

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061418\
 Data File : BF106477.D
 Acq On : 15 Jun 2018 7:16
 Operator : JU/SJ
 Sample : J3475-04
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 061218-DBRI-F-D-B

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	5.196	483	486	492	rBV	89348	88752	2.99%	0.447%
2	5.613	554	557	569	rVB	1148485	1124235	37.92%	5.665%
3	6.607	723	726	735	rBV	910169	842248	28.41%	4.244%
4	6.743	745	749	753	rBV	2070546	1799352	60.70%	9.067%
5	6.966	783	787	790	rBV	825298	660756	22.29%	3.330%
6	7.125	809	814	817	rBV	2622683	2368661	79.90%	11.936%
7	7.531	877	883	886	rBV	1962435	1896154	63.96%	9.555%
8	8.248	1001	1005	1008	rBV	880360	714731	24.11%	3.602%
9	8.801	1095	1099	1102	rBV	122069	100233	3.38%	0.505%
10	9.325	1183	1188	1191	rBV	3014650	2853113	96.24%	14.377%
11	9.713	1250	1254	1259	rBV	320222	256351	8.65%	1.292%
12	10.007	1300	1304	1309	rVB	759163	656214	22.14%	3.307%
13	10.666	1413	1416	1419	rVB	75782	57532	1.94%	0.290%
14	10.719	1421	1425	1428	rVB	321528	283399	9.56%	1.428%
15	10.795	1434	1438	1442	rBV	1197312	1066393	35.97%	5.374%
16	11.495	1554	1557	1561	rBV	796755	659117	22.23%	3.321%
17	12.889	1791	1794	1797	rVB	70636	53868	1.82%	0.271%
18	13.083	1823	1827	1830	rBV	3037764	2964460	100.00%	14.938%
19	13.595	1911	1914	1917	rBV	52207	41102	1.39%	0.207%
20	13.971	1974	1978	1987	rBV	44658	64628	2.18%	0.326%
21	14.148	2004	2008	2012	rBV	872110	765543	25.82%	3.858%
22	15.683	2264	2269	2276	rBV	400705	528503	17.83%	2.663%

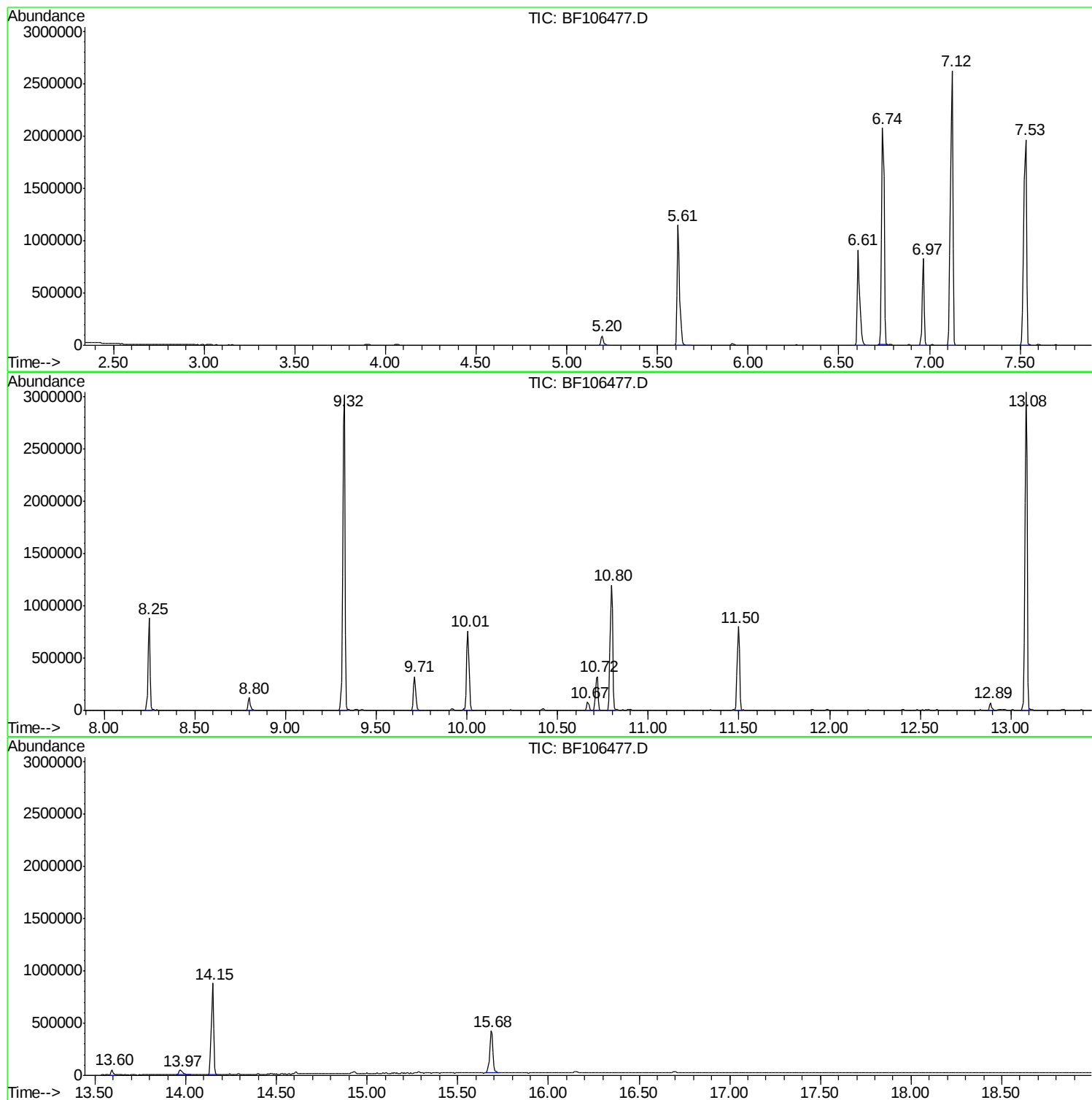
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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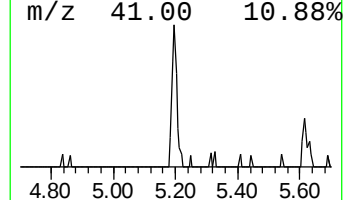
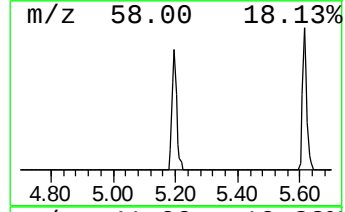
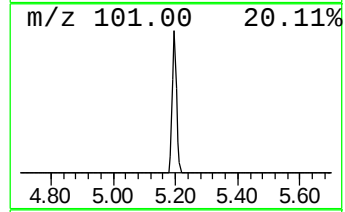
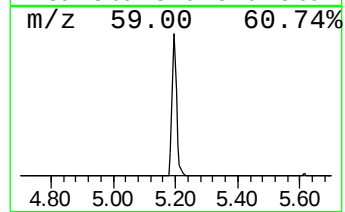
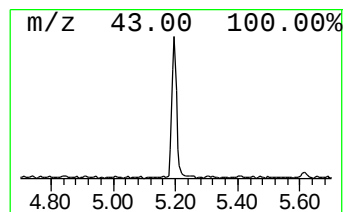
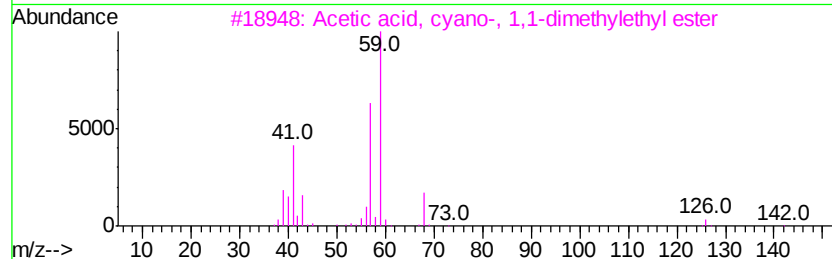
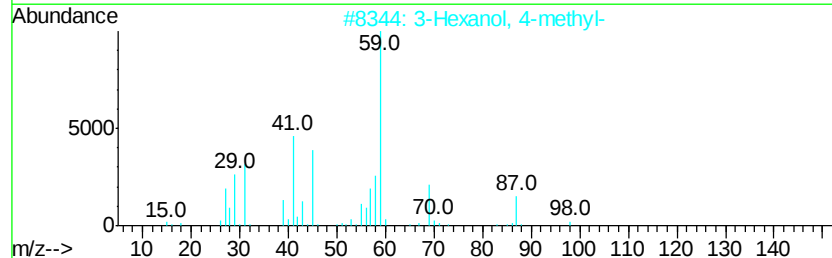
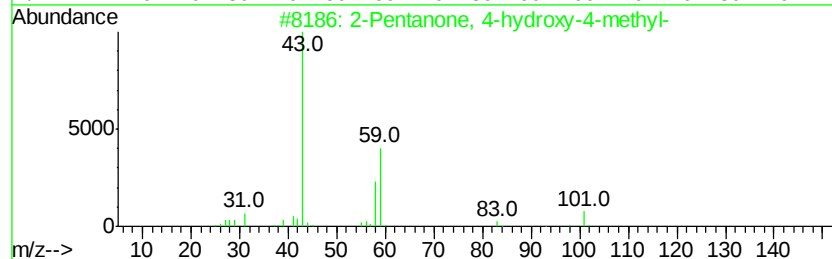
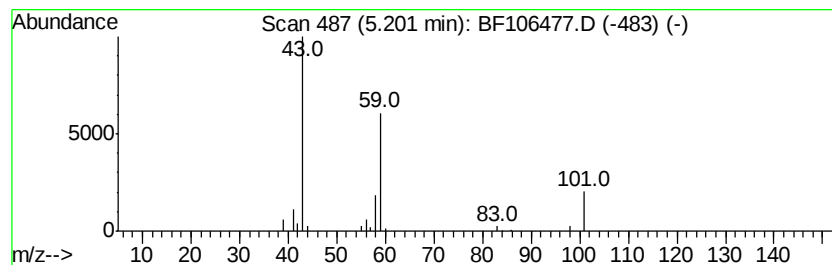
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.69 ng	88752	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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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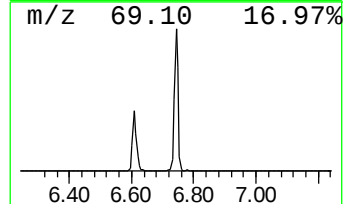
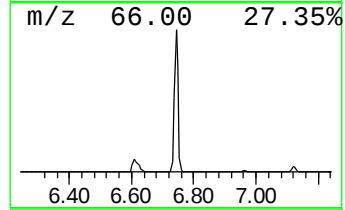
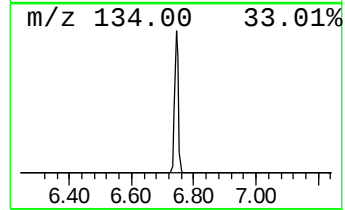
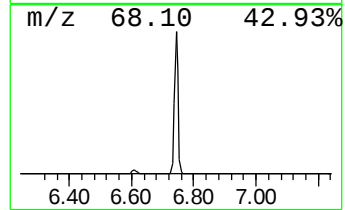
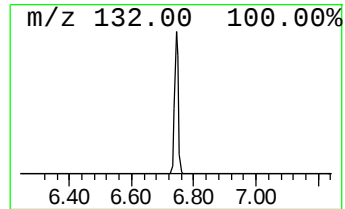
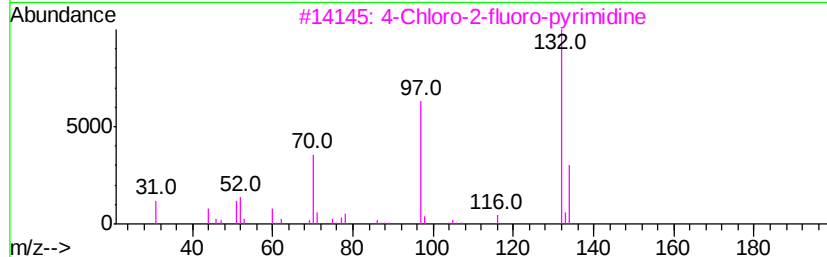
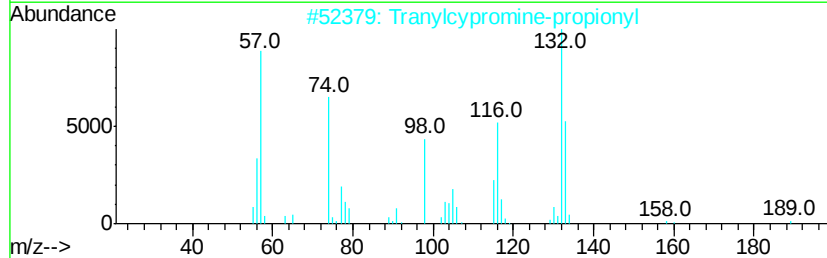
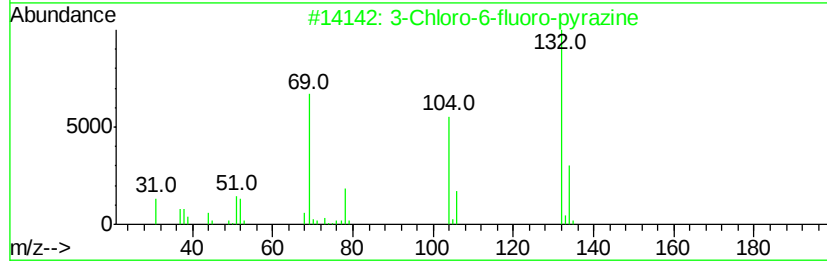
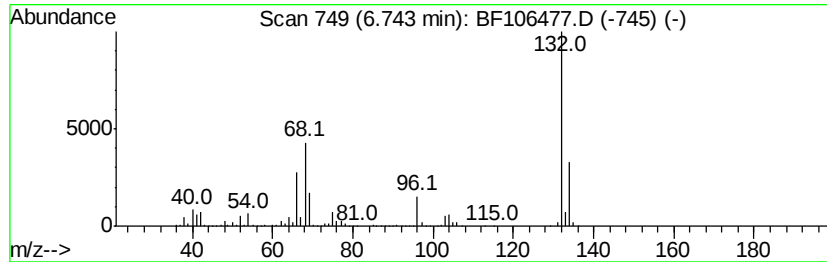
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Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	54.46 ng	1799350	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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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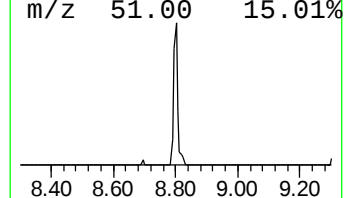
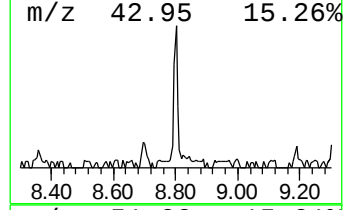
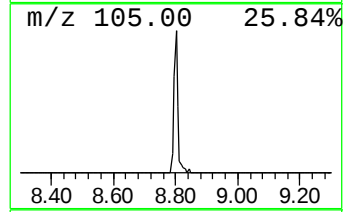
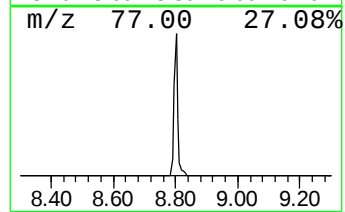
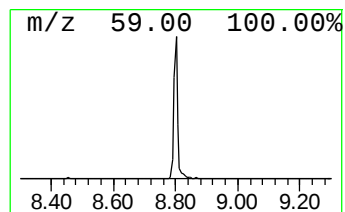
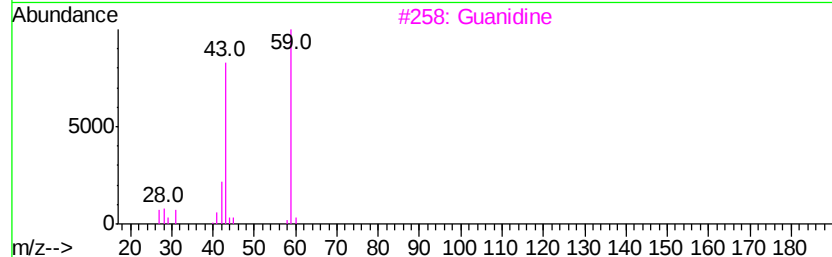
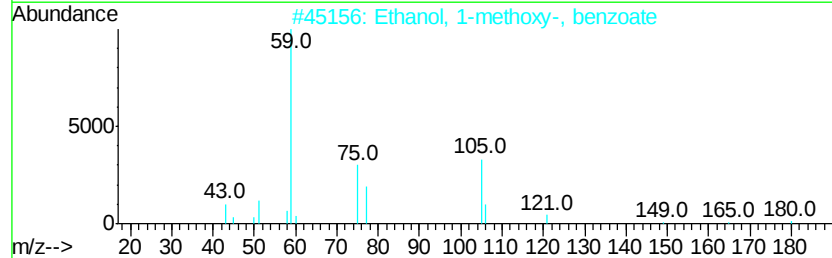
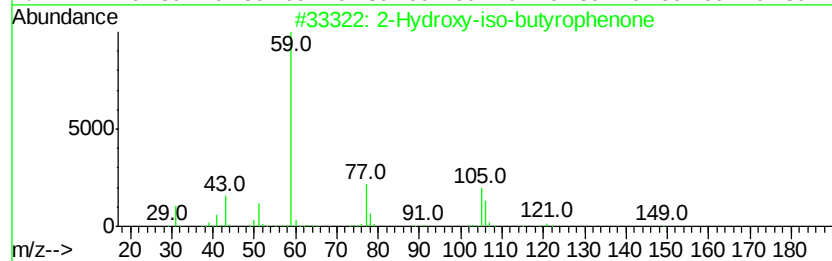
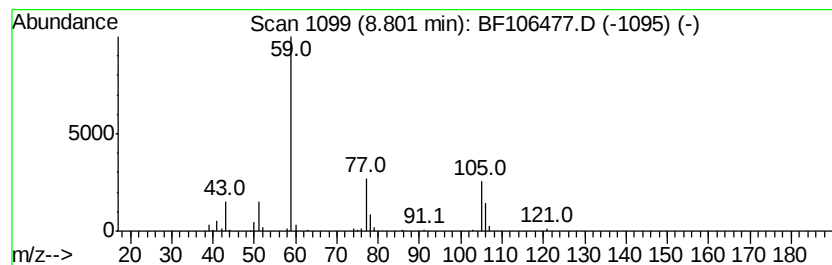
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.80 ng	100233	Napthalene-d8	8.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Guanidine	59	CH5N3	000113-00-8	9
4		Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9



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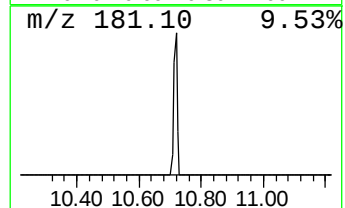
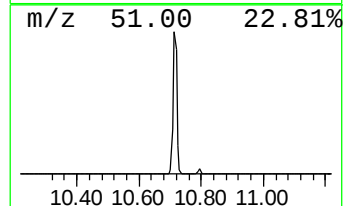
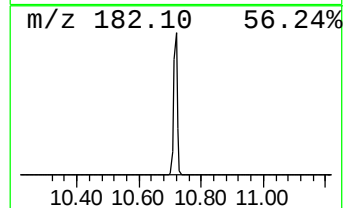
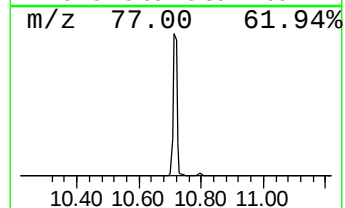
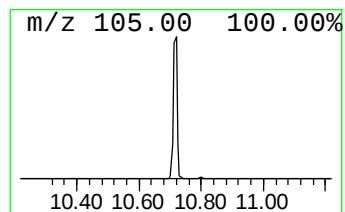
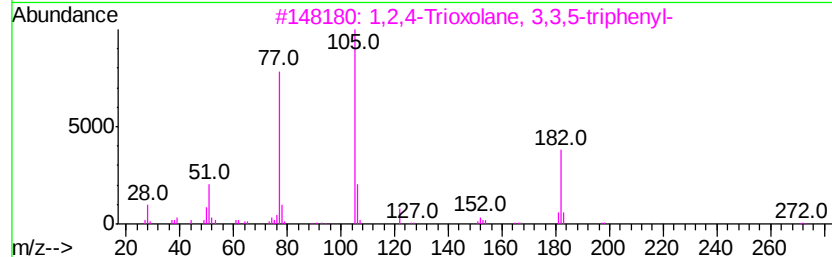
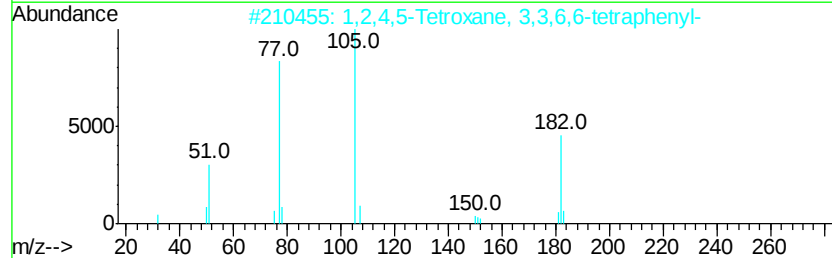
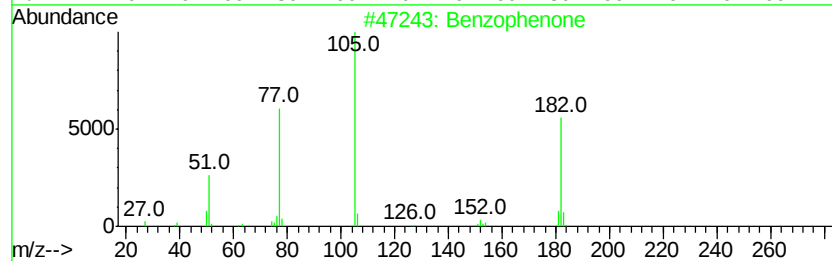
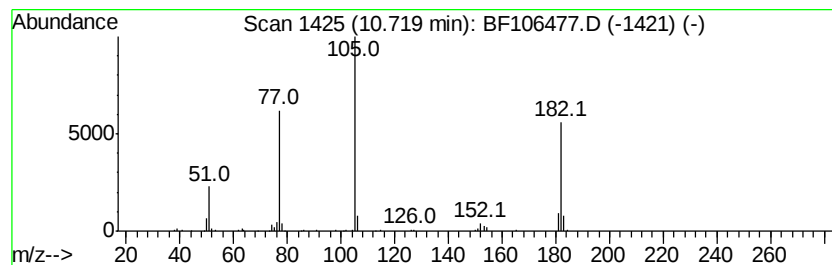
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	8.64 ng	283399	Acenaphthene-d10	10.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
4		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5		Benzopinacol	366	C26H22O2	000464-72-2	47



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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...	5.20	2.7	ng	88752	1	6.97	660756	20.0
unknown6.74	6.74	54.5	ng	1799350	1	6.97	660756	20.0
2-Hydroxy-iso-but...	8.80	2.8	ng	100233	2	8.25	714731	20.0
Benzophenone	10.72	8.6	ng	283399	3	10.01	656214	20.0