

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
 Data File : BF100807.D
 Acq On : 22 Nov 2017 4:13
 Operator : SJ/JU
 Sample : I6466-09
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHAP-2-E(6-7)

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-BF110817.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	5.104	508	513	524	rBV	245588	347126	17.19%	2.083%
2	5.498	574	580	583	rBV	1812225	1808898	89.60%	10.855%
3	6.504	745	751	760	rBV	1713687	1891615	93.70%	11.351%
4	6.645	770	775	778	rBV	1896487	1864015	92.33%	11.185%
5	6.875	810	814	817	rBV	542454	492958	24.42%	2.958%
6	7.028	836	840	843	rBV	1602096	1421867	70.43%	8.532%
7	7.434	904	909	912	rBV	1106607	1148036	56.87%	6.889%
8	8.151	1027	1031	1035	rBV	769014	640089	31.71%	3.841%
9	8.704	1121	1125	1129	rBV	96550	80512	3.99%	0.483%
10	9.228	1209	1214	1217	rBV	2304629	2018763	100.00%	12.114%
11	9.616	1277	1280	1285	rBB	58818	49350	2.44%	0.296%
12	9.910	1326	1330	1334	rBV	804676	669935	33.19%	4.020%
13	10.622	1447	1451	1454	rBV	359426	288351	14.28%	1.730%
14	10.698	1460	1464	1467	rBV	1138691	1003715	49.72%	6.023%
15	11.398	1579	1583	1586	rBV	609642	573282	28.40%	3.440%
16	12.604	1785	1788	1792	rBV	27999	25224	1.25%	0.151%
17	12.839	1823	1828	1831	rBV	27476	26491	1.31%	0.159%
18	12.980	1847	1852	1855	rBV	1465924	1310680	64.92%	7.865%
19	13.863	1998	2002	2006	rBV2	61795	62423	3.09%	0.375%
20	14.033	2027	2031	2034	rBV	545505	483922	23.97%	2.904%
21	14.486	2104	2108	2112	rBV4	15144	25897	1.28%	0.155%
22	15.074	2204	2208	2212	rBV3	16100	25173	1.25%	0.151%
23	15.509	2276	2282	2289	rBV	317251	406267	20.12%	2.438%

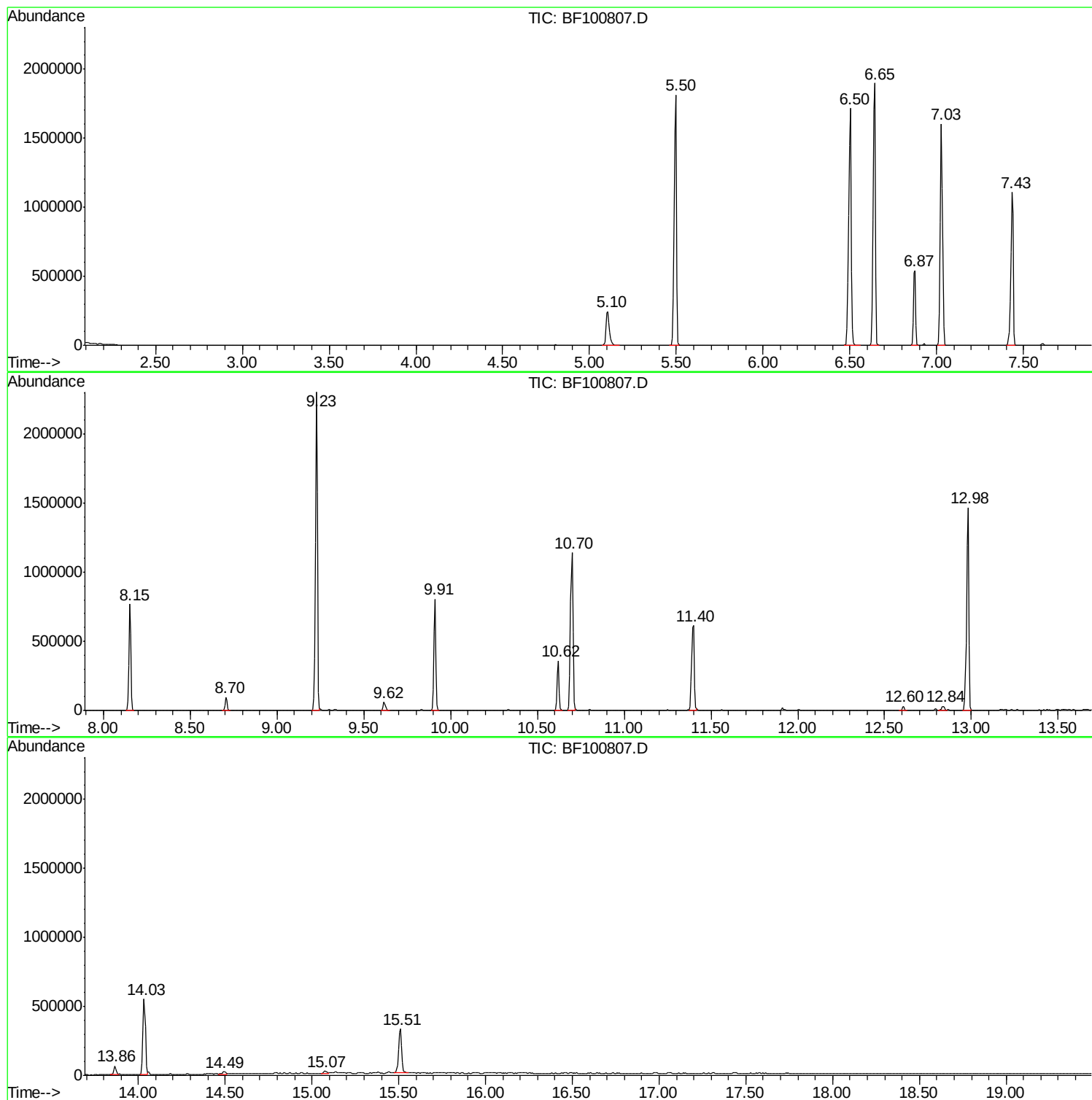
Sum of corrected areas: 16664589

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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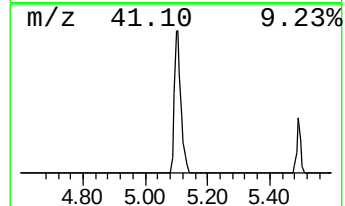
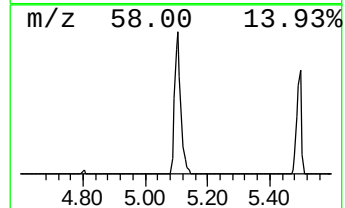
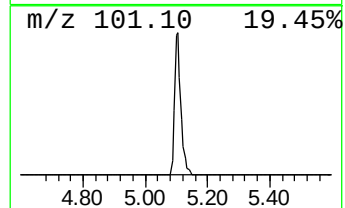
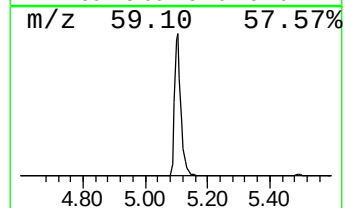
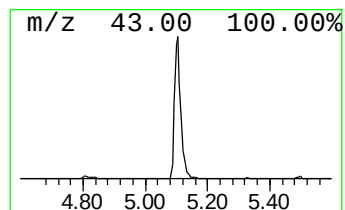
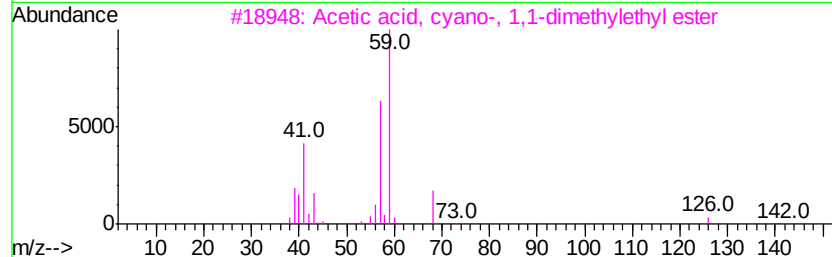
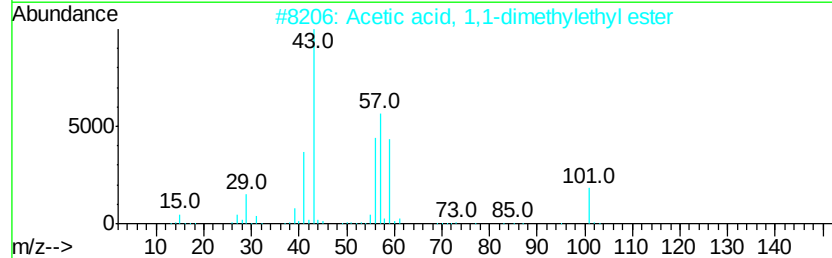
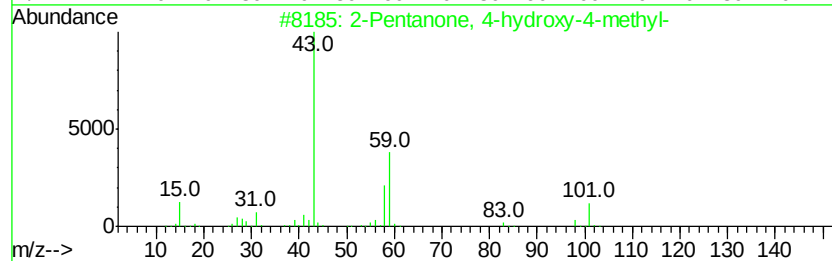
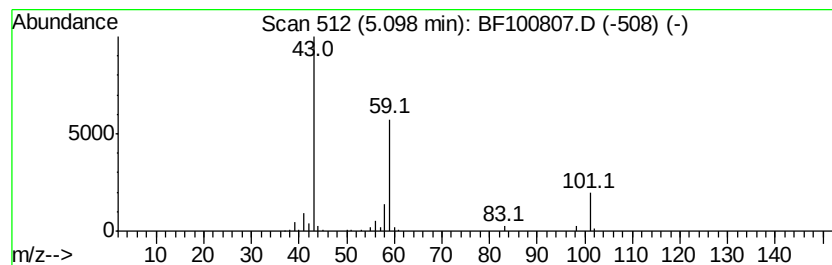
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
5.10	14.08 ng	347126	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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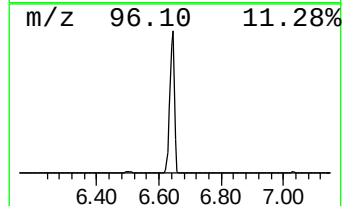
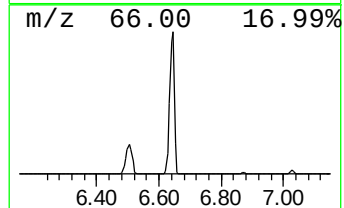
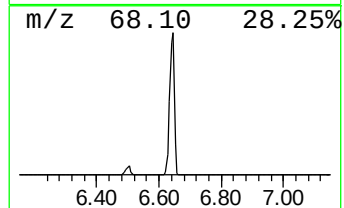
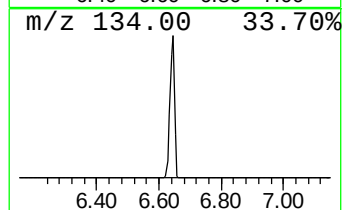
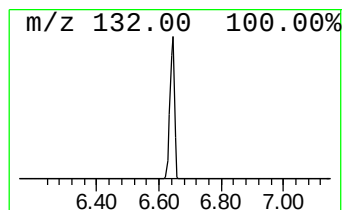
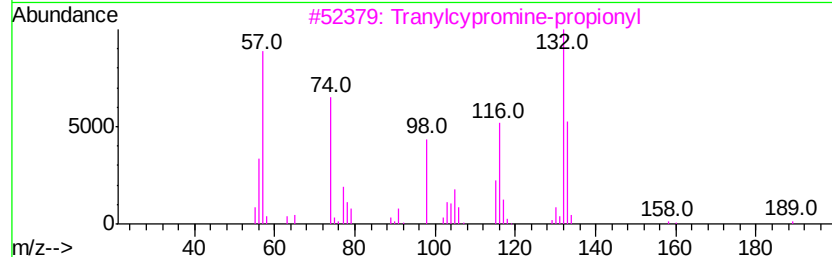
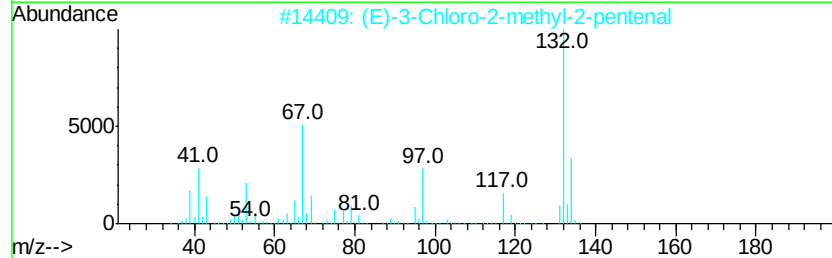
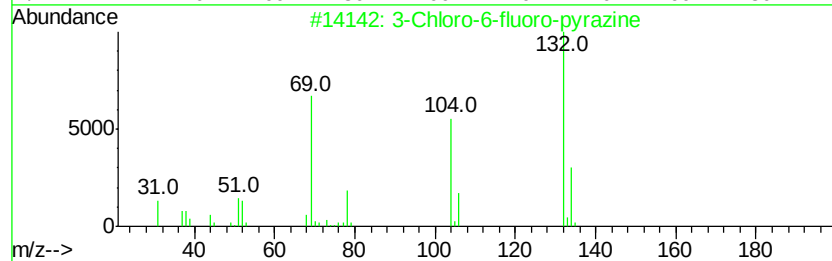
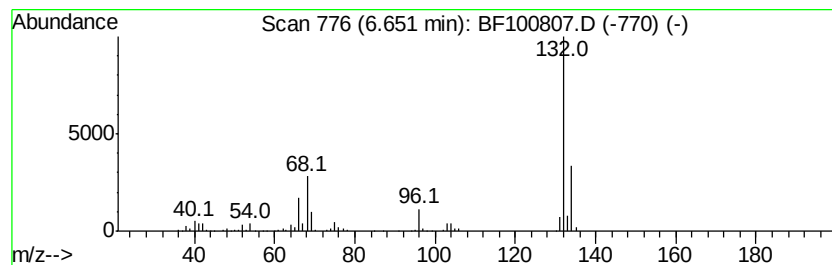
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Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	75.63 ng	1864020	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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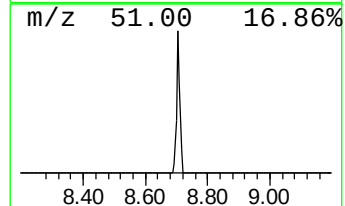
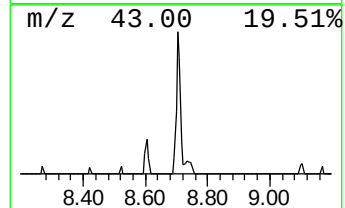
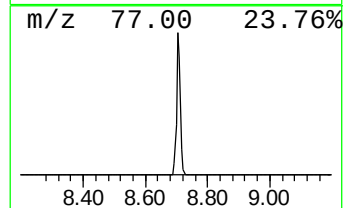
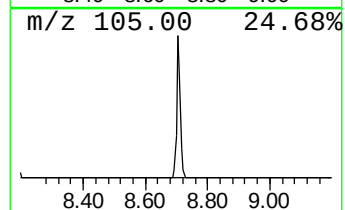
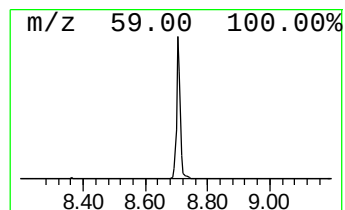
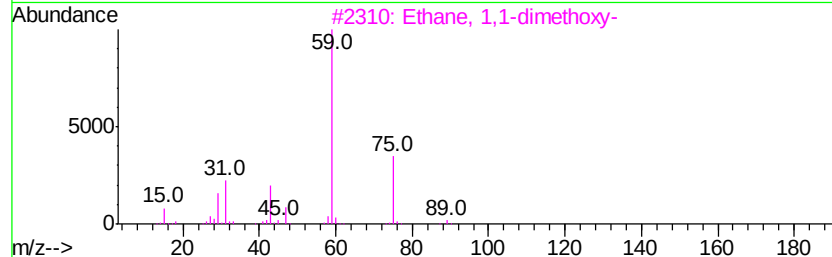
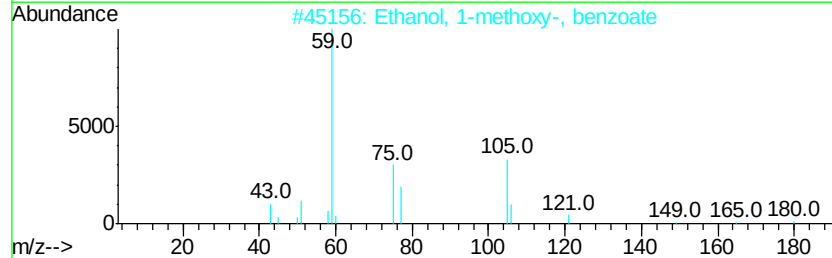
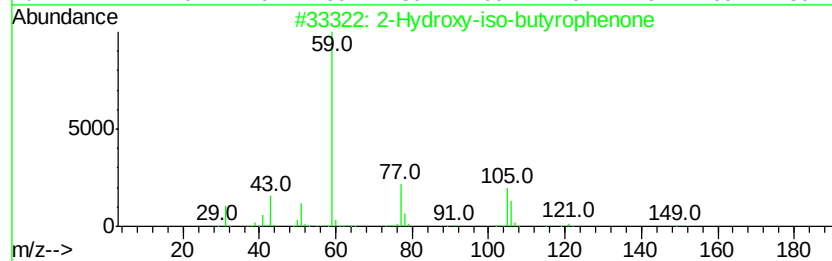
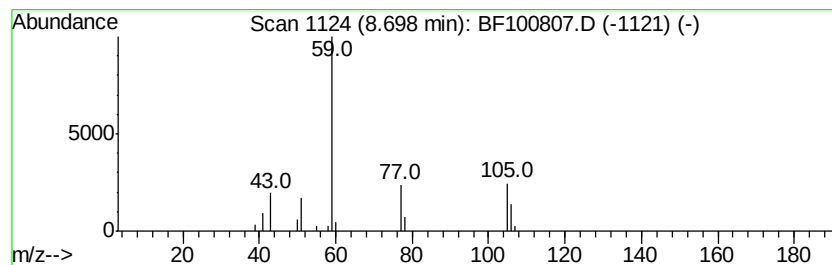
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
8.70	2.52 ng	80512	Naphthalene-d8		8.15	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone		164	C10H12O2	007473-98-5	86
2	Ethanol, 1-methoxy-, benzoate		180	C10H12O3	051835-44-0	64
3	Ethane, 1,1-dimethoxy-		90	C4H10O2	000534-15-6	9
4	Guanidine		59	CH5N3	000113-00-8	7
5	Acetamide		59	C2H5NO	000060-35-5	5



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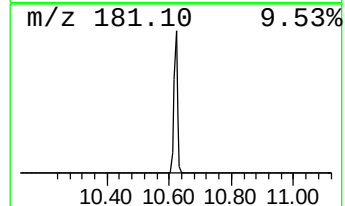
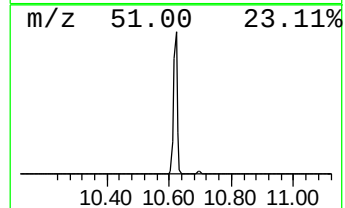
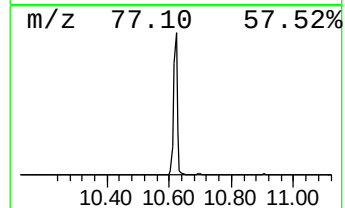
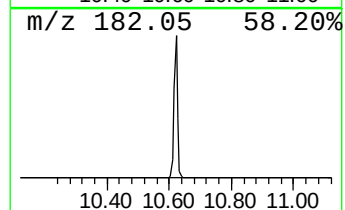
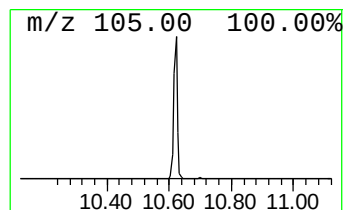
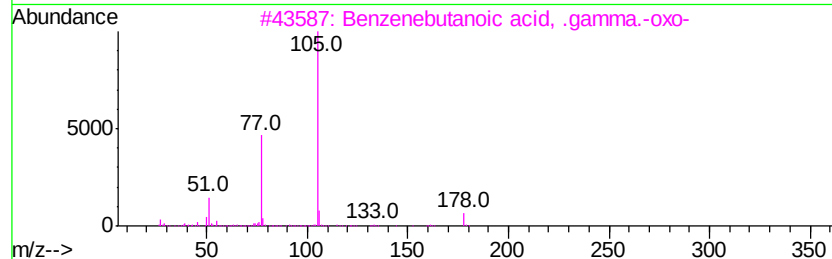
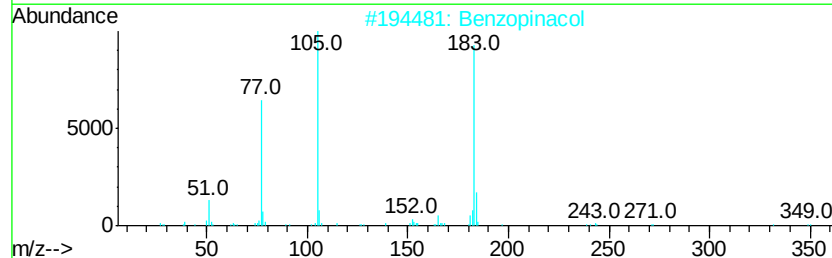
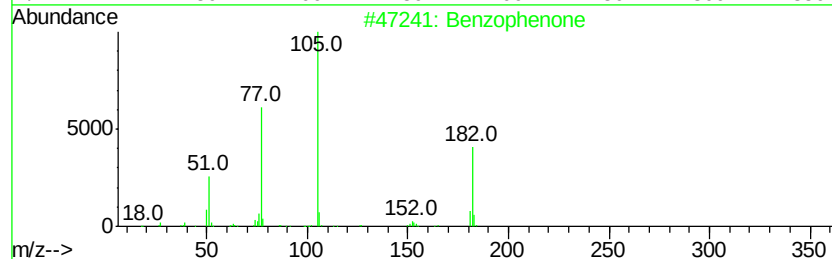
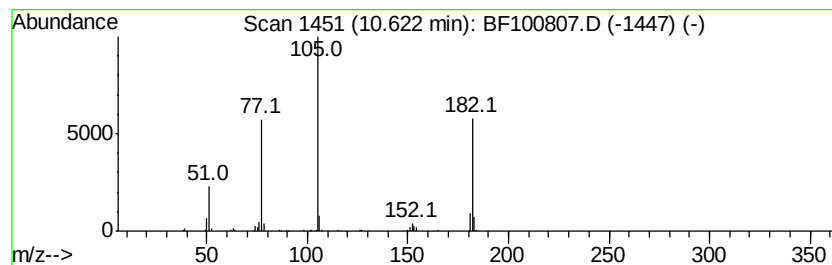
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.62	8.61 ng	288351	Acenaphthene-d10		9.91		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzopinacol	366	C26H22O2	000464-72-2	47
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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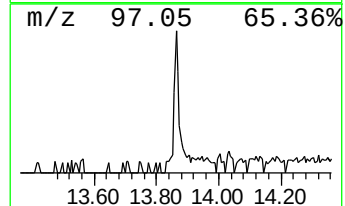
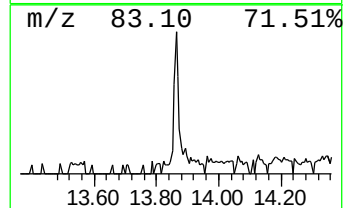
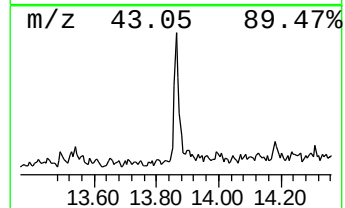
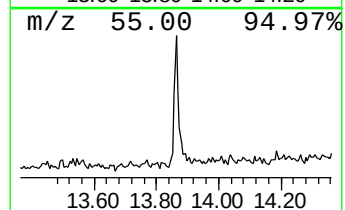
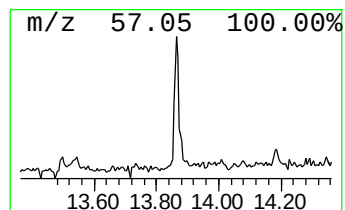
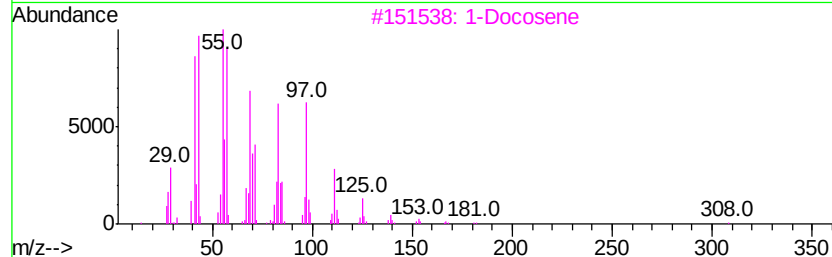
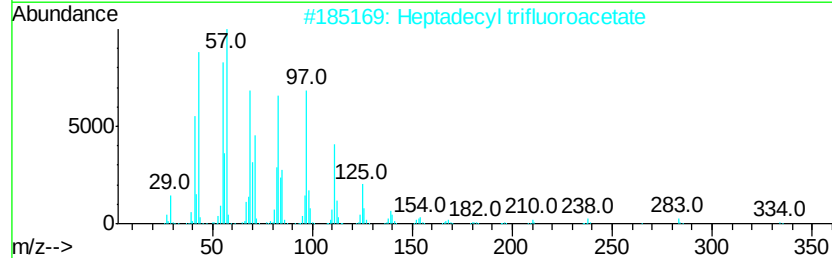
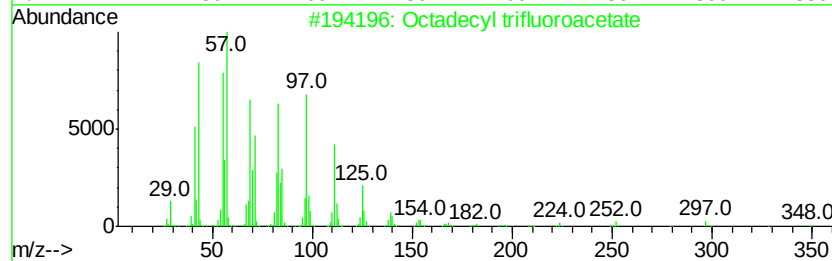
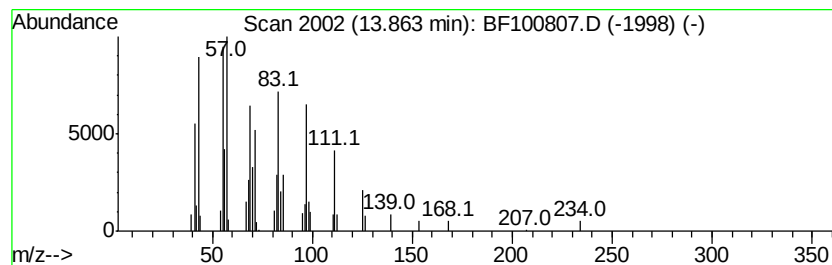
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Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.58 ng	62423	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	14.1	ng	347126	1	6.87	492958	20.0
unknown6.65	6.65	75.6	ng	1864020	1	6.87	492958	20.0
2-Hydroxy-iso-but...	8.70	2.5	ng	80512	2	8.15	640089	20.0
Benzophenone	10.62	8.6	ng	288351	3	9.91	669935	20.0
Octadecyl trifluo...	13.86	2.6	ng	62423	5	14.03	483922	20.0