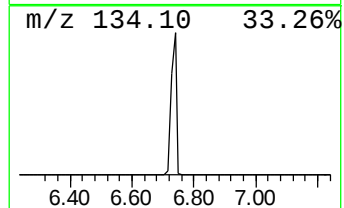
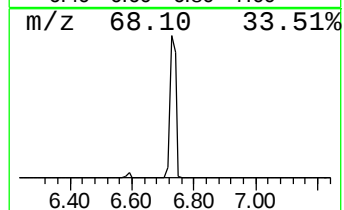
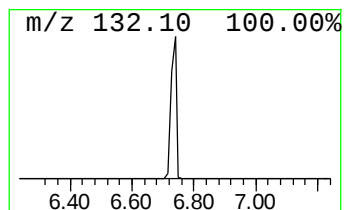
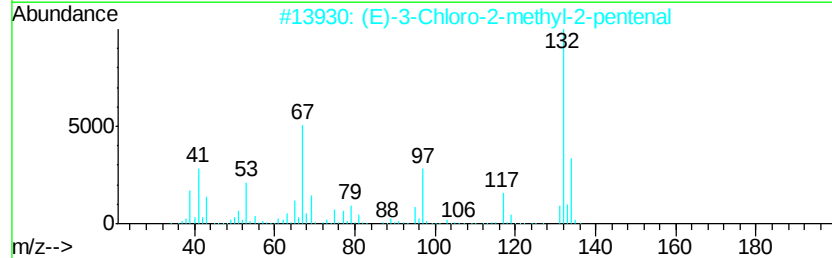
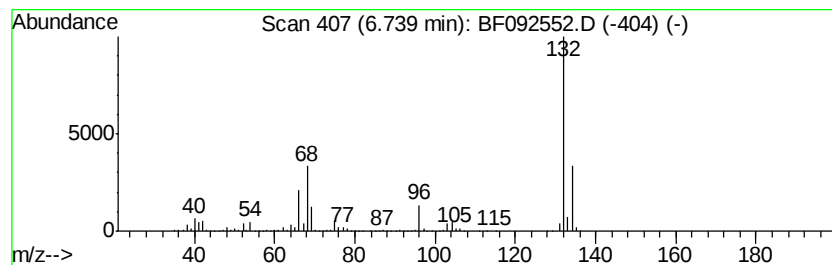
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	66.06 ng	3460620	1,4-Dichlorobenzene-d4	6.97

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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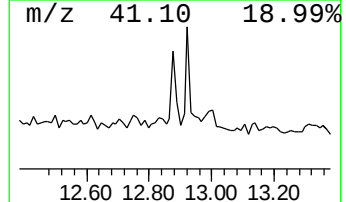
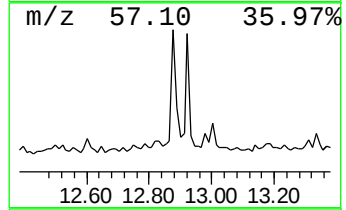
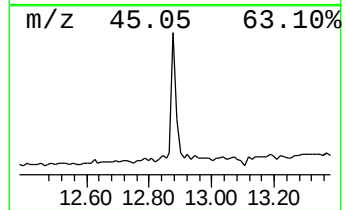
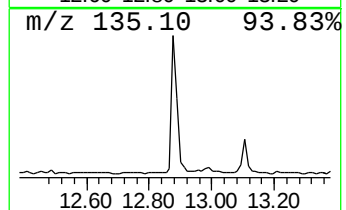
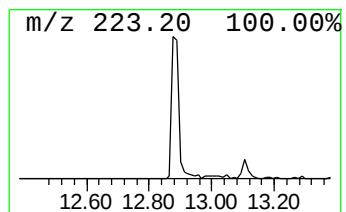
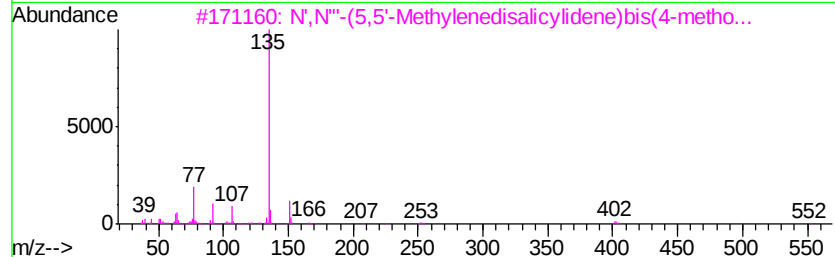
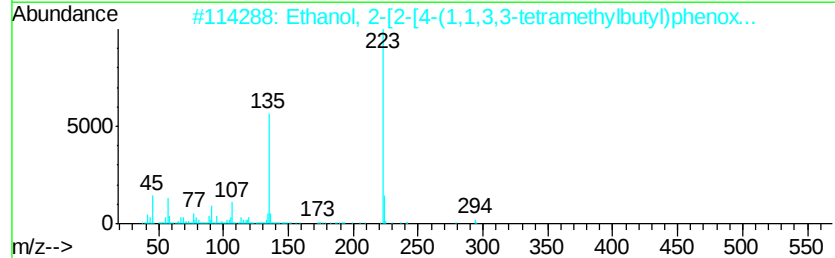
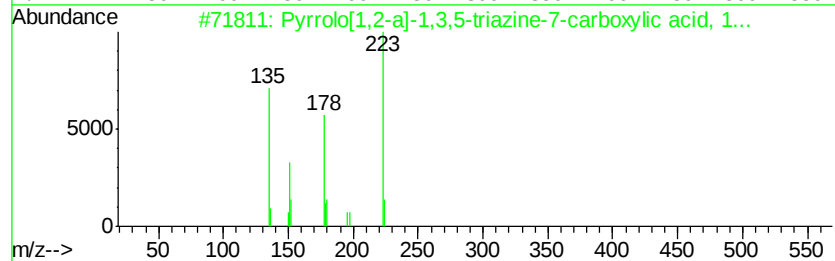
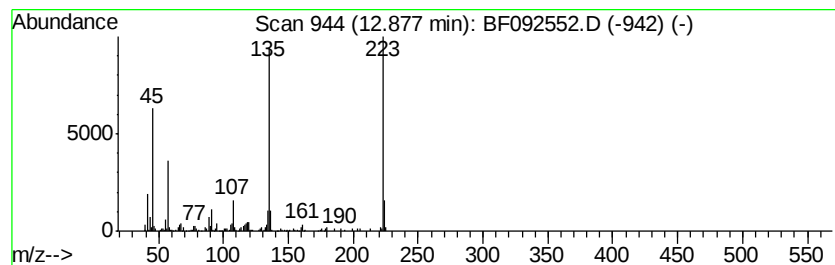
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Peak Number 4 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	2.10 ng	139318	Chrysene-d12	14.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2		Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	58
3		N',N'''-(5,5'-Methylenedisalicyl...	552	C31H28N4O6	328019-12-1	27
4		Pyridine, 4-ethyl-2,6-dimethyl-	135	C9H13N	036917-36-9	27
5		3,5-Dihydropyrrolo(3,2-d)pyrimid...	135	C6H5N3O	005655-01-6	27



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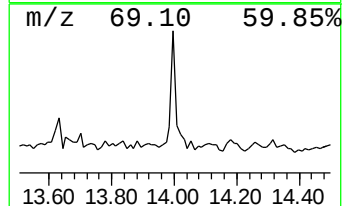
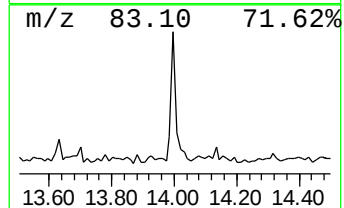
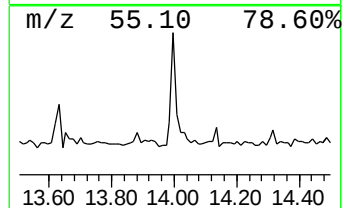
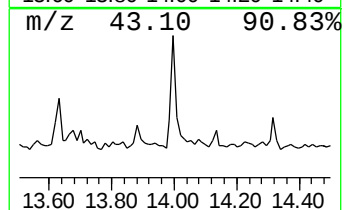
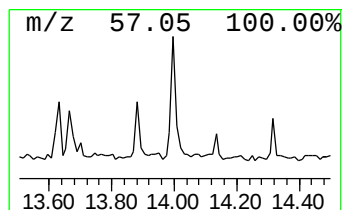
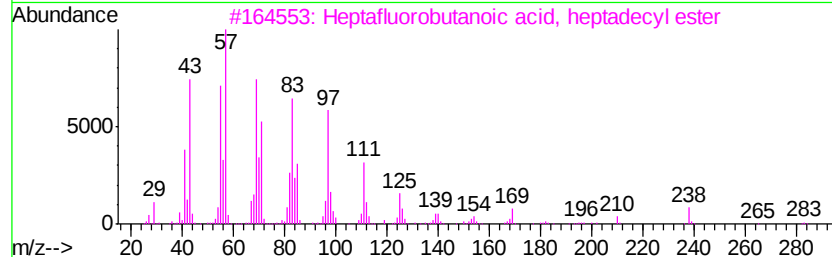
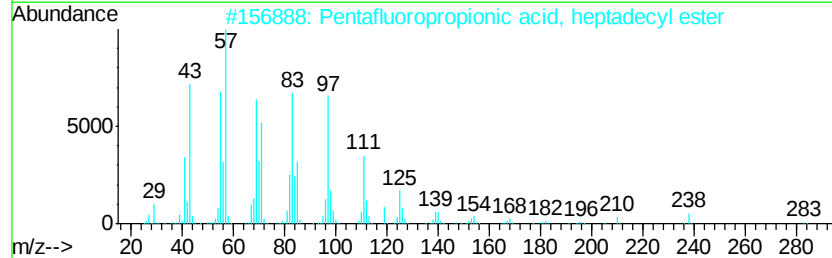
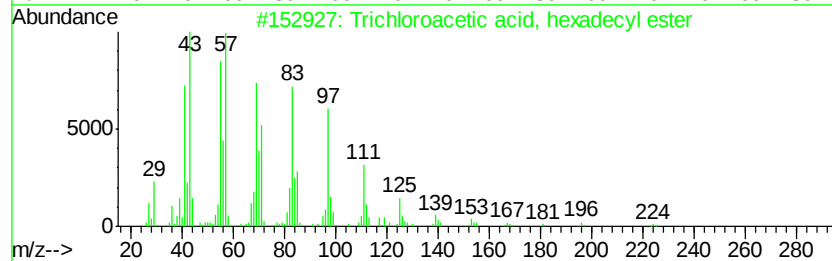
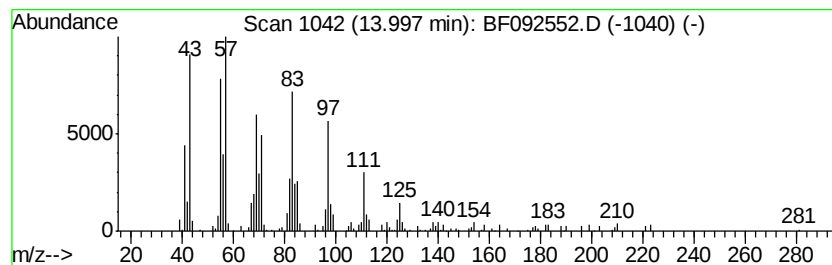
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.44 ng	162158	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	93
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4		Cyclopentadecane	210	C15H30	000295-48-7	92
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	10.8	ng	562953	1	6.97	1047680	20.0
unknown6.74	6.74	66.1	ng	3460620	1	6.97	1047680	20.0
Pyrrolo[1,2-a]-1,...	12.88	2.1	ng	139318	5	14.16	1326500	20.0
Trichloroacetic a...	14.00	2.4	ng	162158	5	14.16	1326500	20.0