

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020916\
 Data File : BF084955.D
 Acq On : 9 Feb 2016 16:42
 Operator : SJ/IZ
 Sample : H1386-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B018(1-3)

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-BF020116.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	4.750	231	233	240	rBV	401386	416412	16.27%	2.980%
2	5.218	272	274	279	rBV	94394	97086	3.79%	0.695%
3	6.281	365	367	374	rVB	246256	217907	8.52%	1.559%
4	6.396	376	377	380	rBV	120435	113111	4.42%	0.809%
5	6.636	395	398	400	rBV	657453	901689	35.24%	6.453%
6	6.784	409	411	414	rBV	493393	418501	16.36%	2.995%
7	7.196	445	447	450	rBV	412907	363190	14.19%	2.599%
8	7.916	508	510	513	rBV	1234927	1233712	48.22%	8.828%
9	9.002	602	605	607	rBV	613209	770500	30.11%	5.514%
10	9.402	638	640	642	rBV	156798	172150	6.73%	1.232%
11	9.619	653	659	661	rBV2	74933	89261	3.49%	0.639%
12	9.665	661	663	666	rVB	1397181	1363056	53.27%	9.754%
13	10.110	700	702	704	rVB	72821	66978	2.62%	0.479%
14	10.328	719	721	725	rBV	21796	40429	1.58%	0.289%
15	10.453	730	732	734	rBV	129401	132878	5.19%	0.951%
16	10.579	740	743	748	rBV	51724	101885	3.98%	0.729%
17	11.036	780	783	784	rBV	24839	35440	1.39%	0.254%
18	11.139	790	792	795	rBV2	1090164	1327820	51.89%	9.502%
19	12.351	896	898	900	rBV	59765	57584	2.25%	0.412%
20	12.568	914	917	920	rBV	39915	58716	2.29%	0.420%
21	12.728	929	931	934	rBV	2729974	2558724	100.00%	18.310%
22	12.899	939	946	948	rBV7	7835	30511	1.19%	0.218%
23	13.208	971	973	976	rVB	314756	271058	10.59%	1.940%
24	13.642	1008	1011	1015	rBV	142475	248869	9.73%	1.781%
25	13.768	1020	1022	1025	rBV	1179979	1235773	48.30%	8.843%
26	14.271	1064	1066	1069	rBV3	26921	60361	2.36%	0.432%
27	14.362	1071	1074	1077	rVB3	22926	53568	2.09%	0.383%
28	14.534	1087	1089	1095	rBV	343982	389107	15.21%	2.784%
29	14.762	1107	1109	1114	rBV	49227	86933	3.40%	0.622%
30	15.025	1130	1132	1135	rVB	34318	36555	1.43%	0.262%
31	15.128	1139	1141	1144	rVV	664131	824265	32.21%	5.898%
32	15.174	1144	1145	1149	rVB2	28855	42203	1.65%	0.302%
33	15.551	1175	1178	1180	rBV2	22475	34940	1.37%	0.250%
34	15.974	1212	1215	1218	rVB2	19214	31098	1.22%	0.223%

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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-BF020116.M
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35	16.385	1248	1251	1254	rVB2	13698	28529	1.11%	0.204%
36	17.048	1306	1309	1312	rVB4	13641	27007	1.06%	0.193%
37	17.723	1366	1368	1374	rBV6	10414	36433	1.42%	0.261%

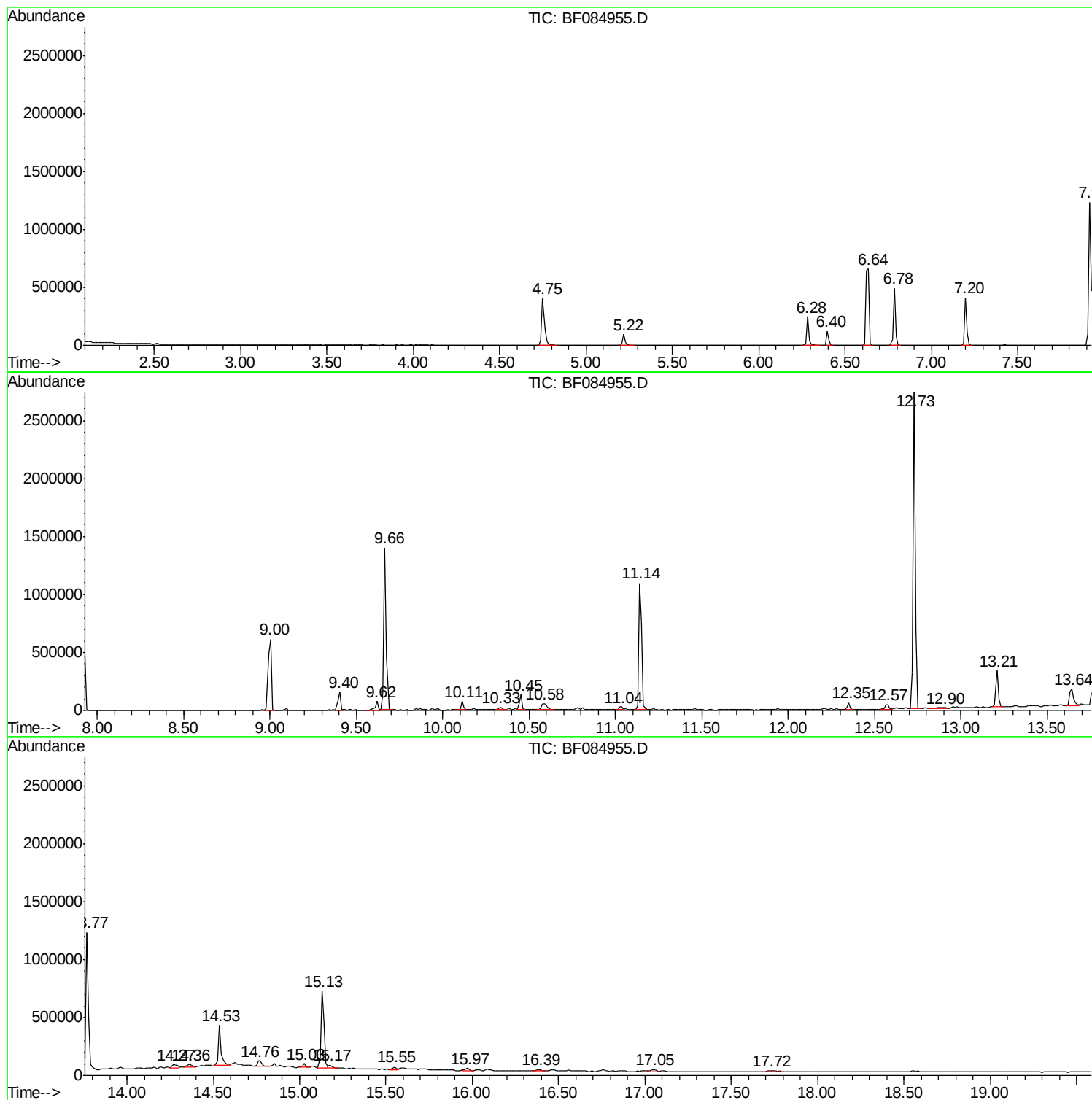
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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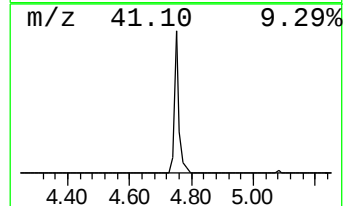
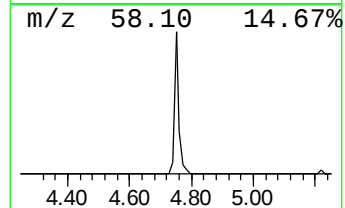
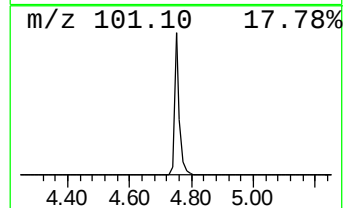
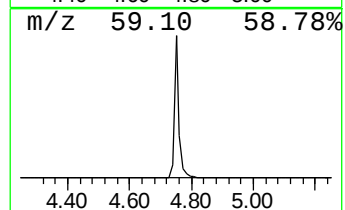
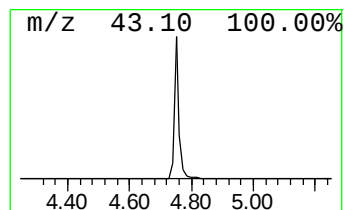
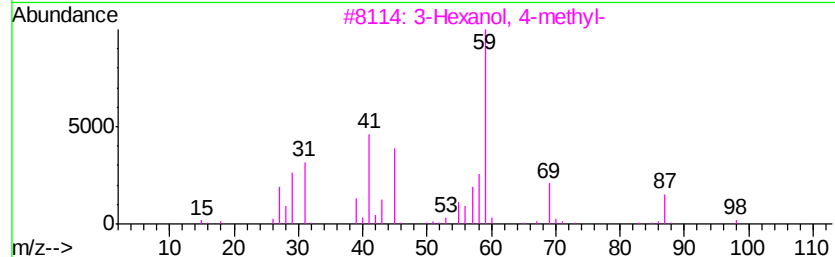
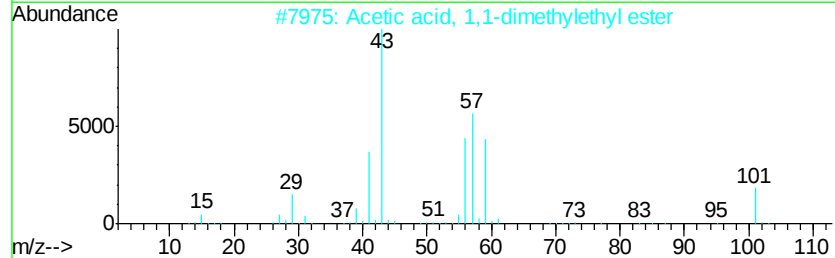
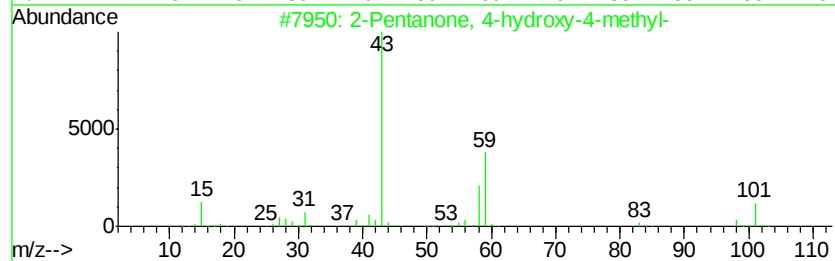
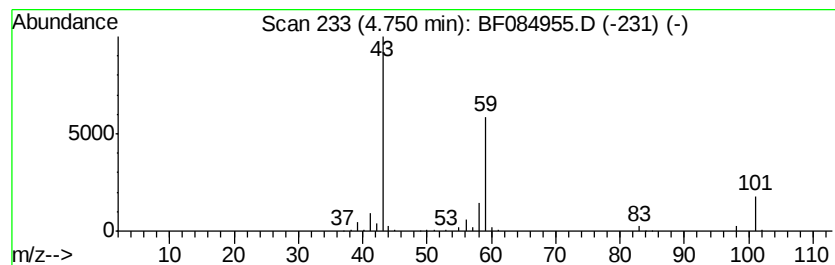
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	9.24 ng	416412	1,4-Dichlorobenzene-d4	6.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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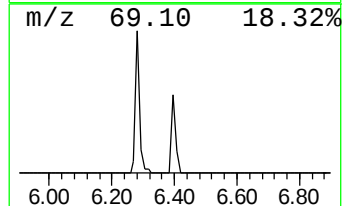
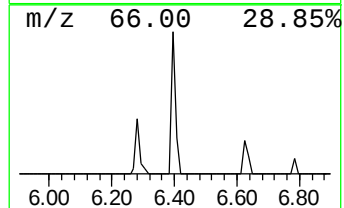
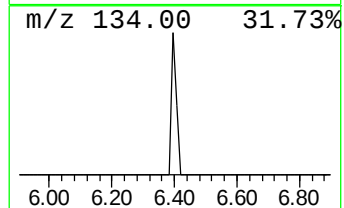
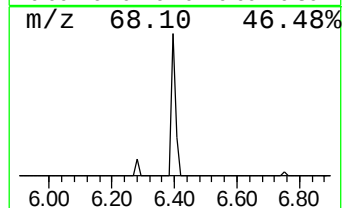
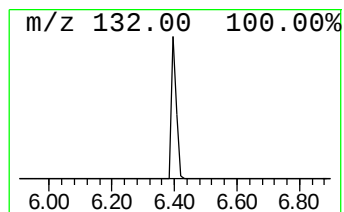
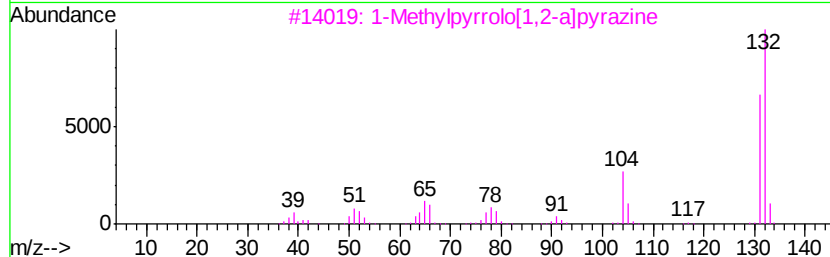
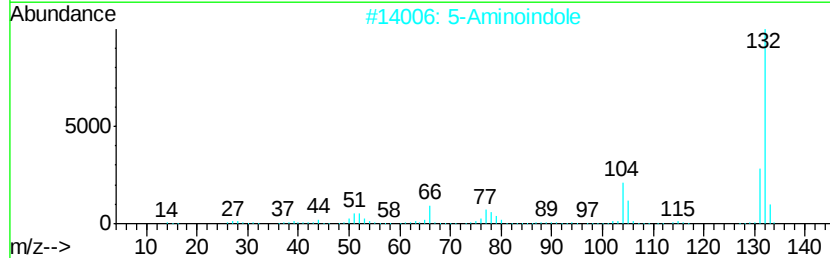
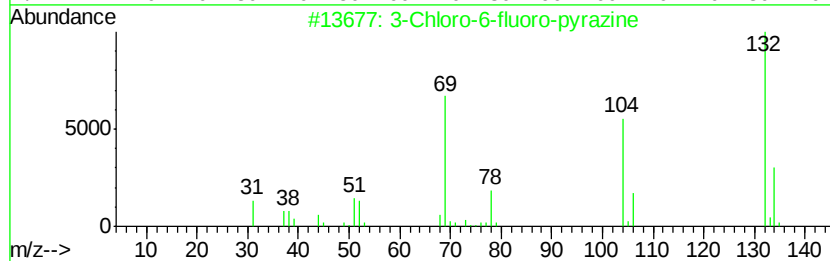
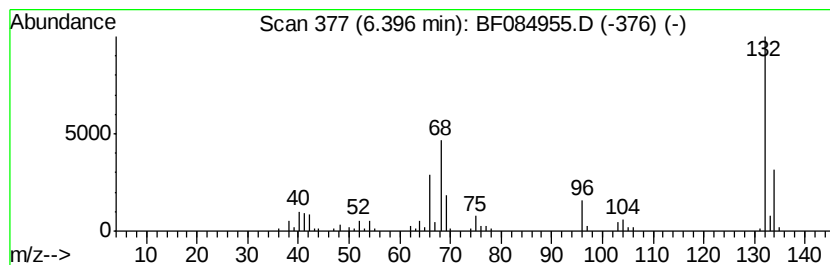
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Peak Number 2 unknown6.40 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	2.51 ng	113111	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	10
3			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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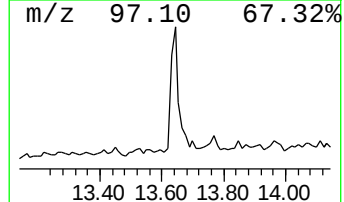
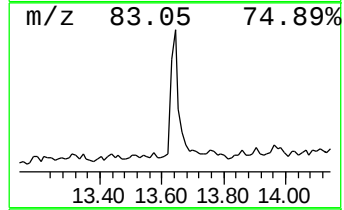
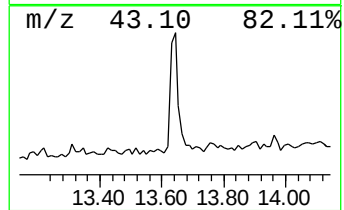
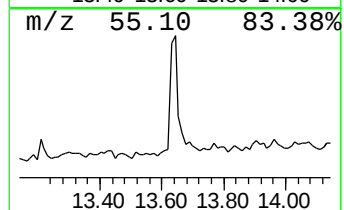
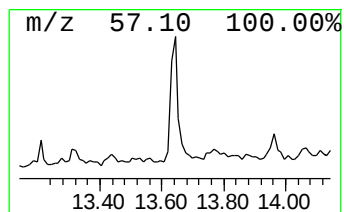
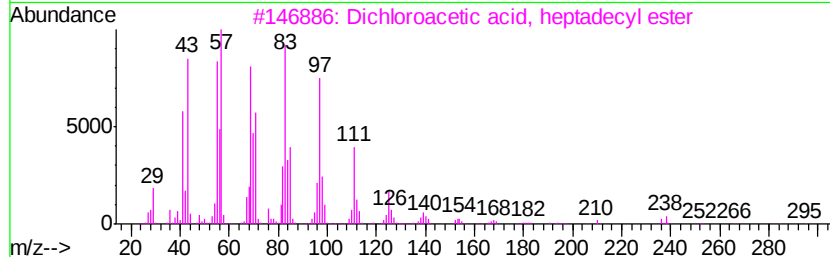
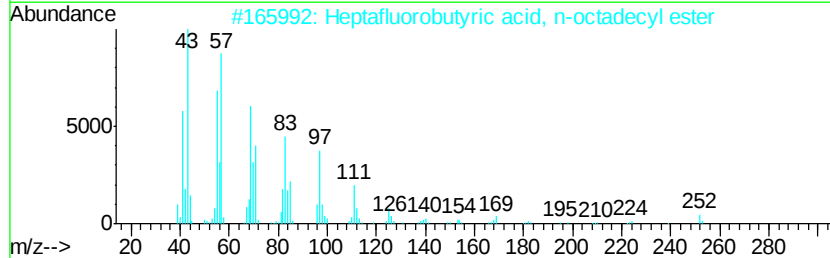
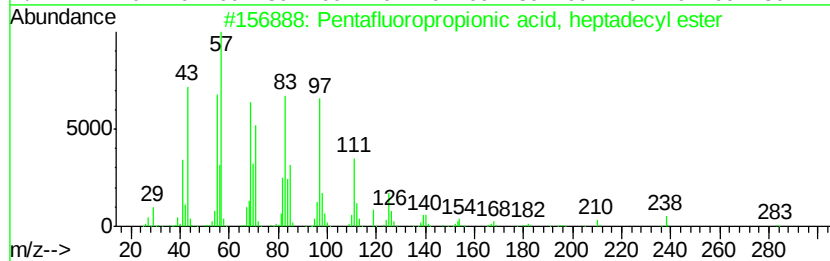
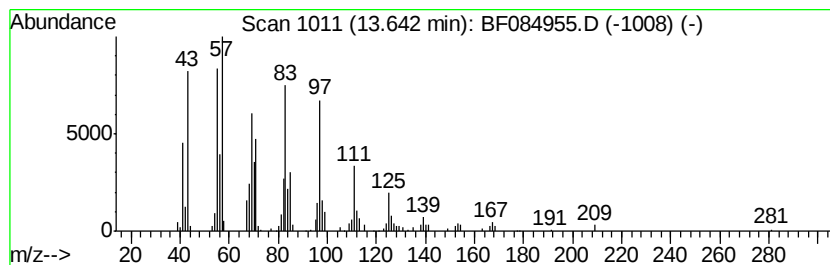
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	4.03 ng	248869	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



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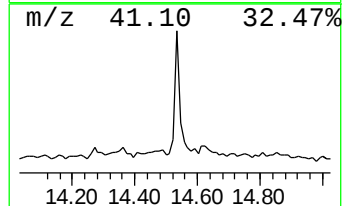
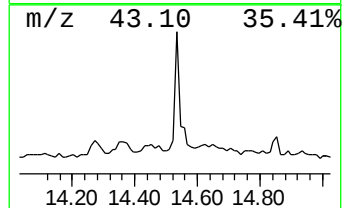
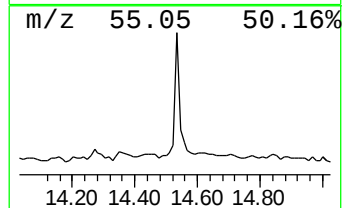
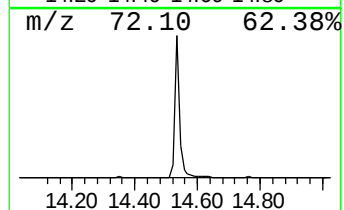
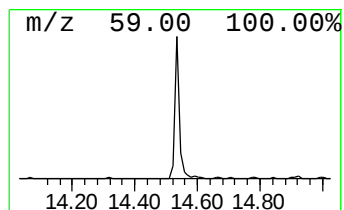
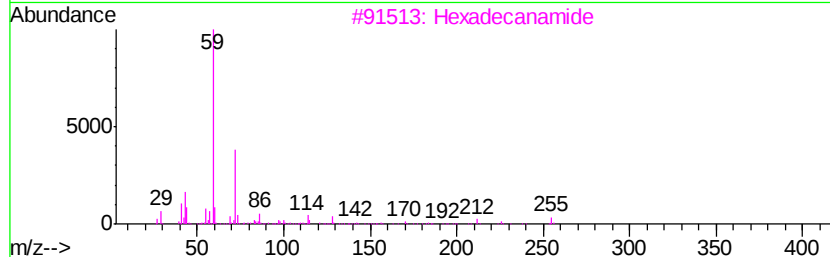
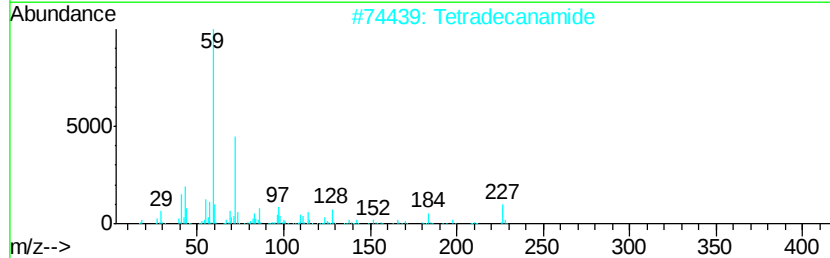
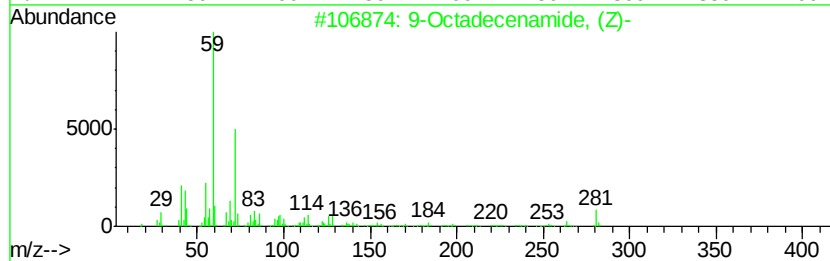
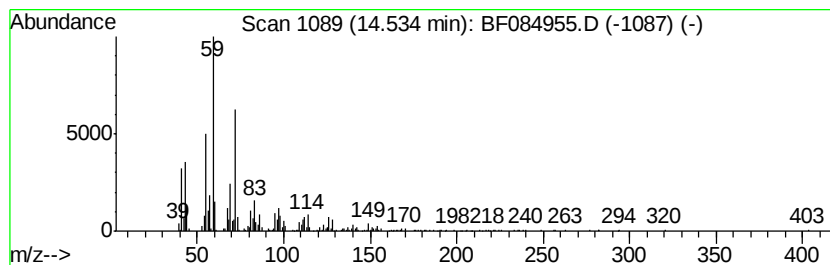
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	9.44 ng	389107	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Tetradecanamide	227	C14H29NO	000638-58-4	78
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.75	9.2	ng	416412	1	6.64	901689	20.0
unknown6.40	6.40	2.5	ng	113111	1	6.64	901689	20.0
Pentafluoropropio...	13.64	4.0	ng	248869	5	13.77	1235770	20.0
9-Octadecenamide,...	14.53	9.4	ng	389107	6	15.13	824265	20.0