

Data Path : Z:\HPCHEM1\BNA G\DATA\BG112817\
 Data File : BG031267.D
 Acq On : 29 Nov 2017 00:51
 Operator : SJ/JU
 Sample : I6590-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BSC-SB-07

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_G\METHODS\8270-BG111017.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	5.203	321	326	337	rVB	39637	64576	1.78%	0.370%
2	5.685	401	408	427	rBV	597668	1056549	29.16%	6.061%
3	7.295	673	682	694	rBV	618080	1160179	32.02%	6.655%
4	7.665	737	745	756	rBV	644457	1147841	31.68%	6.585%
5	8.129	817	824	833	rVB	145839	250945	6.93%	1.440%
6	8.452	872	879	891	rVB	463985	847875	23.40%	4.864%
7	9.299	1015	1023	1039	rBV	334320	673533	18.59%	3.864%
8	10.950	1296	1304	1325	rBV	174618	373878	10.32%	2.145%
9	13.376	1708	1717	1729	rBV	1083341	1780504	49.14%	10.214%
10	14.216	1852	1860	1867	rBV2	18106	40217	1.11%	0.231%
11	14.751	1940	1951	1963	rBV2	371169	634106	17.50%	3.638%
12	16.102	2172	2181	2187	rBV	46667	76805	2.12%	0.441%
13	16.237	2197	2204	2220	rBV	1089076	1774100	48.96%	10.177%
14	17.495	2412	2418	2433	rBV2	631254	1013419	27.97%	5.813%
15	18.259	2542	2548	2556	rBV	74265	111296	3.07%	0.638%
16	18.358	2560	2565	2573	rBV6	18118	42118	1.16%	0.242%
17	20.080	2852	2858	2867	rBV	2755590	3623466	100.00%	20.786%
18	21.373	3074	3078	3086	rBV4	38181	78717	2.17%	0.452%
19	21.760	3137	3144	3157	rBV2	770707	1367313	37.73%	7.844%
20	25.062	3695	3706	3722	rVB2	454147	1314947	36.29%	7.543%

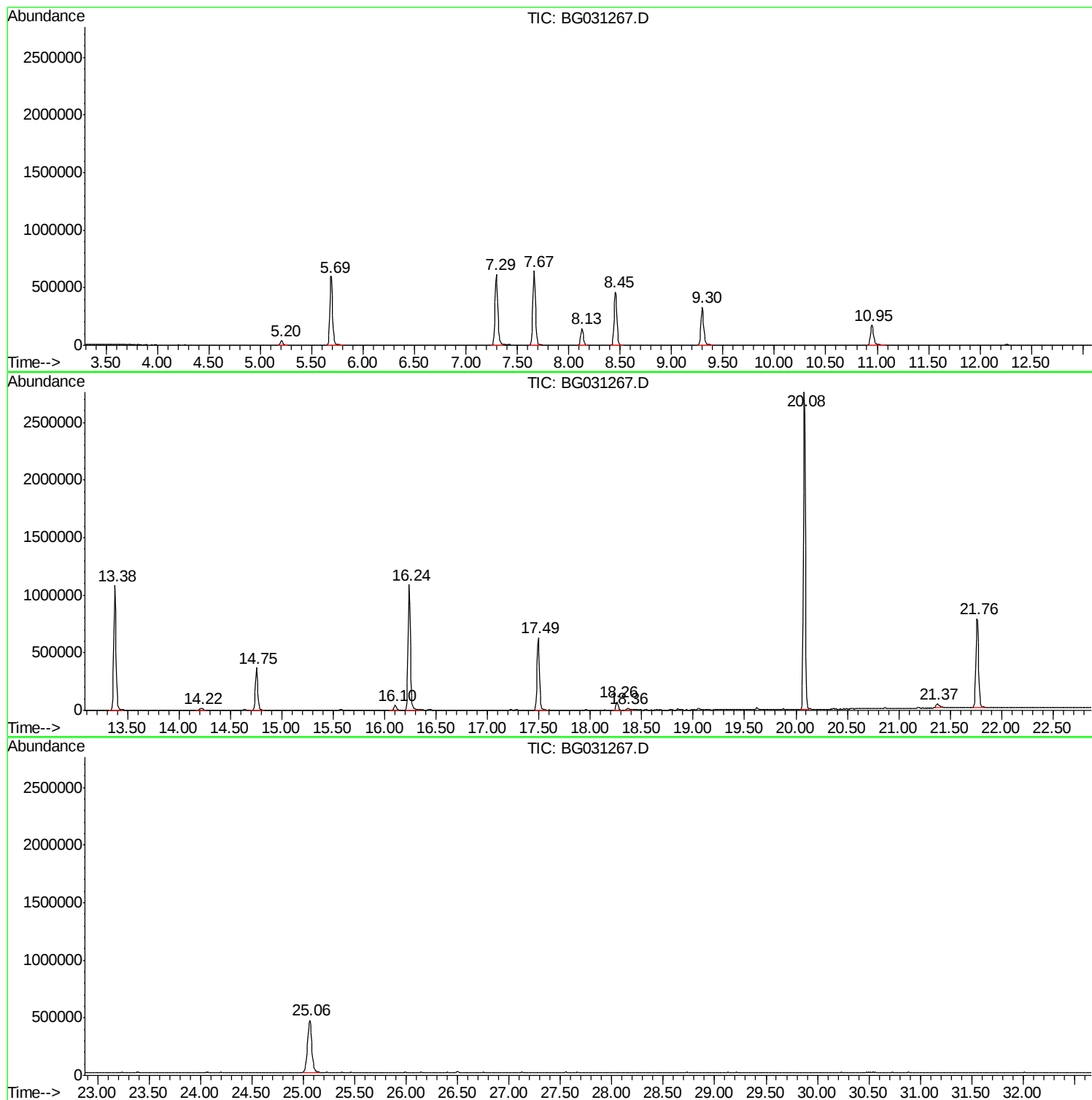
Sum of corrected areas: 17432384

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG111017.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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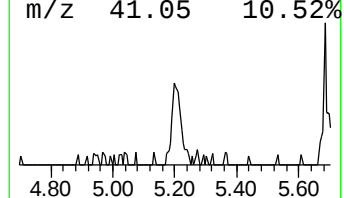
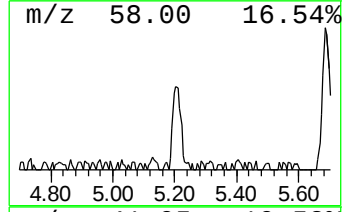
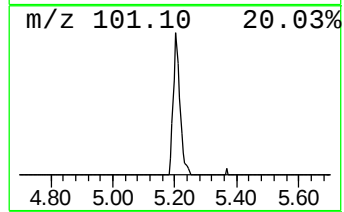
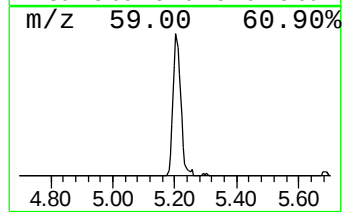
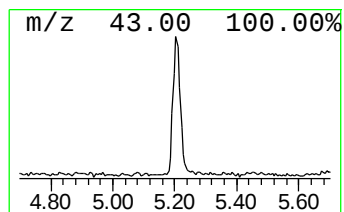
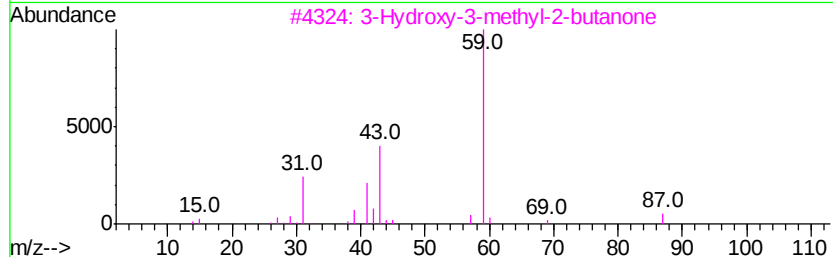
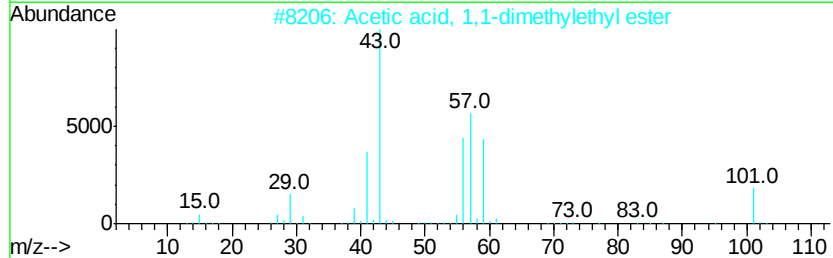
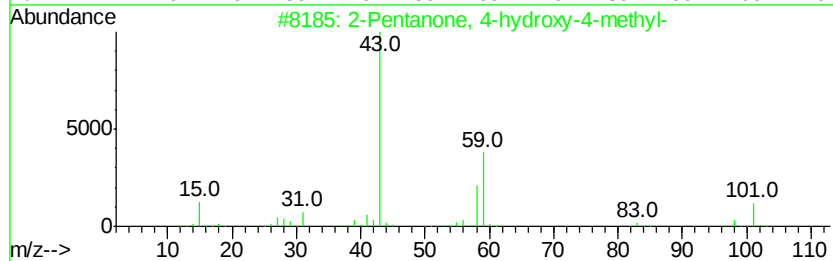
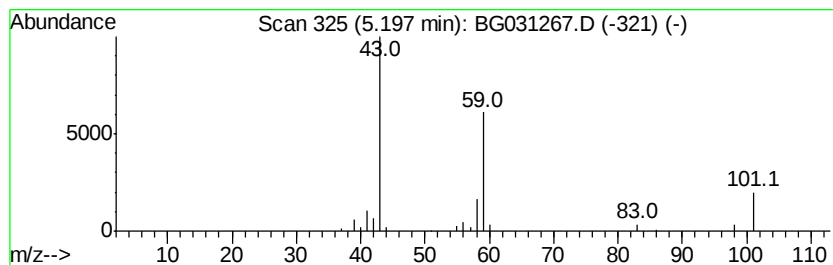
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.20	5.15 ng	64576	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4			1,2-Butanediol	90	C4H10O2	000584-03-2	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17



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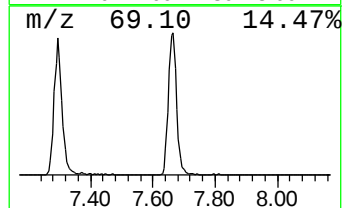
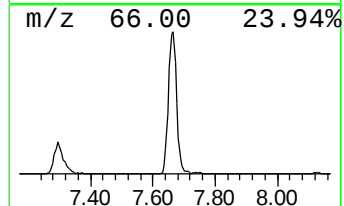
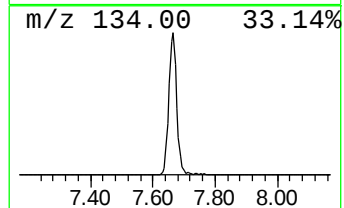
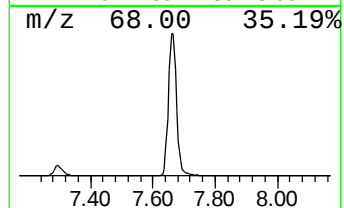
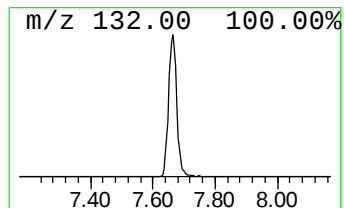
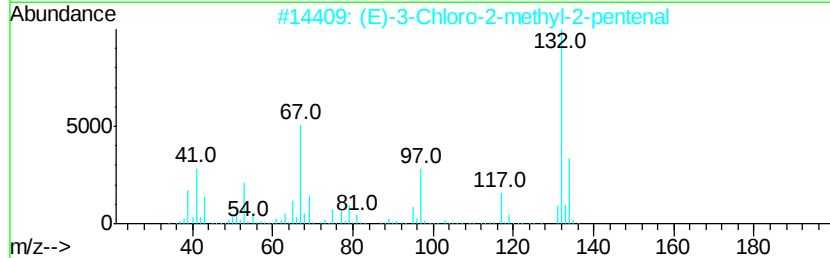
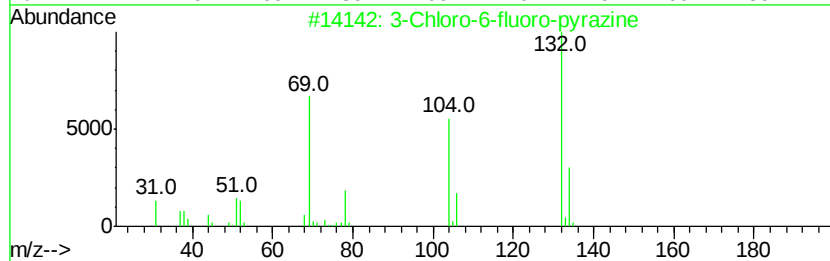
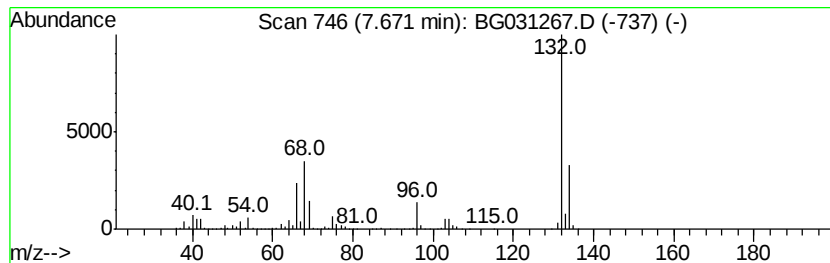
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Peak Number 2 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	91.48 ng	1147840	1,4-Dichlorobenzene-d4	8.13

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	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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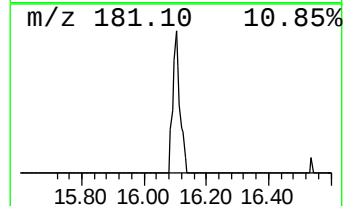
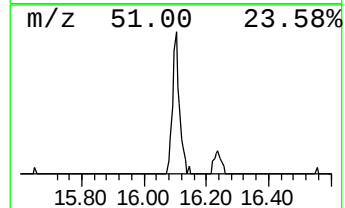
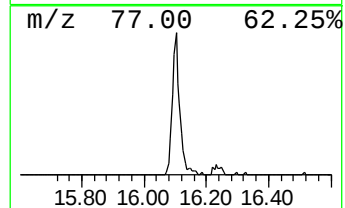
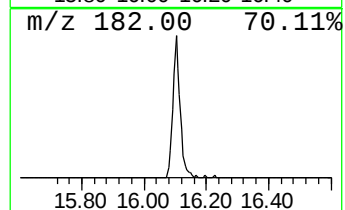
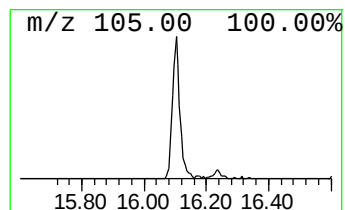
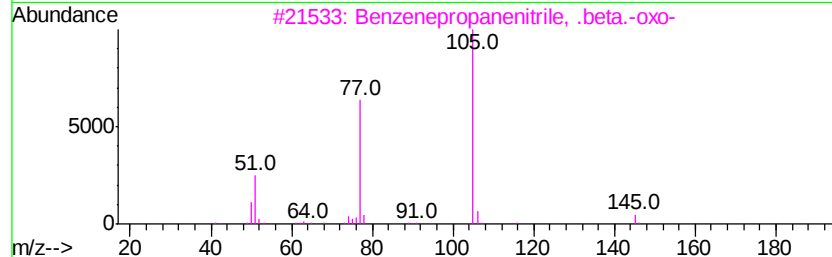
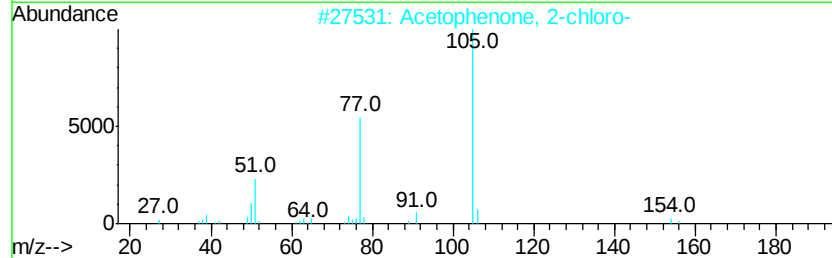
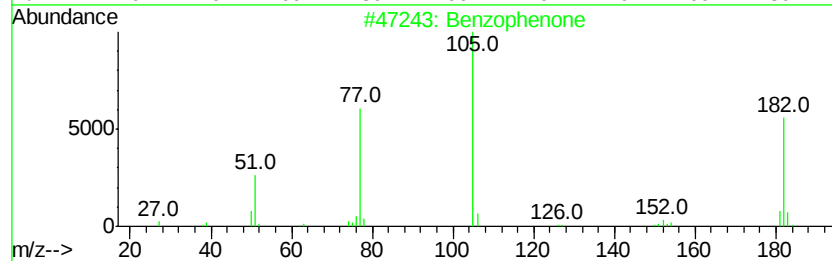
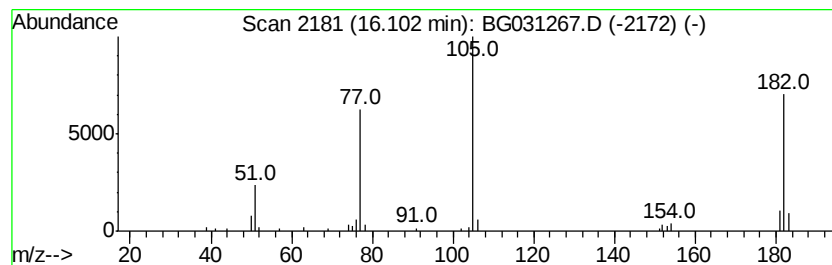
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.42 ng	76805	Acenaphthene-d10	14.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
4			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43



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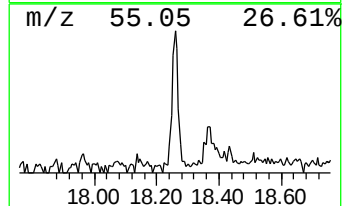
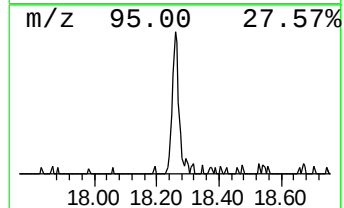
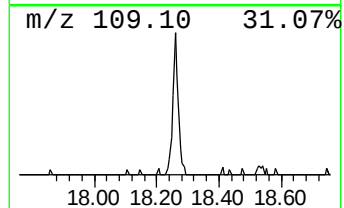
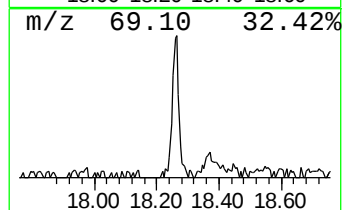
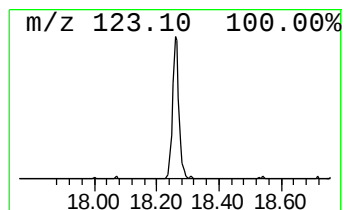
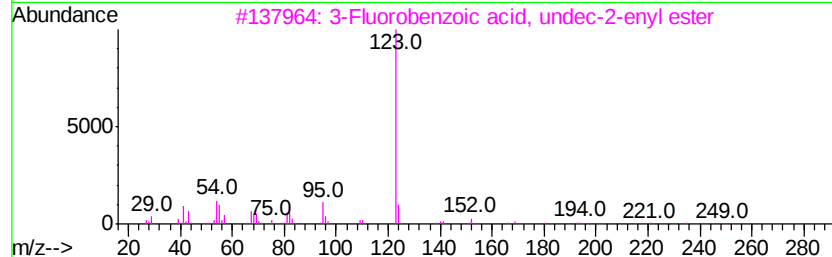
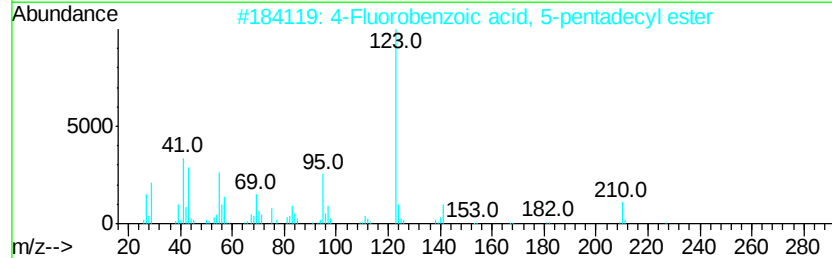
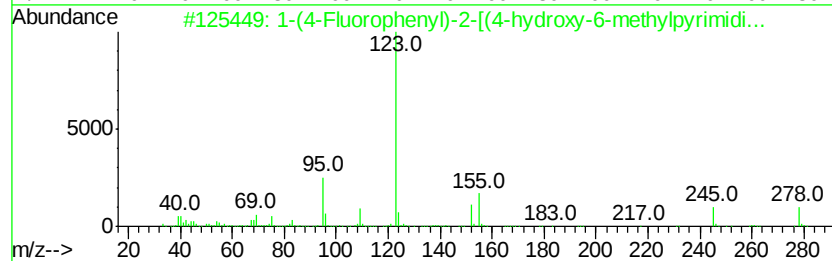
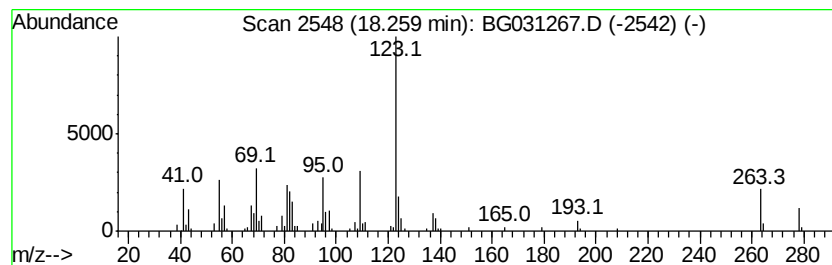
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Peak Number 5 1-(4-Fluorophenyl)-2-[(4-hy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.26	2.20 ng	111296	Phenanthrene-d10	17.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-2-[(4-hydroxy...	278	C13H11FN2O2S	119730-11-9	52
2	4-Fluorobenzoic acid, 5-pentadec...	350	C22H35FO2	1000280-68-6	50
3	3-Fluorobenzoic acid, undec-2-en...	292	C18H25FO2	1000292-60-8	50
4	Phorone	138	C9H14O	000504-20-1	49
5	4-Fluorobenzoic acid, 6-ethyl-3-...	280	C17H25FO2	1000279-07-4	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	5.2	ng	64576	1	8.13	250945	20.0
unknown7.67	7.67	91.5	ng	1147840	1	8.13	250945	20.0
Benzophenone	16.10	2.4	ng	76805	3	14.75	634106	20.0
1-(4-Fluorophenyl...	18.26	2.2	ng	111296	4	17.49	1013420	20.0