

Data Path : Z:\HPCHEM1\BNA F\Data\BF040517\
 Data File : BF094189.D
 Acq On : 5 Apr 2017 15:12
 Operator : SJ/MA
 Sample : PB98041BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98041BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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	1.946	7	10	19	rVB	40791	77979	1.50%	0.185%
2	4.016	357	362	370	rBV	515608	674718	12.97%	1.597%
3	4.410	423	429	432	rBV	3977265	4236319	81.45%	10.025%
4	5.475	603	610	613	rBV	3631520	4270390	82.11%	10.106%
5	5.610	628	633	637	rBV	3914183	4426948	85.12%	10.477%
6	5.863	672	676	680	rBV	1117839	979591	18.83%	2.318%
7	6.045	702	707	710	rVB	3337306	3480962	66.93%	8.238%
8	6.510	780	786	790	rBV	2293760	2843054	54.66%	6.728%
9	7.363	926	931	935	rBV	1301816	1335921	25.69%	3.162%
10	8.692	1150	1157	1160	rBV	4354416	5200916	100.00%	12.308%
11	9.504	1288	1295	1299	rBV2	1419217	1472832	28.32%	3.486%
12	10.480	1454	1461	1464	rBV	2167869	2448526	47.08%	5.795%
13	11.327	1598	1605	1609	rBV	1467014	1507421	28.98%	3.567%
14	11.886	1694	1700	1705	rVB	105001	121891	2.34%	0.288%
15	12.057	1721	1729	1736	rBV4	21403	52982	1.02%	0.125%
16	12.727	1835	1843	1845	rBV5	39348	61500	1.18%	0.146%
17	12.868	1860	1867	1873	rVB	384568	459357	8.83%	1.087%
18	13.168	1914	1918	1922	rVB2	38633	58930	1.13%	0.139%
19	13.310	1934	1942	1946	rBV	3917472	5199343	99.97%	12.304%
20	14.015	2057	2062	2064	rBV3	38701	62440	1.20%	0.148%
21	14.104	2068	2077	2088	rVB3	113583	423292	8.14%	1.002%
22	14.574	2152	2157	2161	rBV	1412252	1434028	27.57%	3.394%
23	15.762	2352	2359	2371	rBV8	125129	398623	7.66%	0.943%
24	16.204	2429	2434	2440	rBV	879128	1027699	19.76%	2.432%

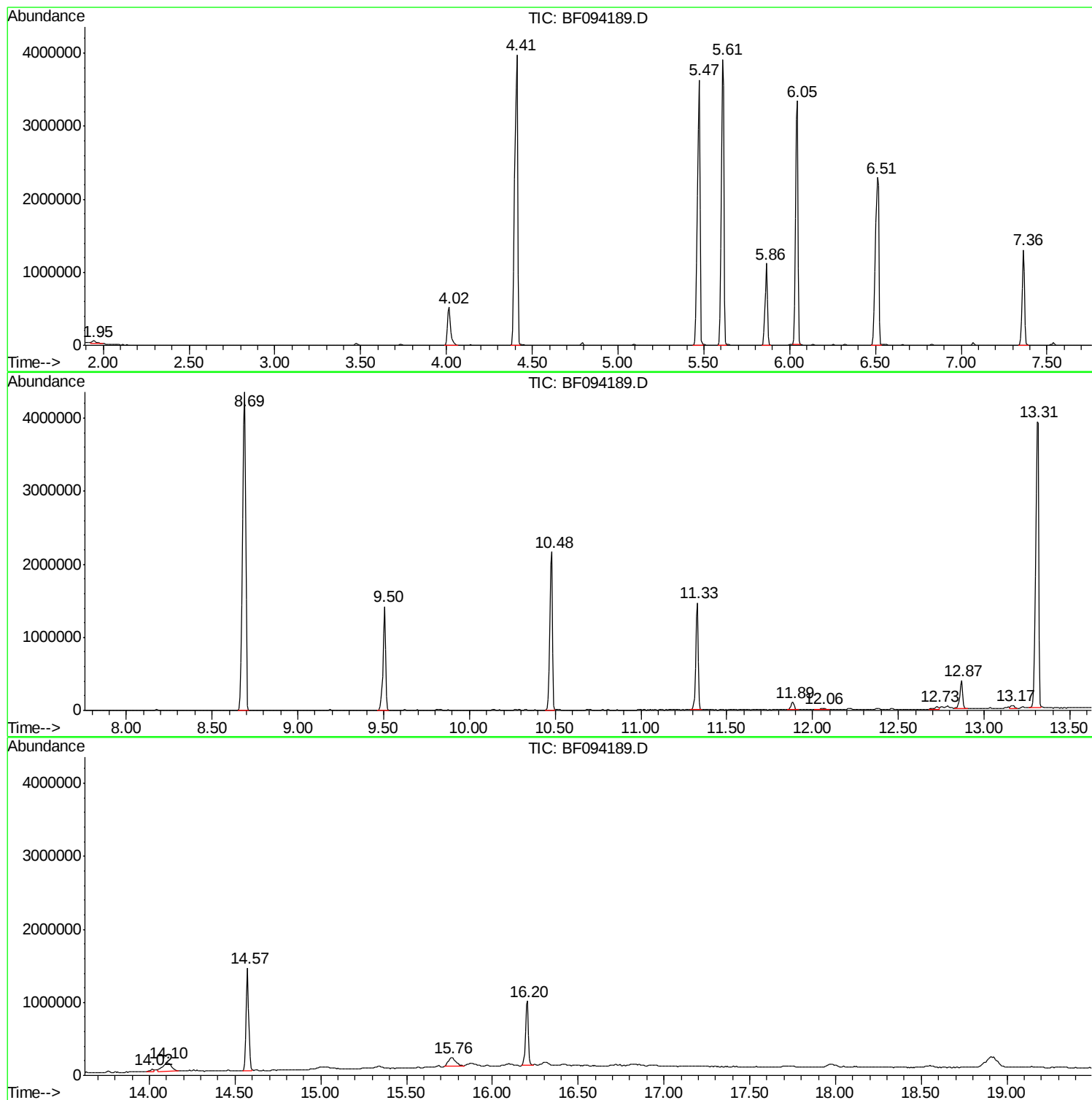
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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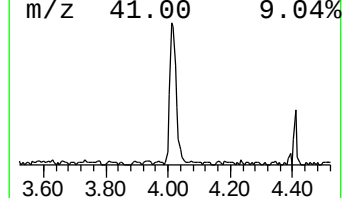
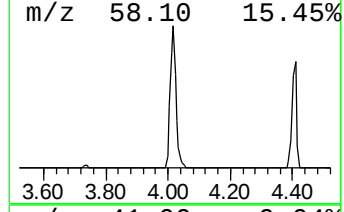
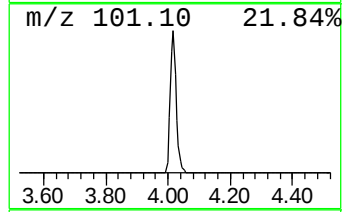
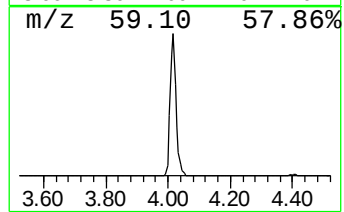
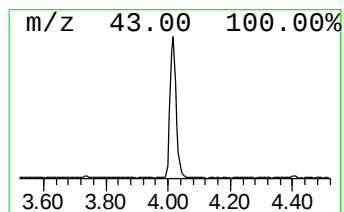
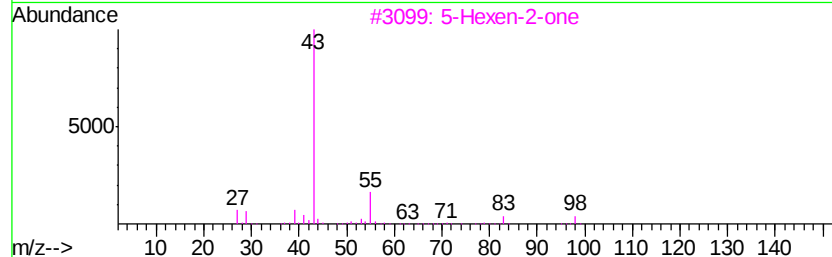
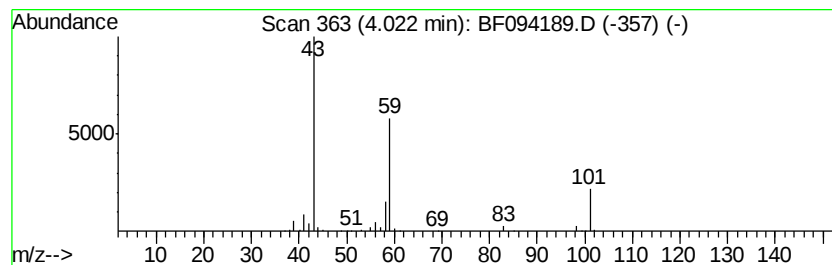
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	13.78 ng	674718	1,4-Dichlorobenzene-d4	5.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	



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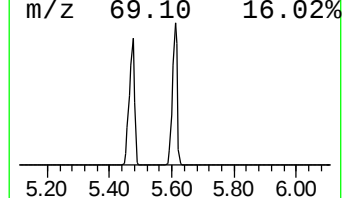
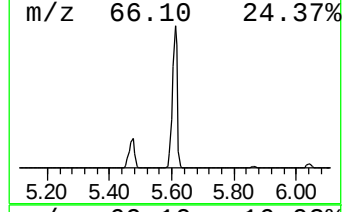
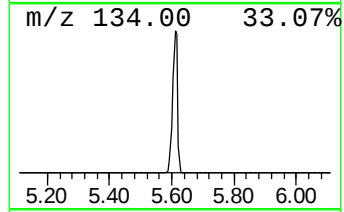
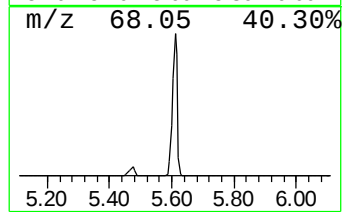
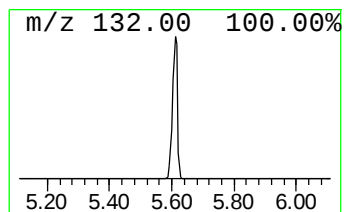
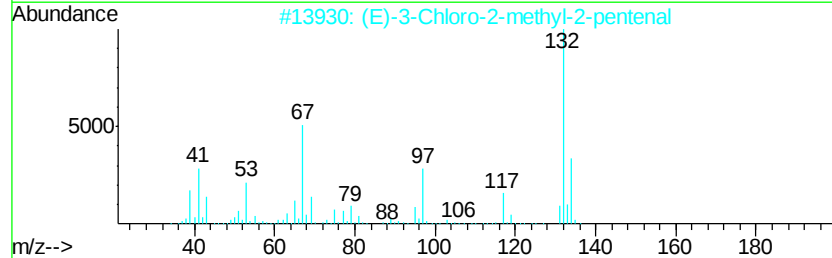
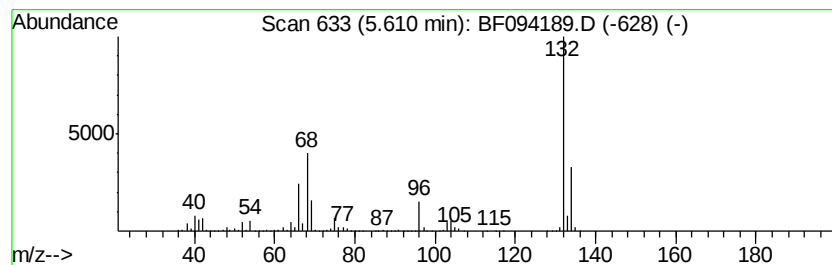
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.61	90.38 ng	4426950	1,4-Dichlorobenzene-d4	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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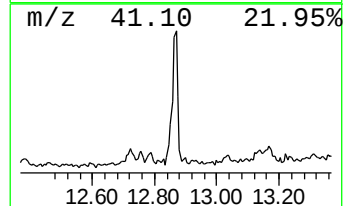
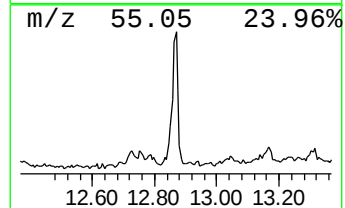
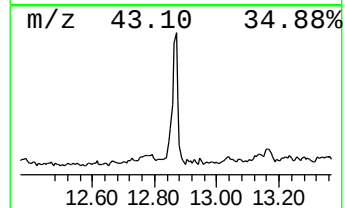
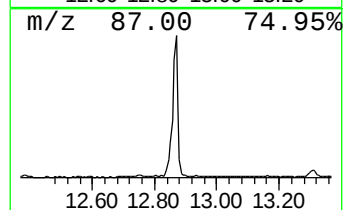
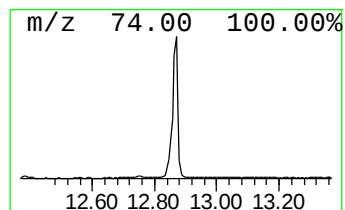
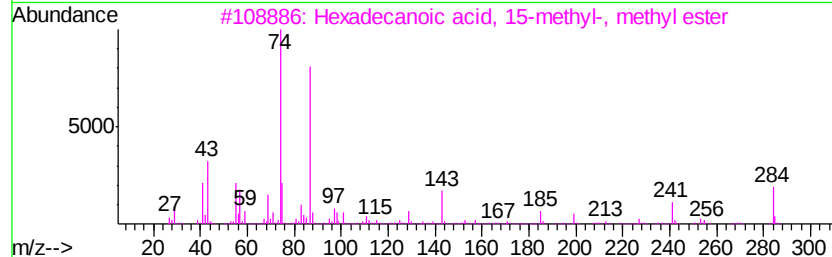
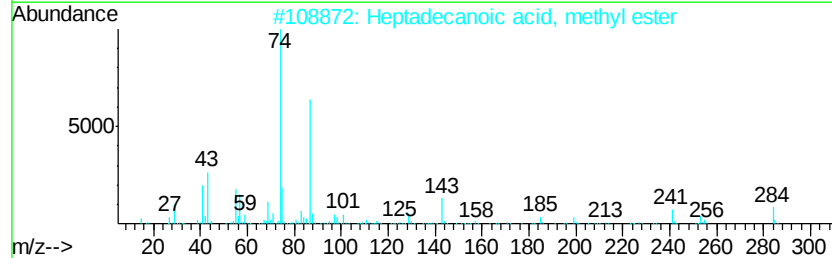
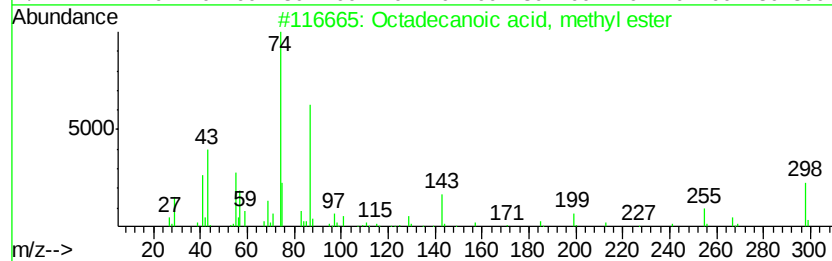
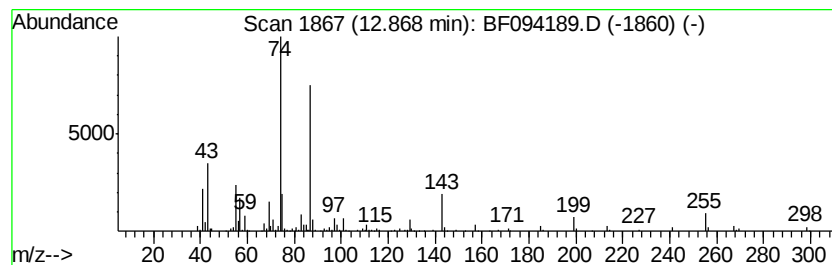
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Peak Number 4 Octadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.87	6.09 ng	459357	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83



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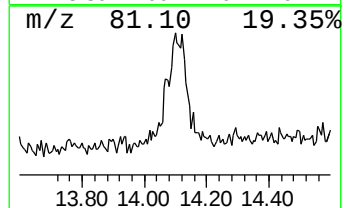
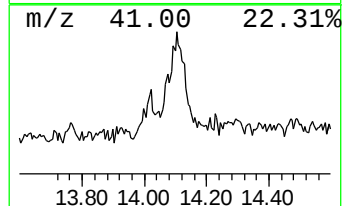
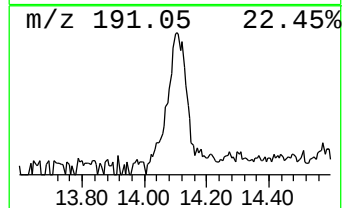
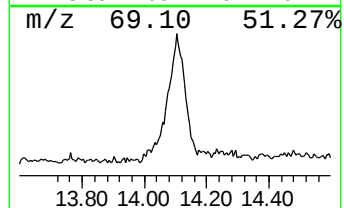
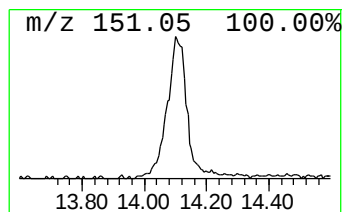
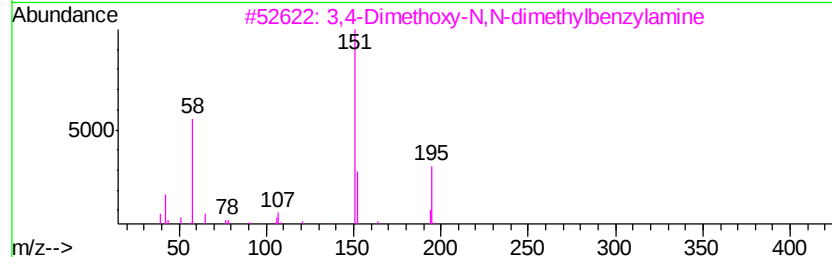
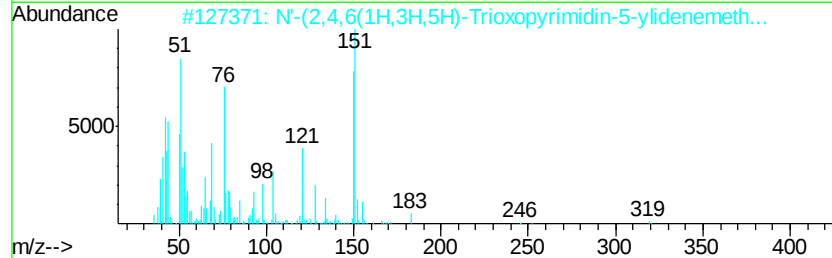
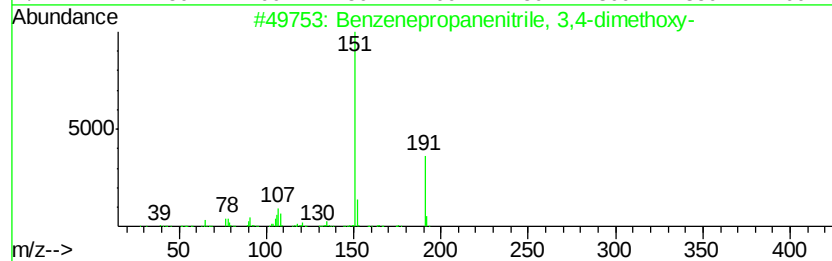
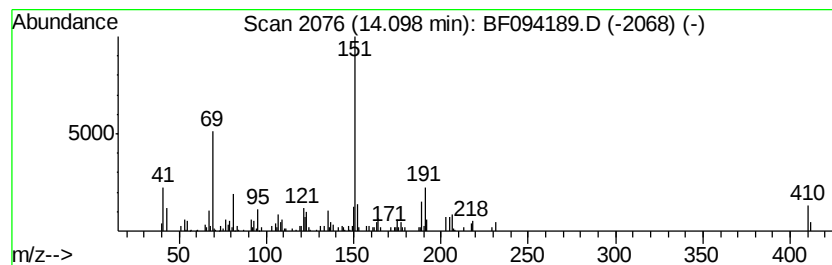
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenepropanenitrile, 3,4-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	5.90 ng	423292	Chrysene-d12	14.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenepropanenitrile, 3,4-dimet...	191	C11H13N02	049621-56-9	50
2		N'-(2,4,6(1H,3H,5H)-Trioxopyrimi...	319	C12H9N5O6	1000225-72-5	46
3		3,4-Dimethoxy-N,N-dimethylbenzyl...	195	C11H17N02	065495-21-8	43
4		Benzaldehyde, 4-methoxy-, oxime	151	C8H9N02	003235-04-9	38
5		Silane, (3,3-dimethylbut-2-yloxy...	208	C12H20OSi	1000163-31-6	38



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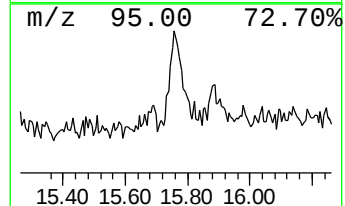
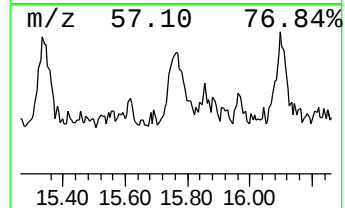
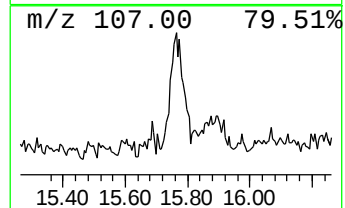
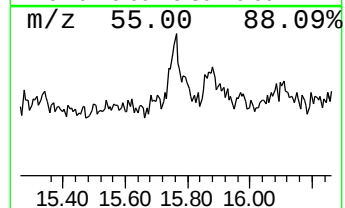
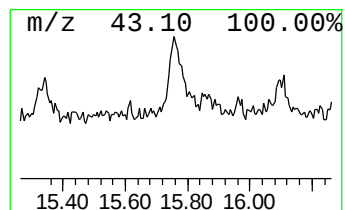
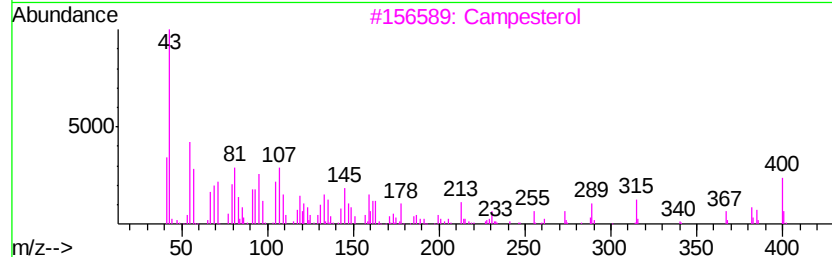
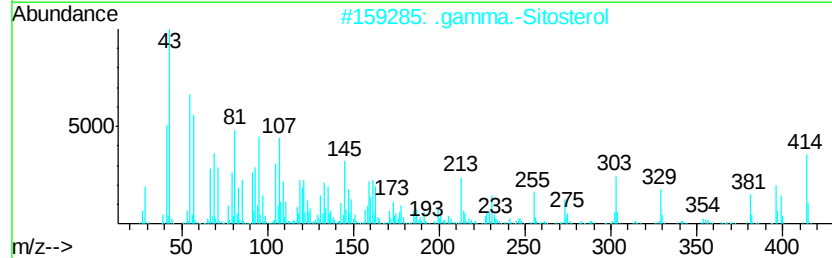
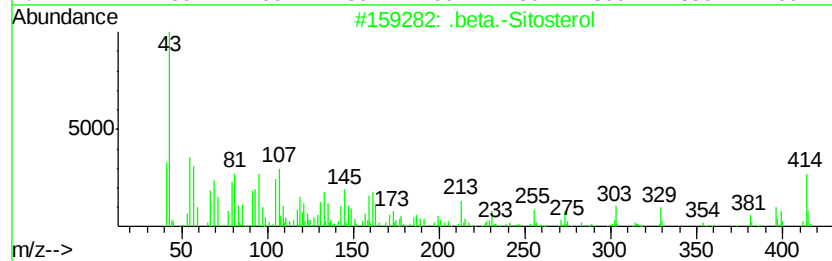
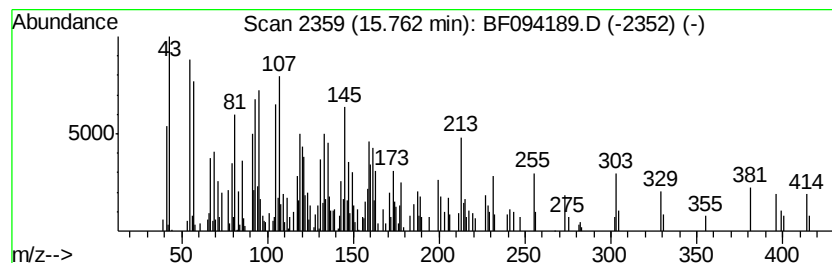
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Peak Number 6 .beta.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.76	7.76 ng	398623	Perylene-d12	16.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	93
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	83
3	Campesterol	400	C28H48O	000474-62-4	58
4	5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	58
5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.02	13.8	ng	674718	1	5.86	979591	20.0
unknown5.61	5.61	90.4	ng	4426950	1	5.86	979591	20.0
Octadecanoic acid...	12.87	6.1	ng	459357	4	11.33	1507420	20.0
Benzenepropanenit...	14.10	5.9	ng	423292	5	14.57	1434030	20.0
.beta.-Sitosterol	15.76	7.8	ng	398623	6	16.20	1027700	20.0