

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
 Data File : BF099979.D
 Acq On : 31 Oct 2017 00:38
 Operator : SJ/JU
 Sample : I6083-05
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 102017-TIFR-F-D-B

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-BF102317.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	4.998	493	495	509	rBV	53309	78417	3.15%	0.540%
2	5.410	562	565	587	rBV	460438	651639	26.18%	4.490%
3	6.434	736	739	757	rBV	304773	462172	18.57%	3.185%
4	6.557	757	760	771	rVB	1386303	1283675	51.57%	8.846%
5	6.786	796	799	813	rBB	525206	462201	18.57%	3.185%
6	6.939	822	825	840	rBV	1877516	1753126	70.43%	12.081%
7	7.357	892	896	915	rBV	1247346	1308025	52.54%	9.014%
8	8.069	1014	1017	1036	rBV	760445	637930	25.63%	4.396%
9	8.627	1110	1112	1119	rBV	34831	35792	1.44%	0.247%
10	9.145	1196	1200	1203	rBV	2879517	2489351	100.00%	17.154%
11	9.545	1265	1268	1277	rBB	33367	31293	1.26%	0.216%
12	9.827	1312	1316	1328	rVB	728797	702363	28.21%	4.840%
13	10.492	1426	1429	1434	rBB	61042	52434	2.11%	0.361%
14	10.539	1434	1437	1447	rBV	207497	167010	6.71%	1.151%
15	10.621	1447	1451	1464	rBV	928244	862275	34.64%	5.942%
16	11.321	1566	1570	1578	rBV	682548	630450	25.33%	4.344%
17	12.910	1835	1840	1843	rBV	1958823	1985793	79.77%	13.684%
18	13.786	1984	1989	1996	rBV2	22215	32751	1.32%	0.226%
19	13.974	2018	2021	2032	rBV	500913	468999	18.84%	3.232%
20	15.456	2269	2273	2285	rBV2	301245	416114	16.72%	2.867%

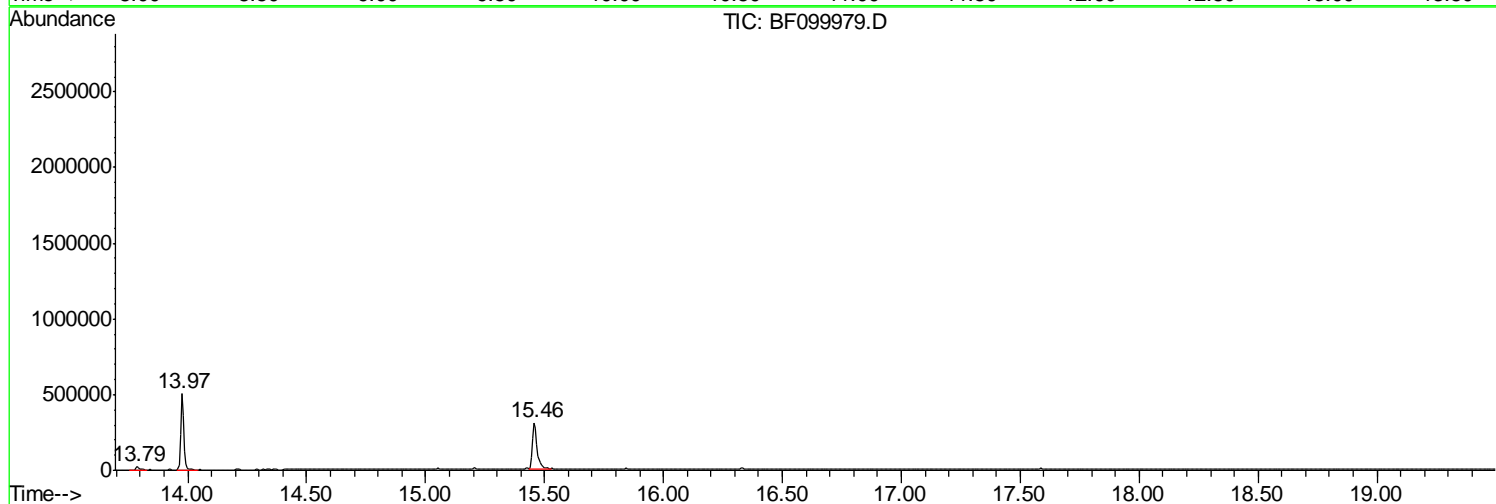
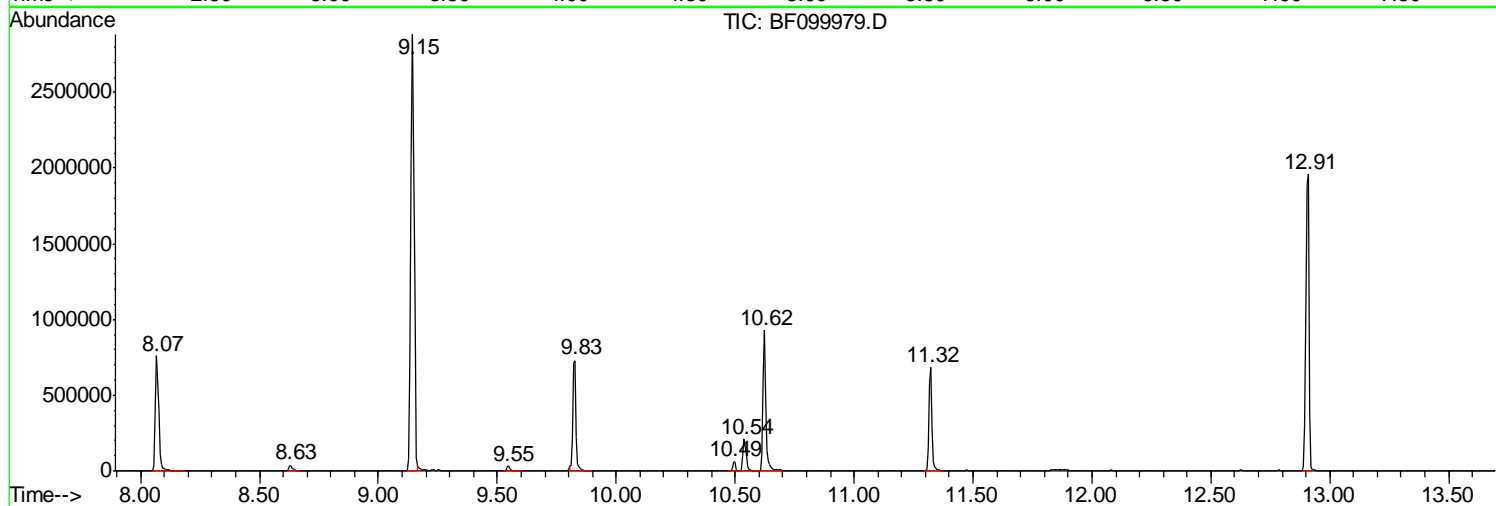
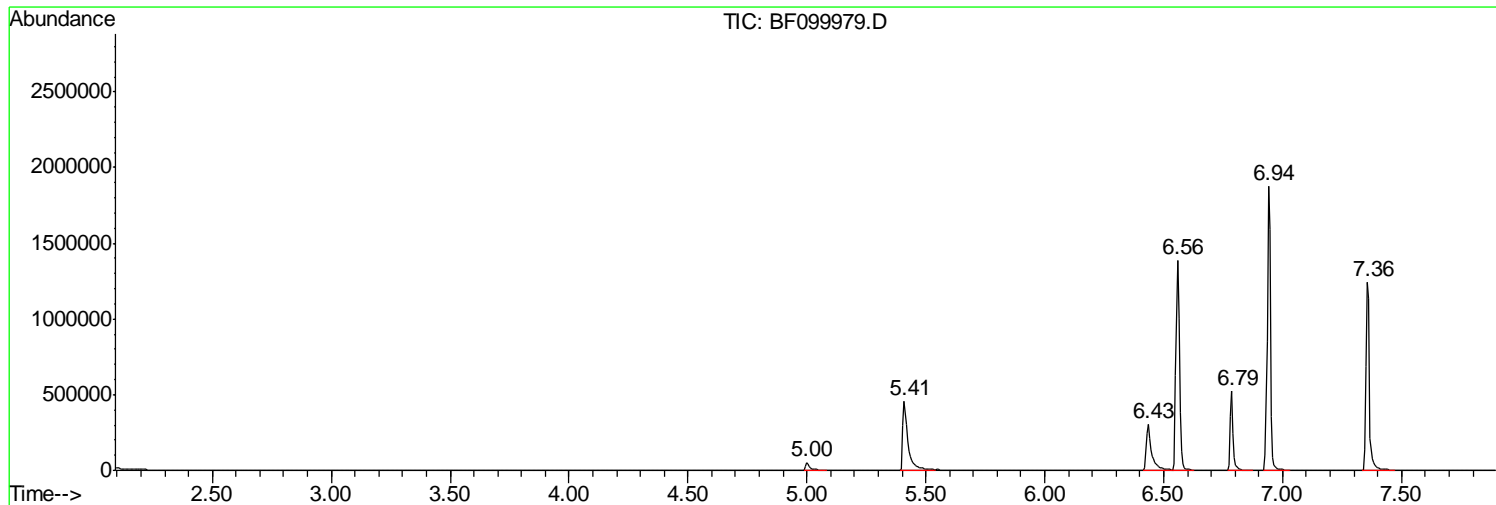
Sum of corrected areas: 14511810

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.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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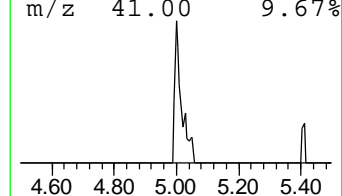
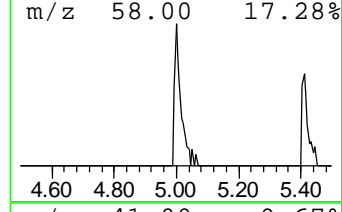
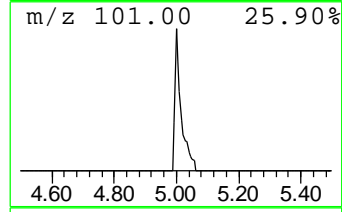
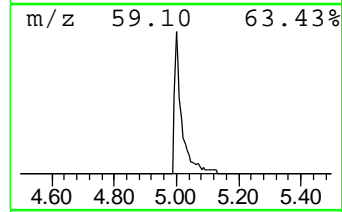
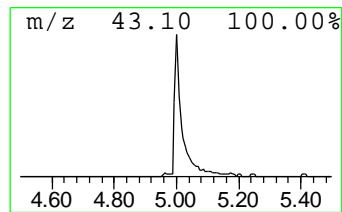
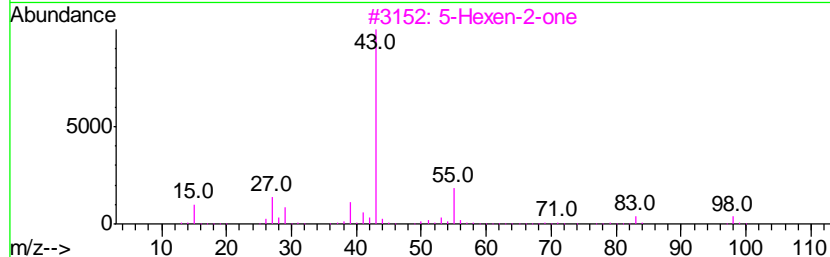
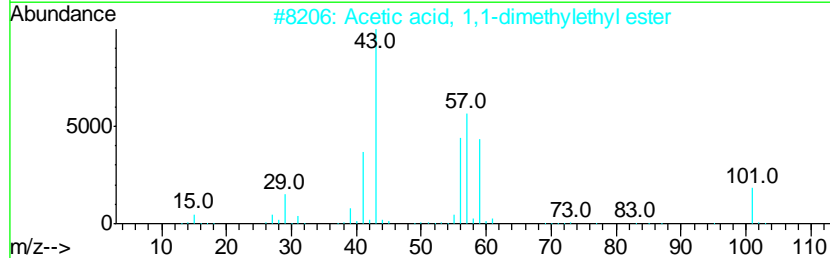
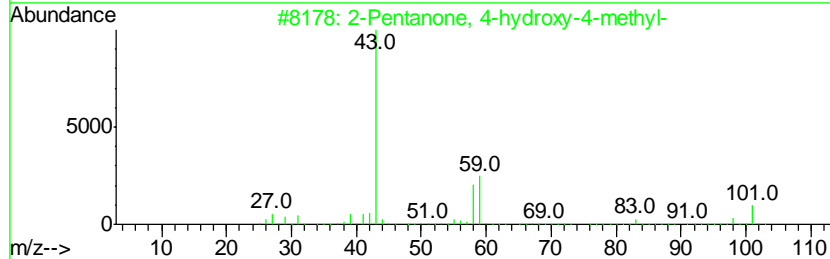
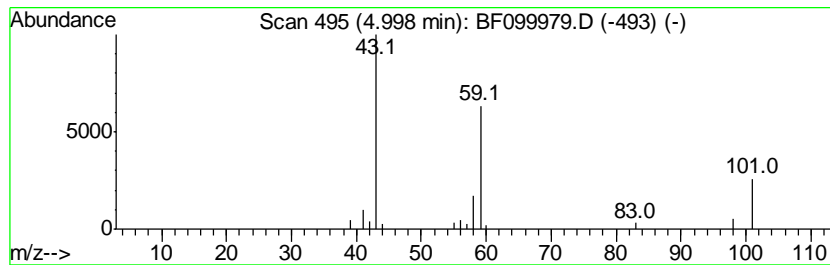
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.39 ng	78417	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		3-Hexanol	102	C6H14O	000623-37-0	9
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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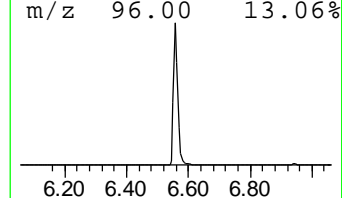
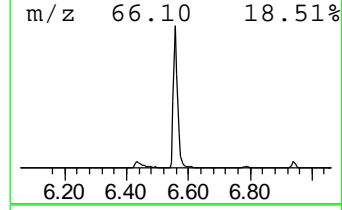
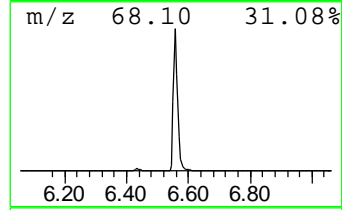
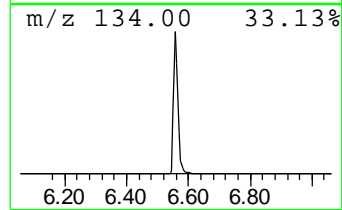
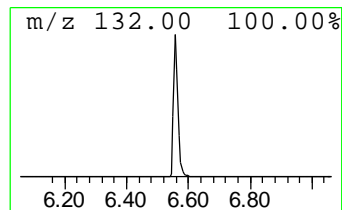
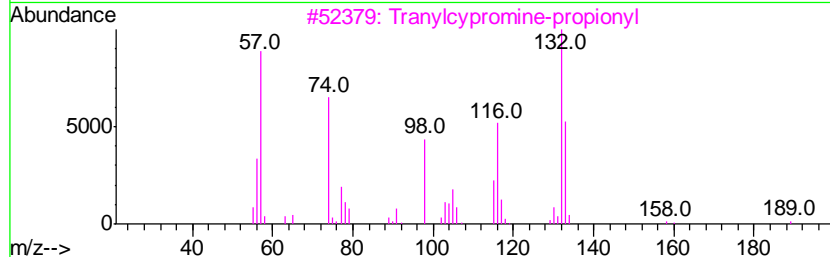
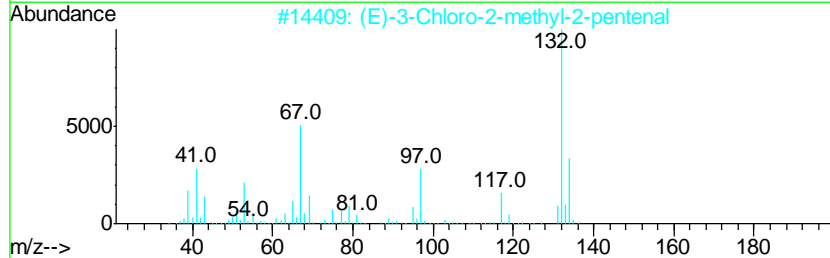
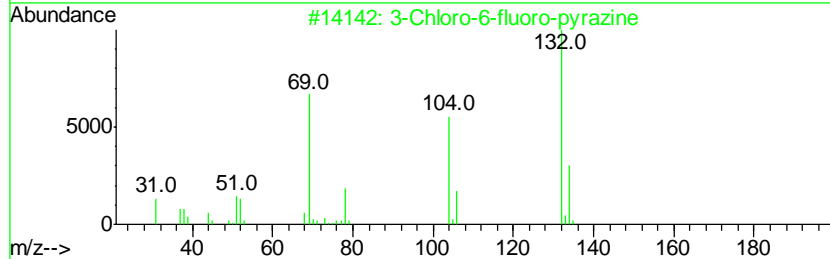
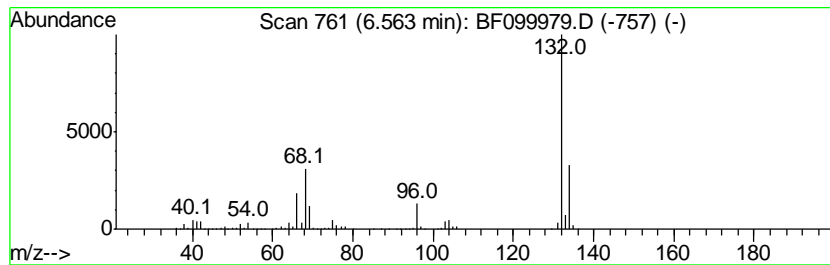
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 Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	55.55 ng	1283680	1,4-Dichlorobenzene-d4	6.79

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	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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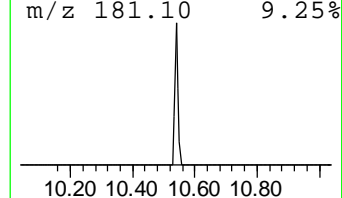
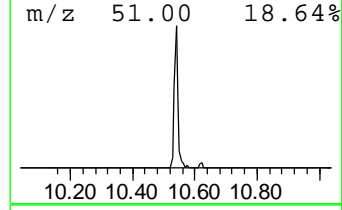
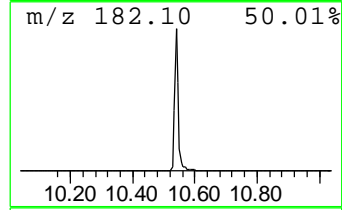
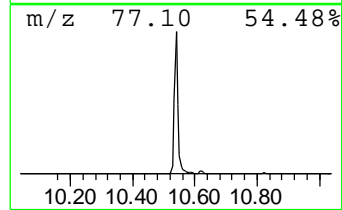
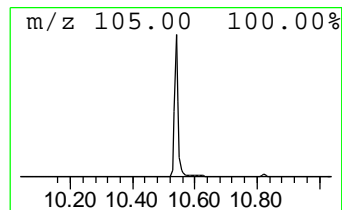
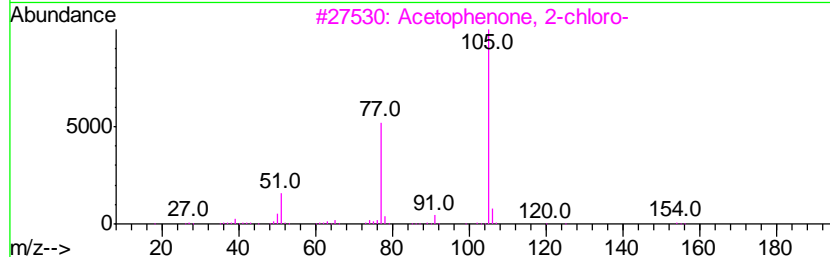
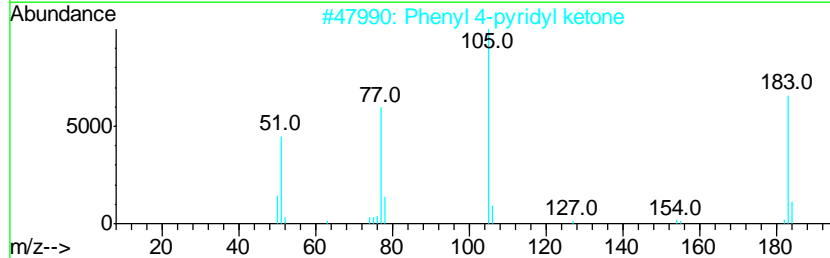
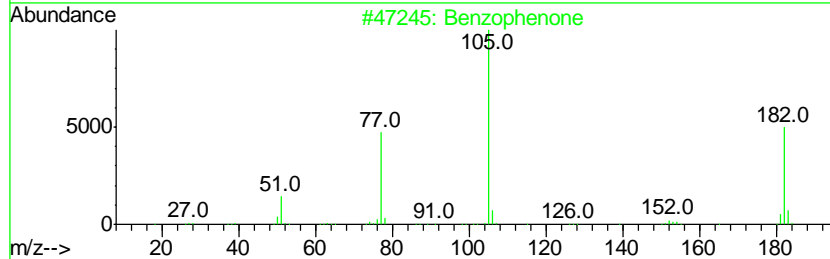
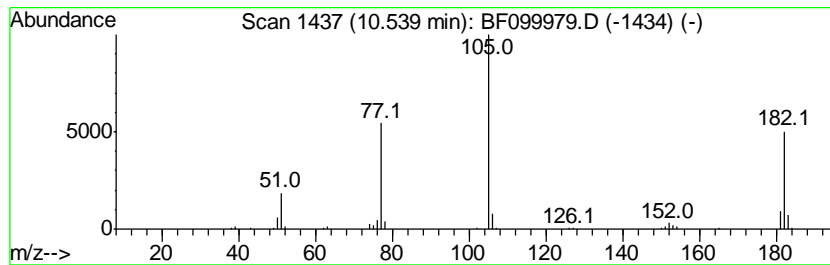
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 Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	4.76 ng	167010	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	97
2		Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4		Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	43
5		Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	43



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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...	5.00	3.4	ng	78417	1	6.79	462201	20.0
unknown6.56	6.56	55.5	ng	1283680	1	6.79	462201	20.0
Benzophenone	10.54	4.8	ng	167010	3	9.82	702363	20.0