

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
 Data File : BF104683.D
 Acq On : 20 Apr 2018 19:13
 Operator : JU/SJ
 Sample : J2477-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-022

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-BF040618.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	5.010	492	497	505	rBV	70003	89809	4.31%	0.474%
2	5.422	563	567	570	rBV	2240230	2034754	97.73%	10.744%
3	6.075	672	678	681	rBV	219332	189605	9.11%	1.001%
4	6.445	736	741	748	rBV	1982060	2018422	96.94%	10.658%
5	6.498	748	750	755	rVB	28840	23571	1.13%	0.124%
6	6.575	759	763	766	rBV	2424868	2082081	100.00%	10.994%
7	6.804	798	802	805	rBV	836637	659734	31.69%	3.484%
8	6.957	824	828	832	rBV	1798021	1640251	78.78%	8.661%
9	7.369	893	898	901	rBV	1412149	1175355	56.45%	6.206%
10	8.087	1017	1020	1026	rBV	972065	804780	38.65%	4.250%
11	8.128	1026	1027	1040	rVB2	19035	25365	1.22%	0.134%
12	9.163	1199	1203	1213	rBV	2277975	2030681	97.53%	10.723%
13	9.557	1266	1270	1278	rBV	145583	132932	6.38%	0.702%
14	9.769	1303	1306	1310	rVB	58497	48352	2.32%	0.255%
15	9.845	1315	1319	1327	rVV	876983	801076	38.47%	4.230%
16	10.269	1388	1391	1394	rVB	67157	55349	2.66%	0.292%
17	10.486	1422	1428	1430	rBV	18921	23230	1.12%	0.123%
18	10.633	1450	1453	1464	rVV	1185580	1087781	52.24%	5.744%
19	10.739	1468	1471	1480	rVB	62363	60937	2.93%	0.322%
20	11.186	1544	1547	1550	rBV	25478	24909	1.20%	0.132%
21	11.333	1568	1572	1578	rBV	829832	724540	34.80%	3.826%
22	12.916	1837	1841	1845	rBV	1697161	1640685	78.80%	8.663%
23	13.774	1982	1987	1990	rBV	119857	145079	6.97%	0.766%
24	13.810	1990	1993	2005	rVB	211915	235266	11.30%	1.242%
25	13.974	2018	2021	2029	rBV	610542	630409	30.28%	3.329%
26	14.445	2098	2101	2107	rBV7	24194	41426	1.99%	0.219%
27	14.821	2162	2165	2169	rVB	36336	35778	1.72%	0.189%
28	15.445	2266	2271	2279	rBV	360532	475829	22.85%	2.513%

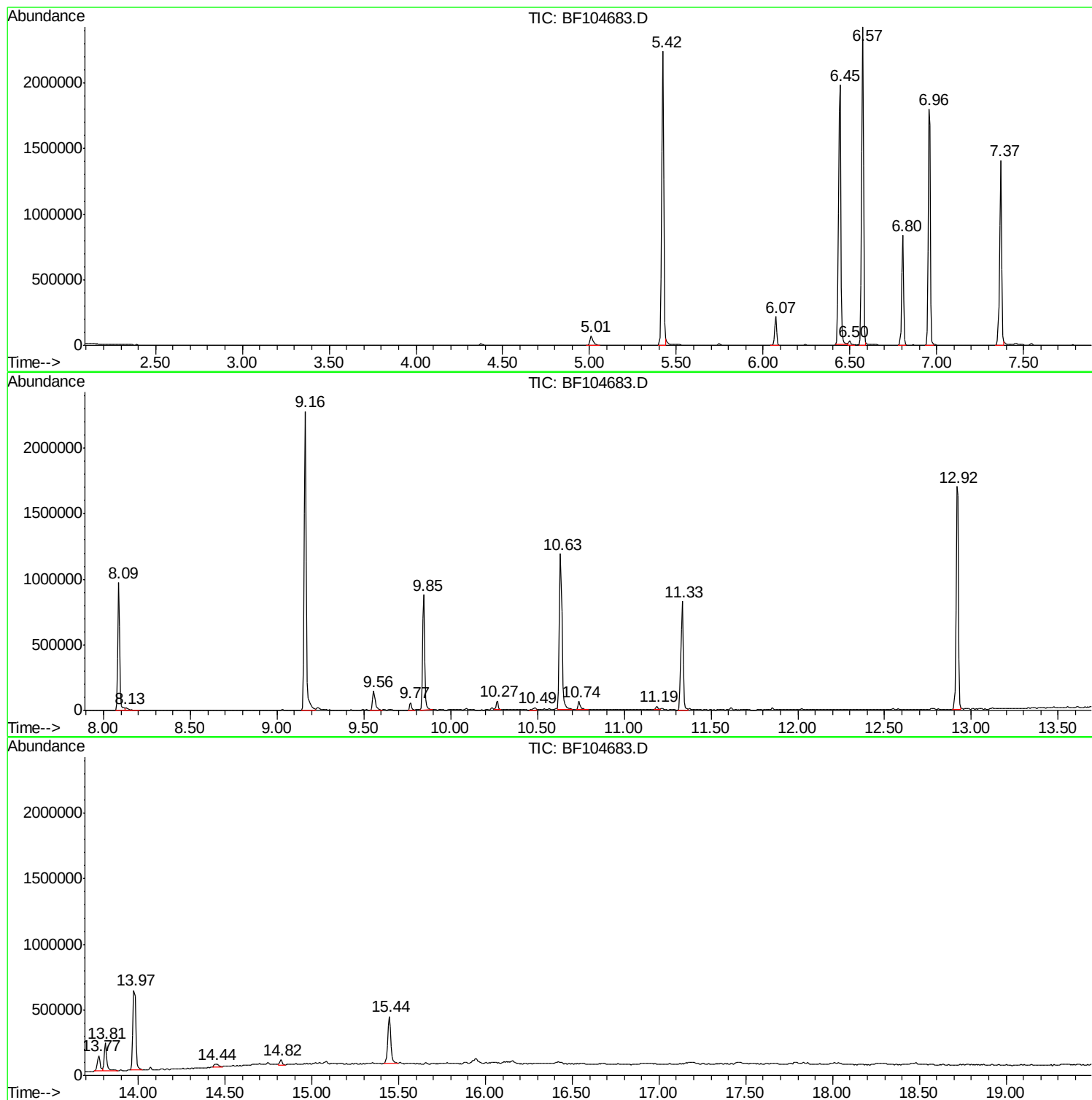
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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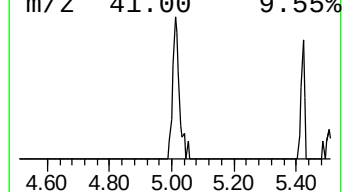
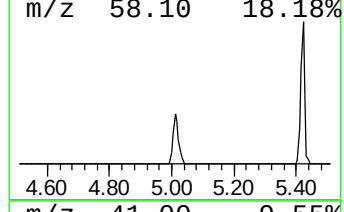
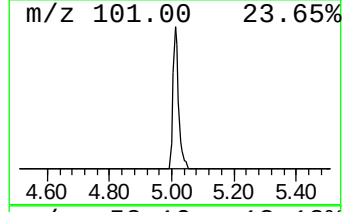
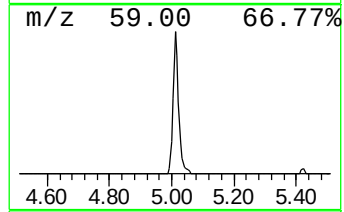
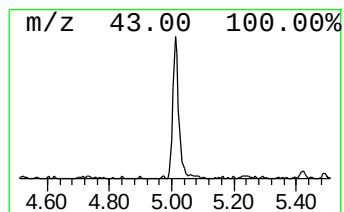
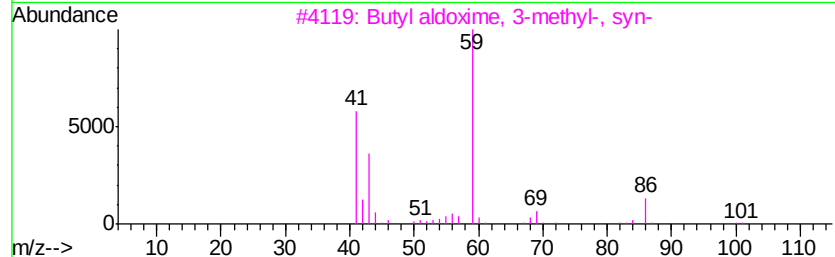
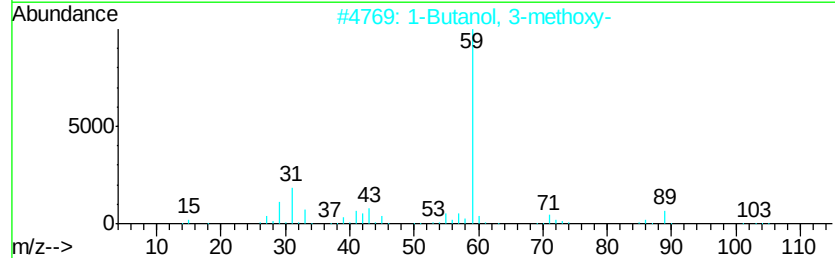
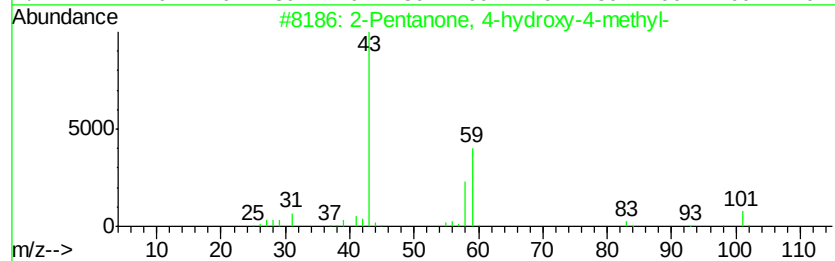
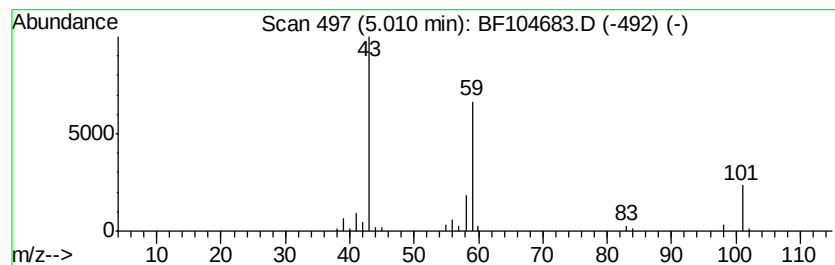
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.72 ng	89809	1,4-Dichlorobenzene-d4	6.80

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	25
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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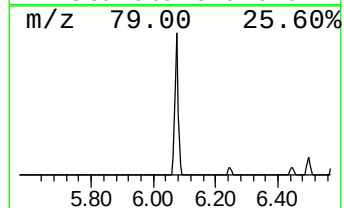
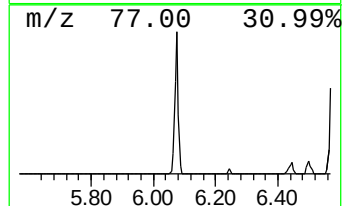
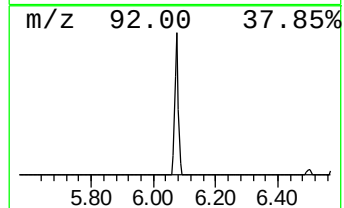
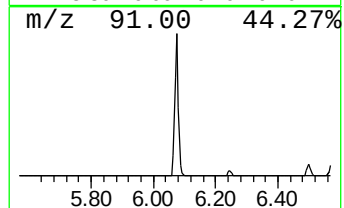
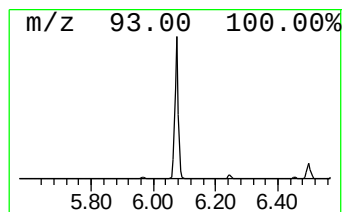
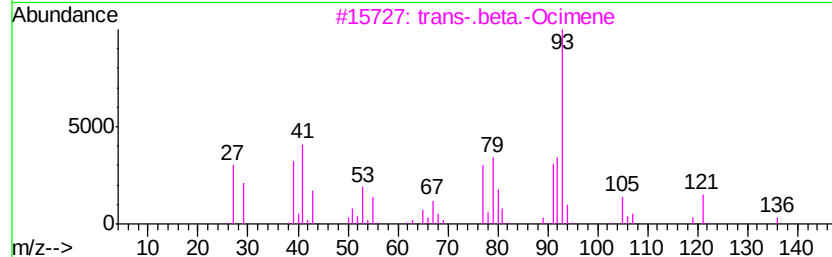
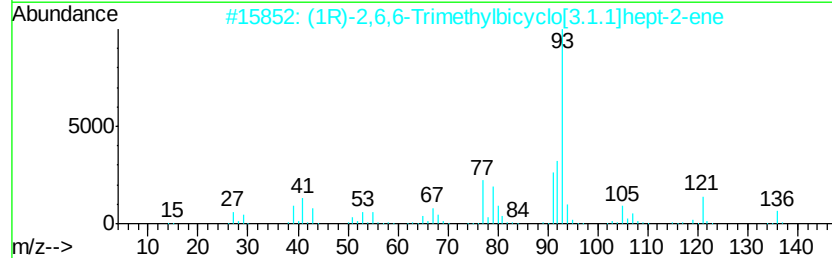
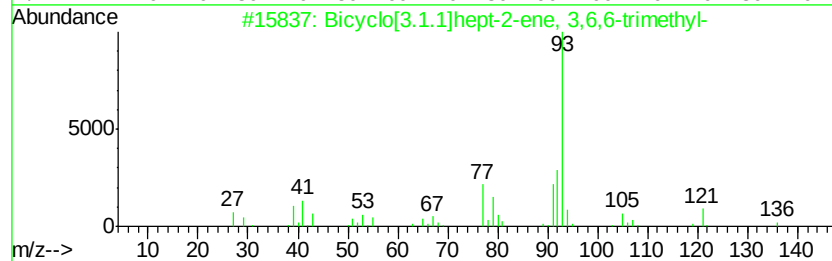
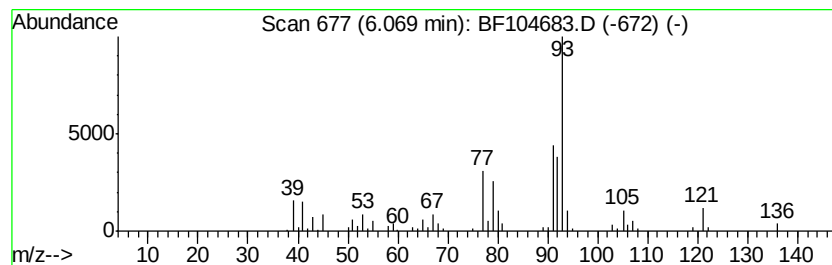
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.07	5.75 ng	189605	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	95
2			(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
3			trans-.beta.-Ocimene	136	C10H16	003779-61-1	91
4			Tricyclo[2.2.1.0(2,6)]heptane, 1,4-dichloro-	136	C10H16	000508-32-7	91
5			.alpha.-Pinene	136	C10H16	000080-56-8	90



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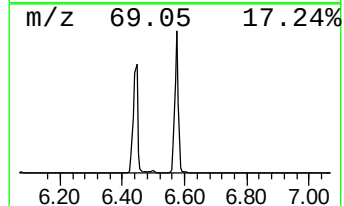
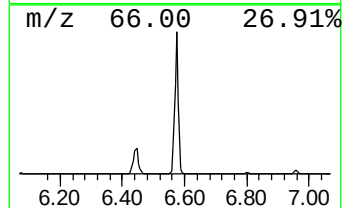
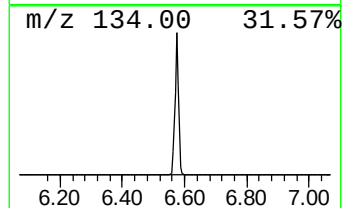
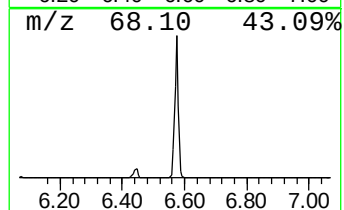
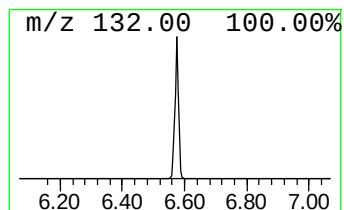
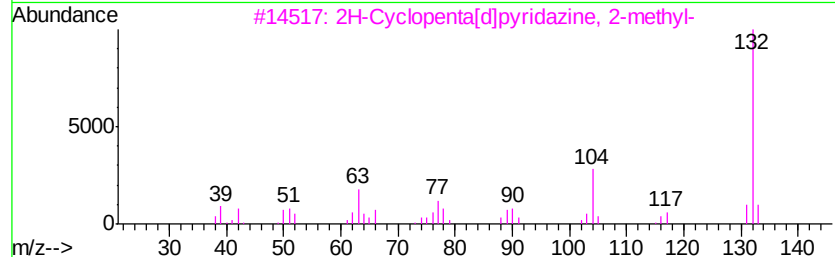
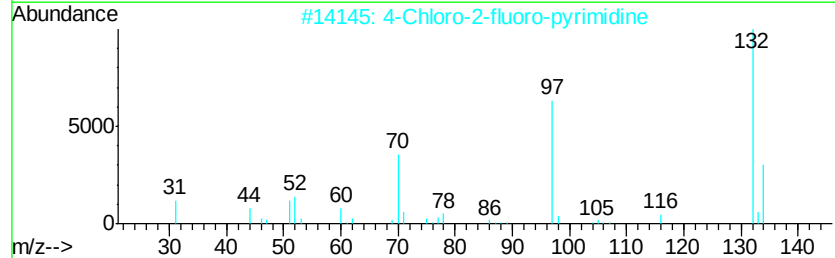
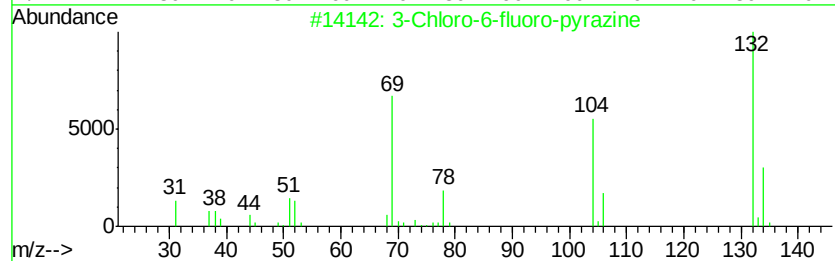
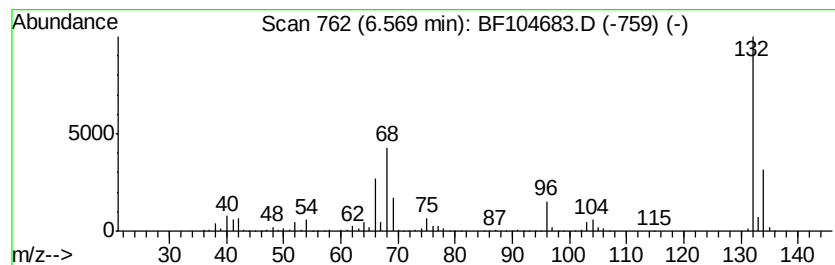
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Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	63.12 ng	2082080	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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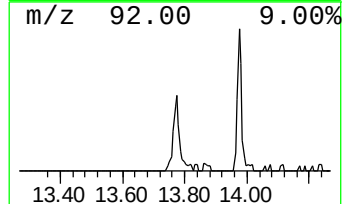
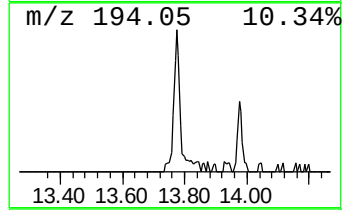
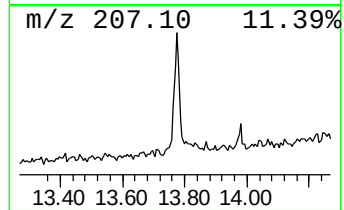
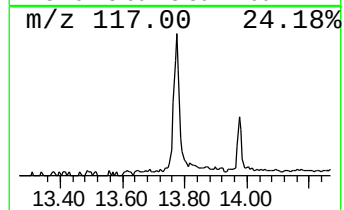
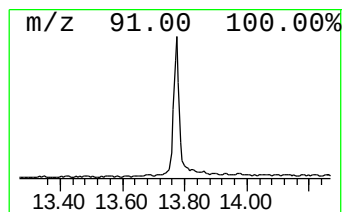
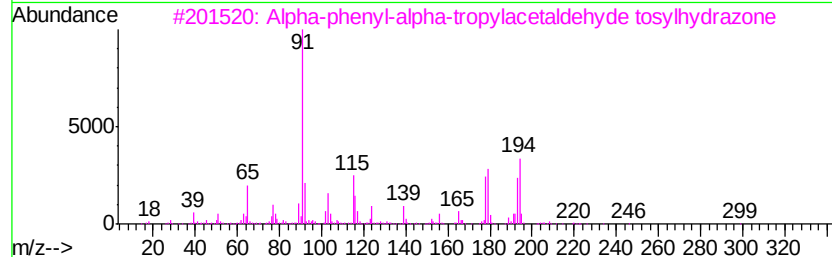
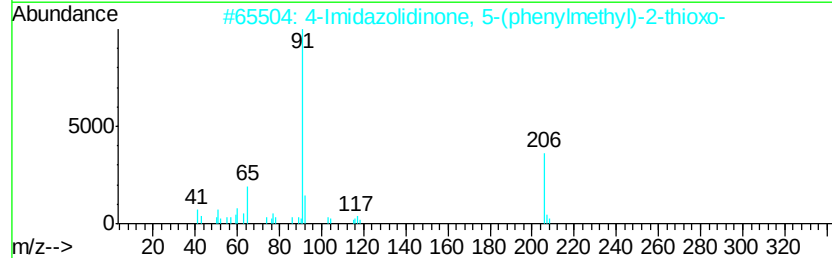
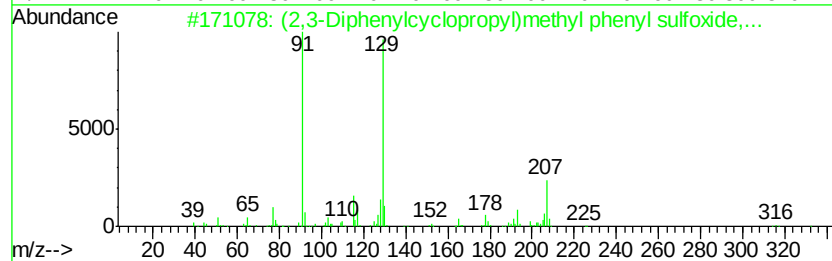
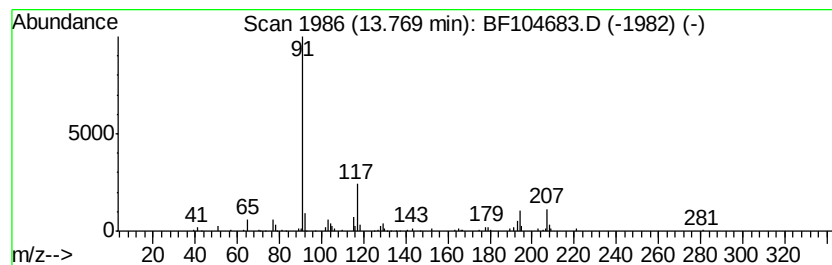
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Peak Number 5 unknown13.77 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.60 ng	145079	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	32
2		4-Imidazolidinone, 5-(phenylmeth...	206	C10H10N2OS	006330-09-2	25
3		Alpha-phenyl-alpha-troplacetal...	378	C22H22N2O2S	022532-16-7	22
4		Benzenemethanamine, N-(phenylmet...	195	C14H13N	000780-25-6	12
5		2,5-Diphenyltetrazole	222	C13H10N4	018039-45-7	10



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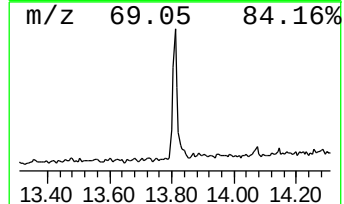
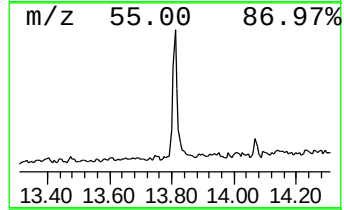
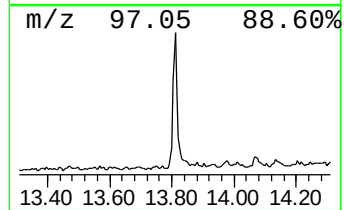
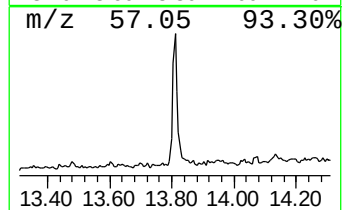
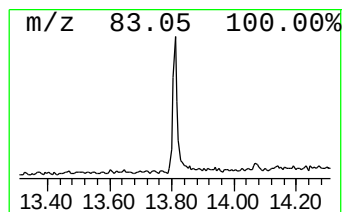
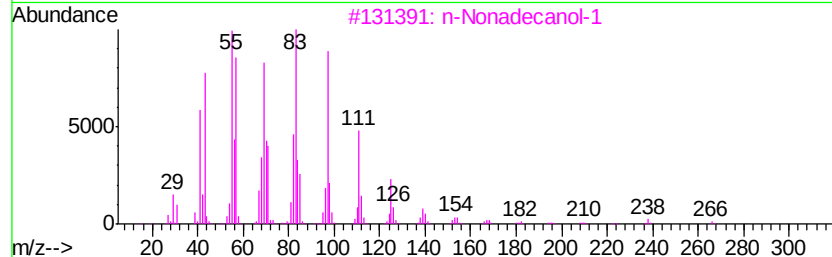
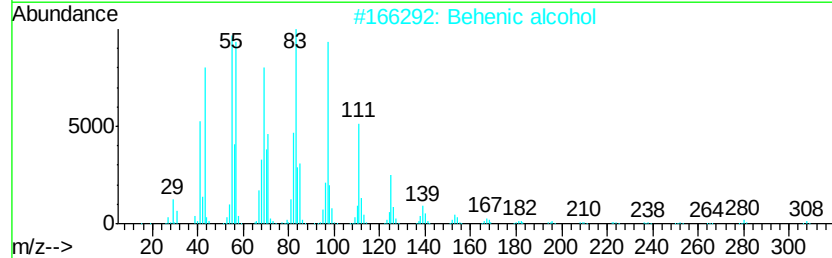
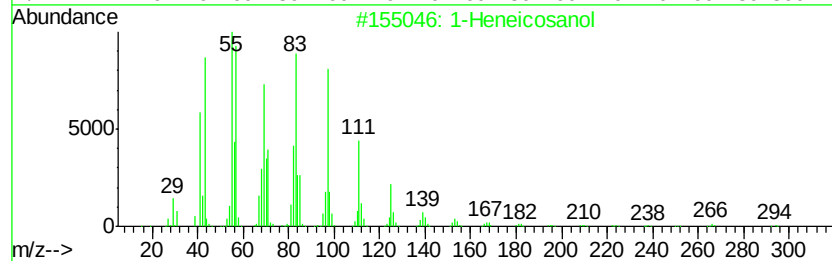
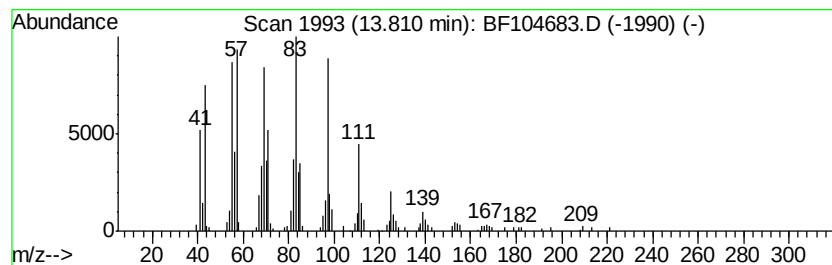
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Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	7.46 ng	235266	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	2.7	ng	89809	1	6.80	659734	20.0
Bicyclo[3.1.1]hep...	6.07	5.8	ng	189605	1	6.80	659734	20.0
unknown6.57	6.57	63.1	ng	2082080	1	6.80	659734	20.0
unknown13.77	13.77	4.6	ng	145079	5	13.97	630409	20.0
1-Heneicosanol	13.81	7.5	ng	235266	5	13.97	630409	20.0