

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061318\
 Data File : BF106424.D
 Acq On : 14 Jun 2018 6:36
 Operator : JU/SJ
 Sample : J3447-02
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-20

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	5.190	482	485	491	rVB	120442	122641	3.24%	0.437%
2	5.613	553	557	565	rVB	1482593	1668303	44.02%	5.946%
3	5.760	576	582	585	rBV	65556	61350	1.62%	0.219%
4	6.613	723	727	733	rBV	1009985	1133311	29.90%	4.039%
5	6.678	733	738	742	rVB	50699	61411	1.62%	0.219%
6	6.748	746	750	753	rBV	3046078	2718321	71.72%	9.688%
7	6.966	783	787	790	rBV	1038291	832844	21.98%	2.968%
8	7.125	808	814	817	rVB	2810142	2711626	71.55%	9.664%
9	7.242	829	834	836	rBV2	40859	40458	1.07%	0.144%
10	7.284	840	841	845	rVB	50617	41349	1.09%	0.147%
11	7.531	876	883	886	rVB	2402331	2325437	61.36%	8.288%
12	7.619	895	898	901	rVB3	62825	65373	1.72%	0.233%
13	7.695	905	911	913	rBV5	38433	60013	1.58%	0.214%
14	7.731	913	917	922	rBV6	41203	72713	1.92%	0.259%
15	7.807	927	930	933	rVV2	114418	94337	2.49%	0.336%
16	7.836	933	935	940	rVB2	43376	44895	1.18%	0.160%
17	7.931	948	951	953	rVB	85983	66422	1.75%	0.237%
18	7.984	953	960	964	rVB2	47082	73896	1.95%	0.263%
19	8.172	984	992	996	rBV6	24499	51172	1.35%	0.182%
20	8.207	996	998	1001	rVB	53495	40537	1.07%	0.144%
21	8.248	1001	1005	1008	rBV	1347529	1085361	28.64%	3.868%
22	9.325	1183	1188	1191	rBV	4070449	3789952	100.00%	13.507%
23	9.713	1250	1254	1257	rBV	306306	246192	6.50%	0.877%
24	9.919	1285	1289	1292	rBV	79942	62996	1.66%	0.225%
25	10.007	1300	1304	1308	rVB	1402348	1176318	31.04%	4.192%
26	10.419	1372	1374	1377	rVB2	107205	83010	2.19%	0.296%
27	10.801	1434	1439	1442	rBV	2500539	2345808	61.90%	8.360%
28	10.895	1452	1455	1464	rVB	92131	103342	2.73%	0.368%
29	11.342	1528	1531	1534	rBV	50703	38825	1.02%	0.138%
30	11.495	1553	1557	1561	rBV	1332620	1157288	30.54%	4.125%
31	12.007	1641	1644	1649	rBV	91329	92528	2.44%	0.330%
32	13.083	1822	1827	1830	rBV	3525213	3447458	90.96%	12.287%
33	13.966	1973	1977	1983	rBV	151925	152456	4.02%	0.543%
34	14.142	2003	2007	2011	rBV	1088240	951954	25.12%	3.393%

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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

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35	15.001	2149	2153	2157	rVB	93155	93031	2.45%	0.332%
36	15.677	2262	2268	2277	rVB	735827	945458	24.95%	3.370%

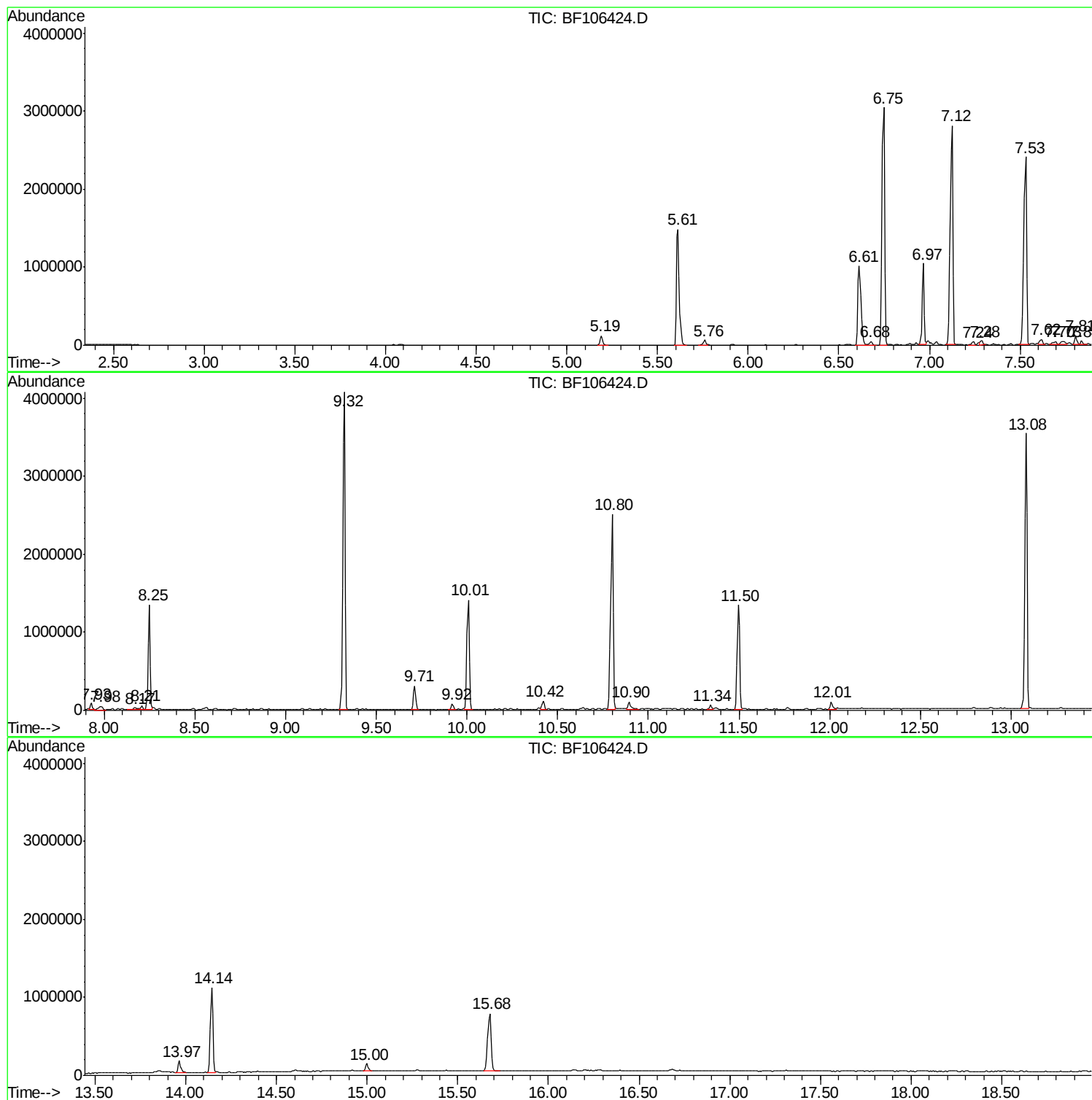
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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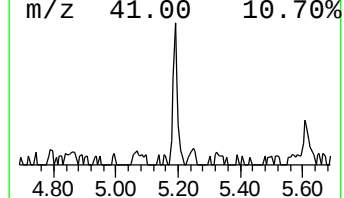
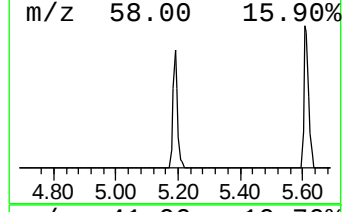
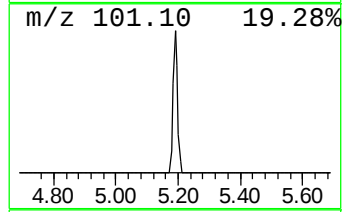
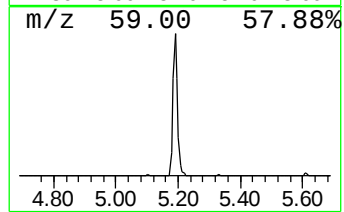
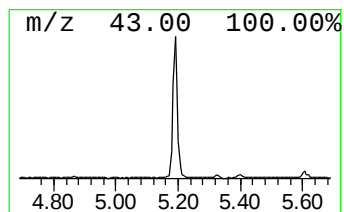
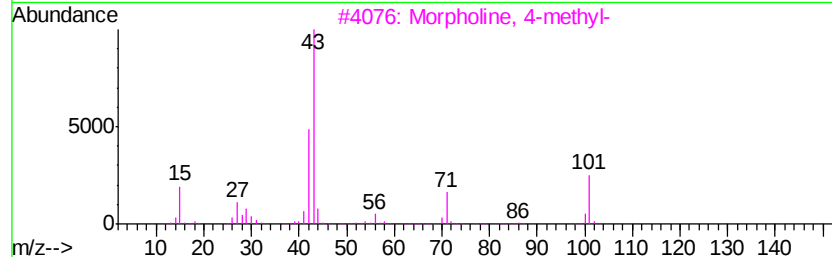
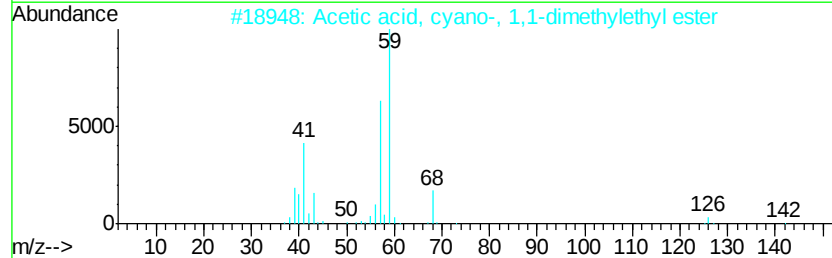
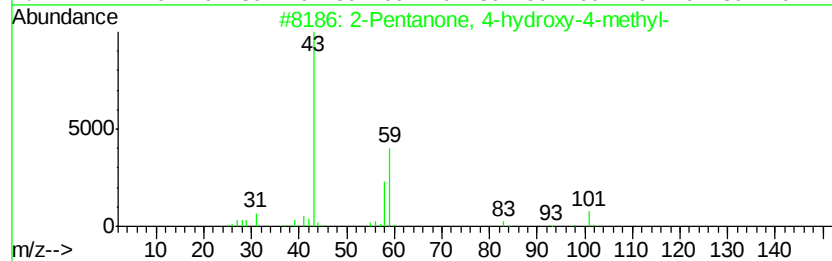
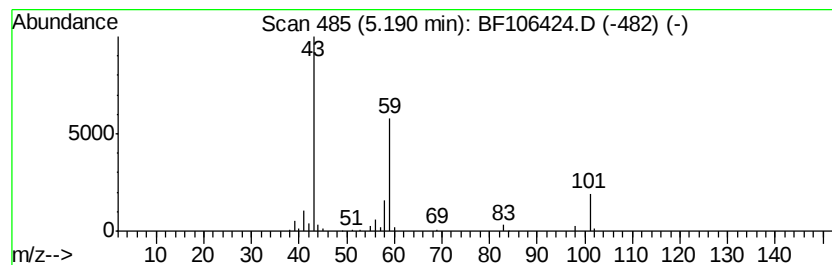
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.95 ng	122641	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	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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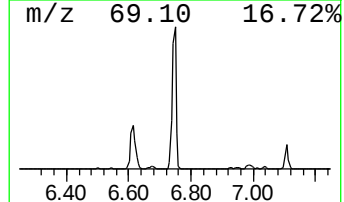
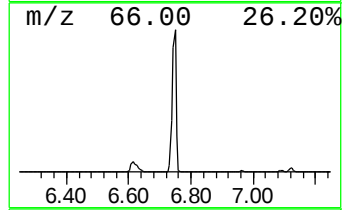
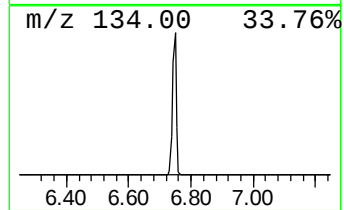
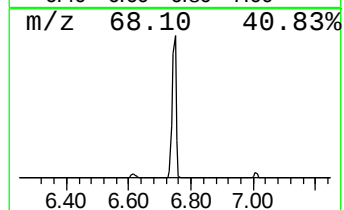
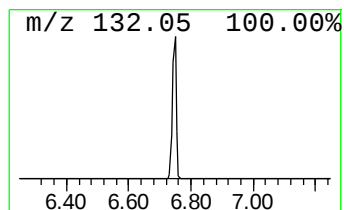
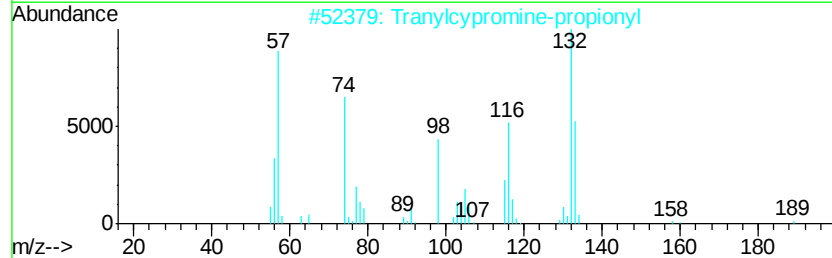
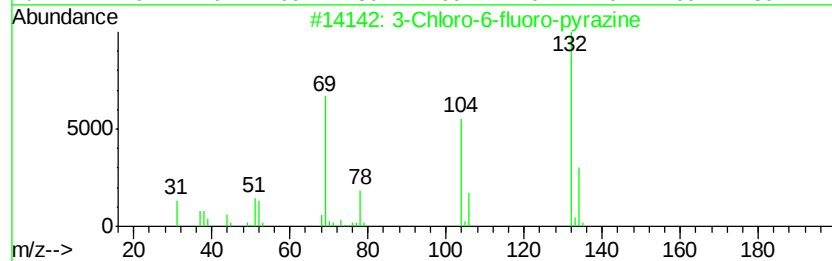
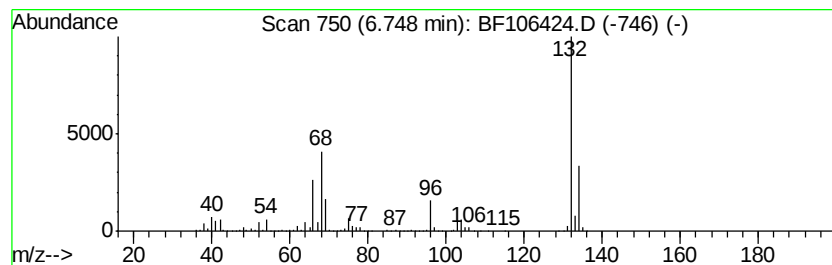
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	65.28 ng	2718320	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	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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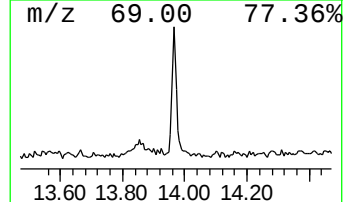
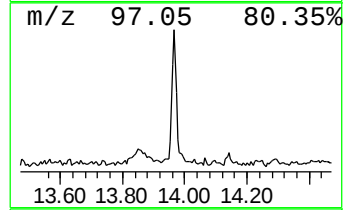
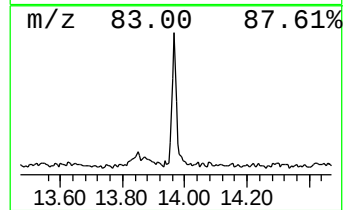
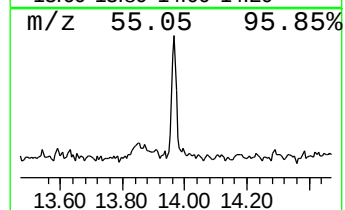
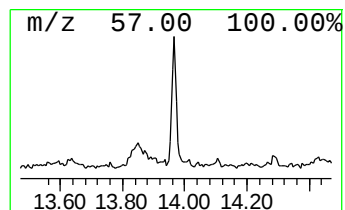
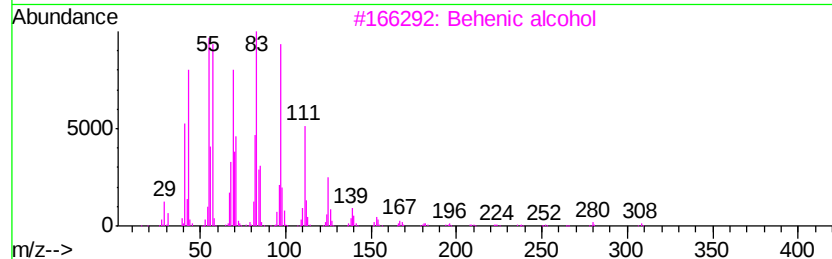
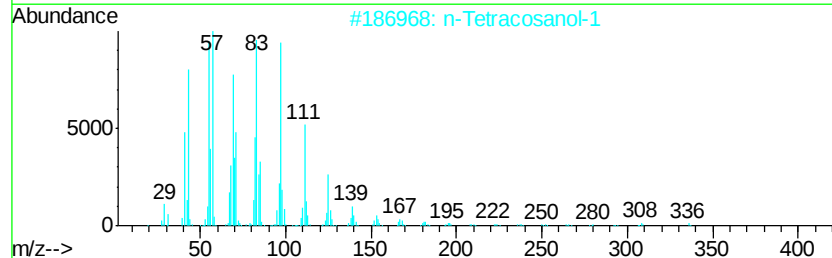
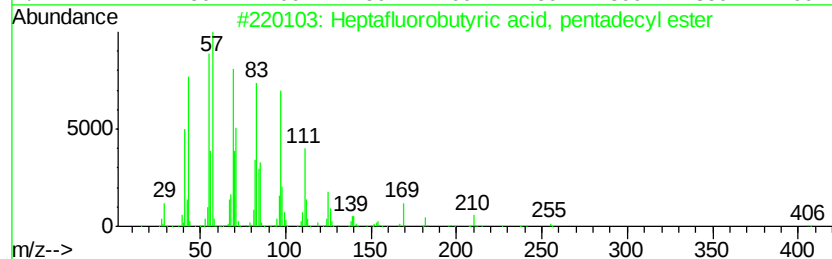
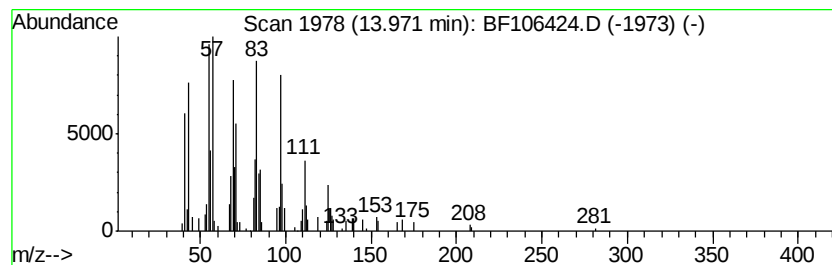
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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.20 ng	152456	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	3.0	ng	122641	1	6.97	832844	20.0
unknown6.75	6.75	65.3	ng	2718320	1	6.97	832844	20.0
Heptafluorobutyri...	13.97	3.2	ng	152456	5	14.14	951954	20.0