

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104352.D
 Acq On : 7 Apr 2018 12:02
 Operator : JU/SJ
 Sample : J2255-07
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040418-DBRI-E-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-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	4.998	492	495	502	rVB	111587	108664	2.70%	0.466%
2	5.404	559	564	567	rBV	1310786	1120943	27.84%	4.806%
3	6.416	732	736	745	rVB	842784	717392	17.82%	3.076%
4	6.569	757	762	765	rBV	2278059	2094373	52.03%	8.980%
5	6.622	768	771	777	rBV	64838	52397	1.30%	0.225%
6	6.804	798	802	805	rBV	937224	797718	19.82%	3.420%
7	6.963	824	829	832	rVB	2875387	2820294	70.06%	12.092%
8	7.369	892	898	901	rBV	2285508	2271543	56.43%	9.740%
9	8.086	1016	1020	1023	rVB	1328056	1056710	26.25%	4.531%
10	9.163	1198	1203	1206	rBV	3945668	4025673	100.00%	17.261%
11	9.557	1266	1270	1273	rBV	97704	89645	2.23%	0.384%
12	9.774	1303	1307	1310	rBV	75678	66297	1.65%	0.284%
13	9.839	1313	1318	1322	rVB2	1284669	1133881	28.17%	4.862%
14	10.274	1384	1392	1395	rBV2	94843	94885	2.36%	0.407%
15	10.627	1447	1452	1455	rBV	1639356	1445239	35.90%	6.197%
16	10.745	1469	1472	1477	rBV	89764	79308	1.97%	0.340%
17	11.327	1567	1571	1574	rBV	1075254	880573	21.87%	3.776%
18	12.739	1808	1811	1815	rBV	119104	91184	2.27%	0.391%
19	12.921	1837	1842	1845	rBV	2798771	2651951	65.88%	11.371%
20	13.445	1927	1931	1934	rBV	71215	58417	1.45%	0.250%
21	13.809	1990	1993	2004	rBV	195420	192722	4.79%	0.826%
22	13.968	2016	2020	2023	rBV	892594	743213	18.46%	3.187%
23	15.427	2263	2268	2273	rBV2	568089	689137	17.12%	2.955%
24	16.403	2428	2434	2440	rBV2	23139	40595	1.01%	0.174%

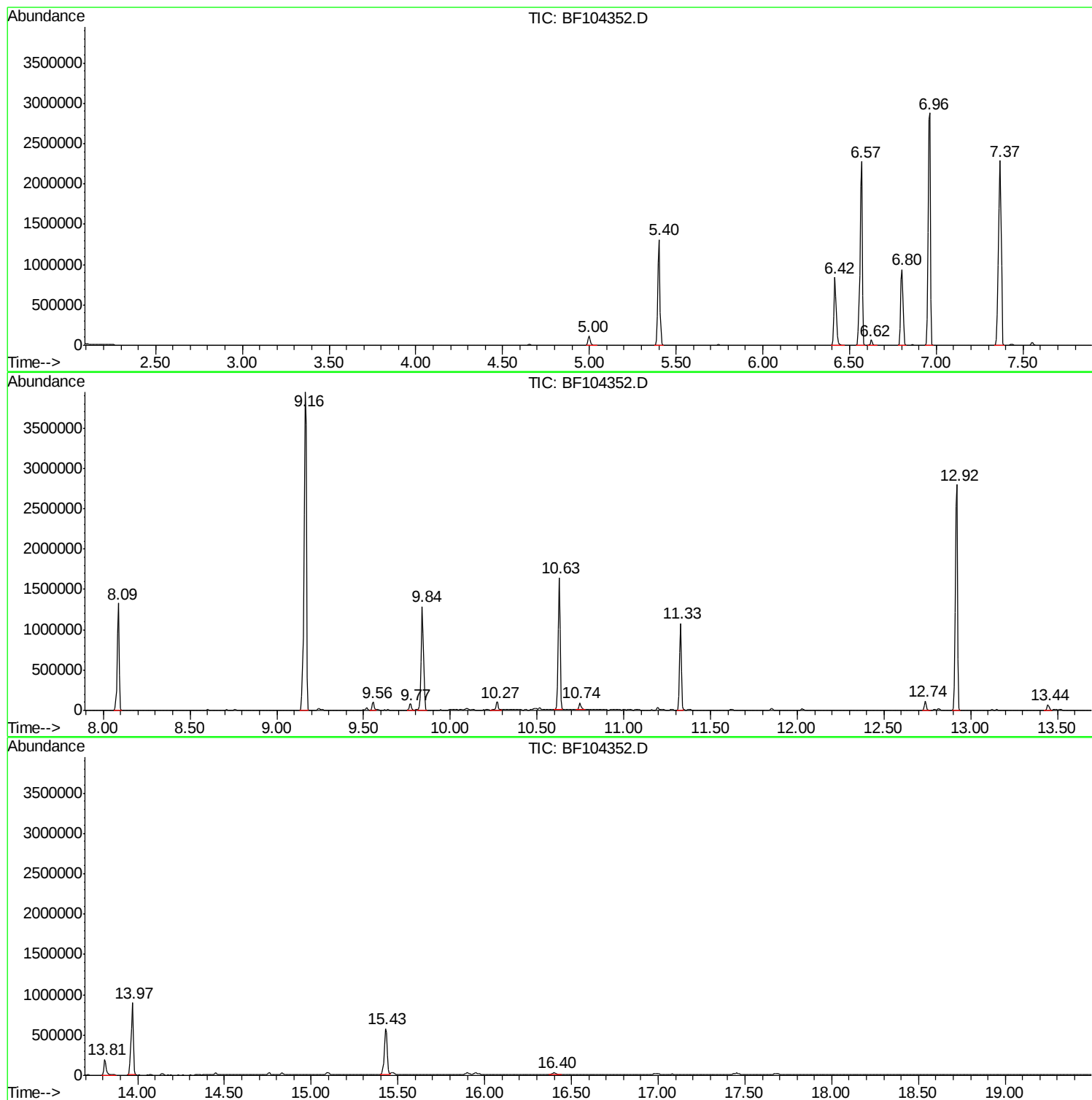
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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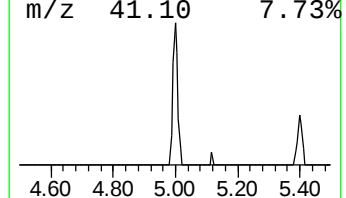
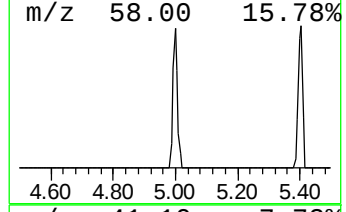
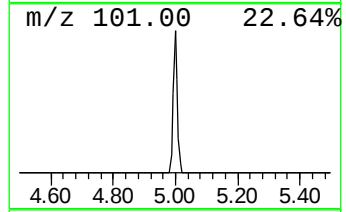
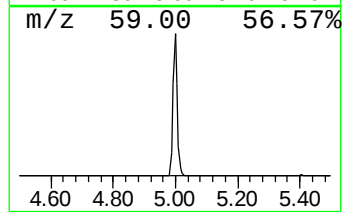
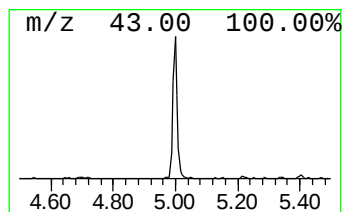
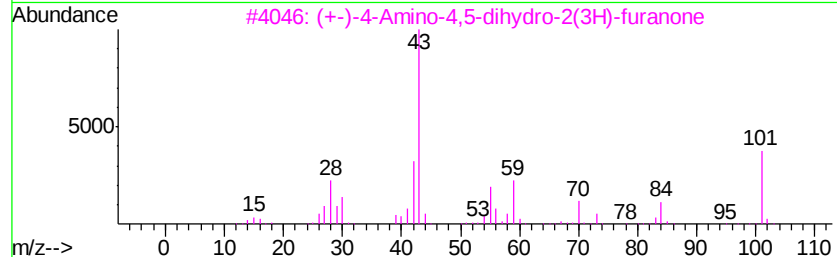
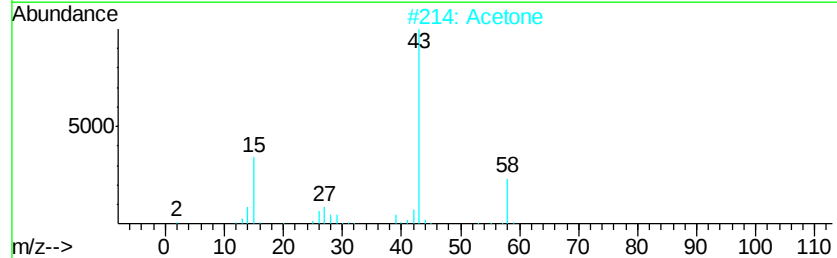
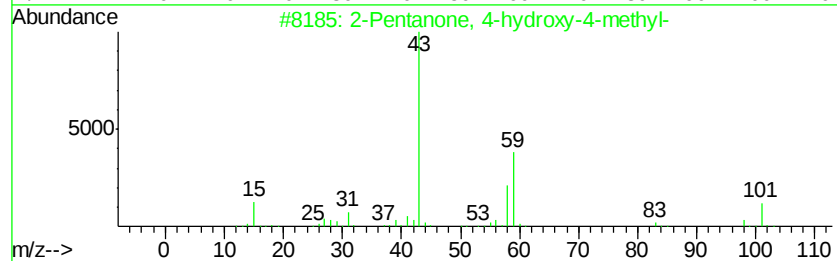
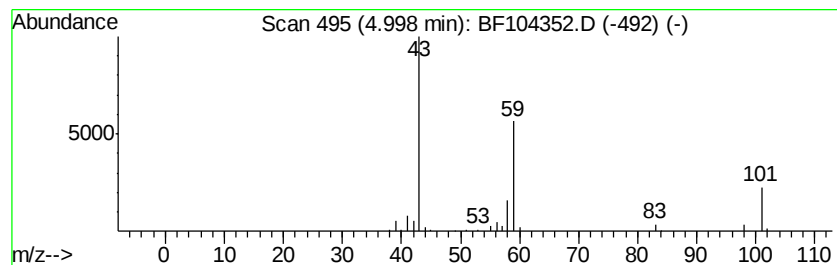
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.72 ng	108664	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	50
2			Acetone	58	C3H6O	000067-64-1	10
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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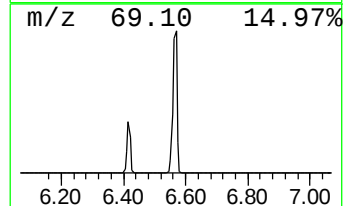
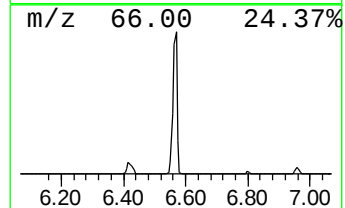
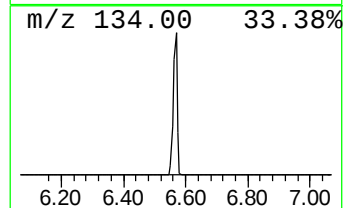
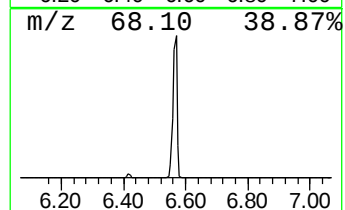
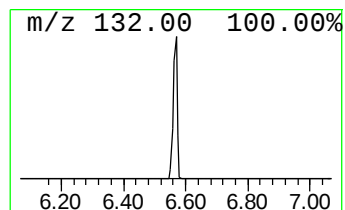
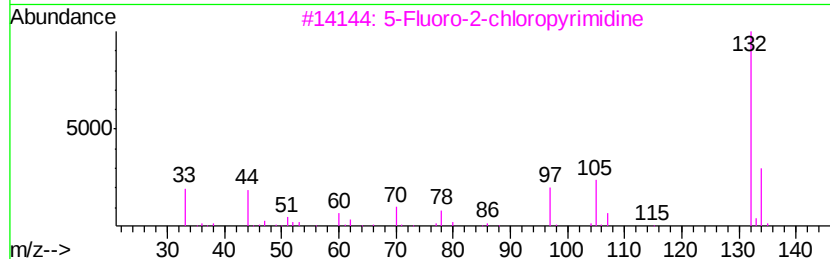
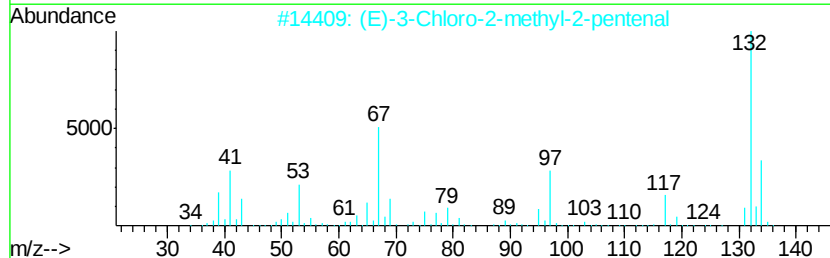
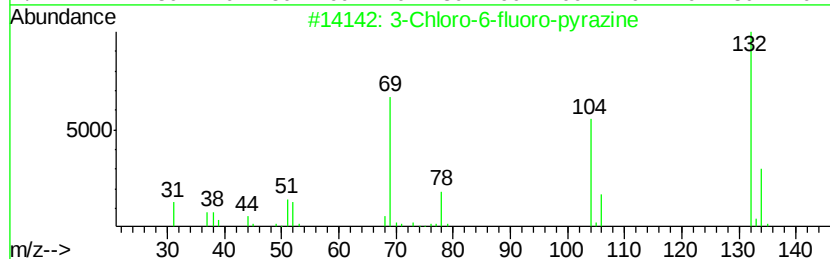
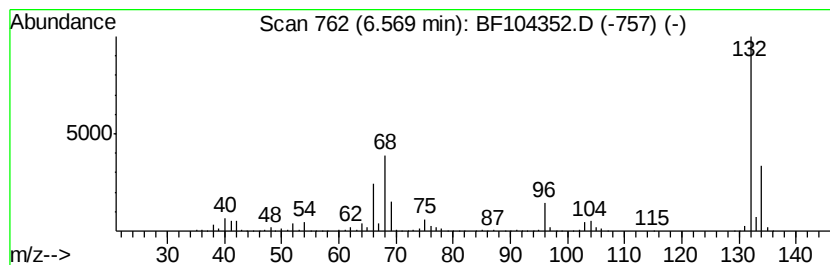
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	52.51 ng	2094370	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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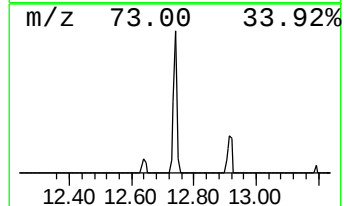
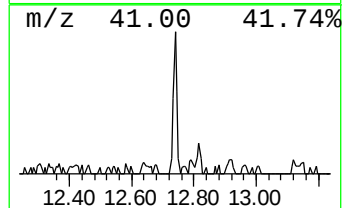
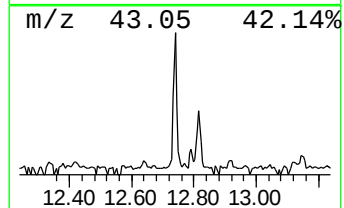
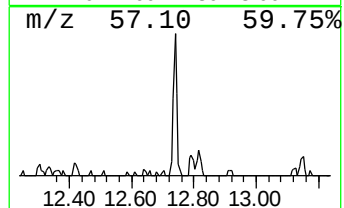
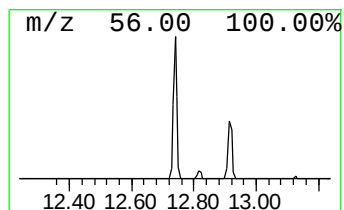
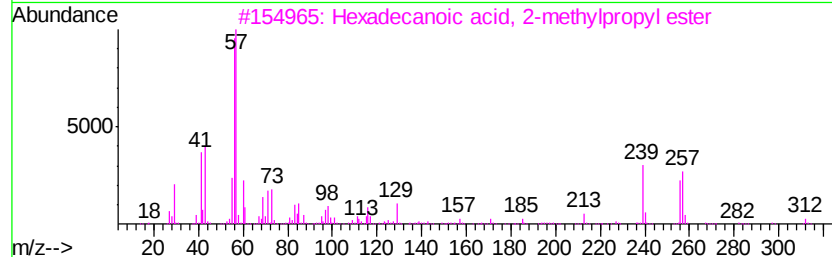
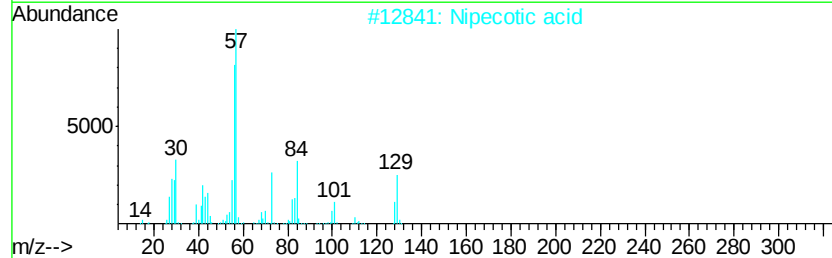
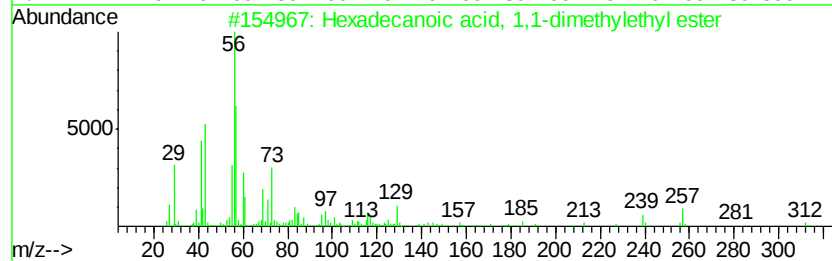
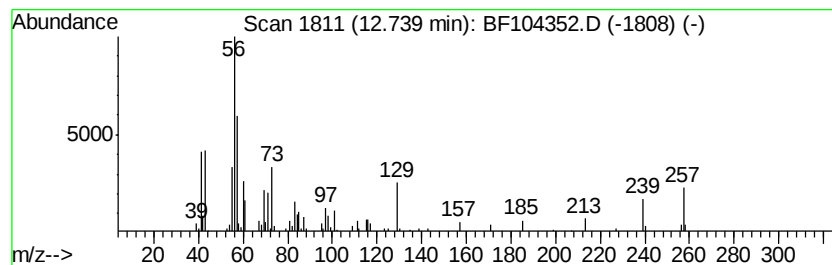
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Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.45 ng	91184	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
2		Nipecotic acid	129	C6H11NO2	000498-95-3	50
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
4		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	41
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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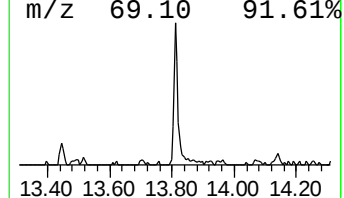
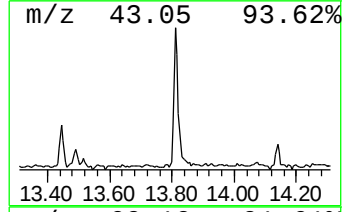
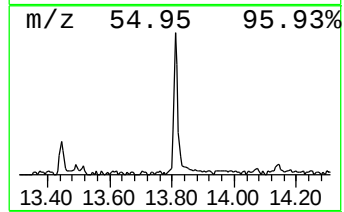
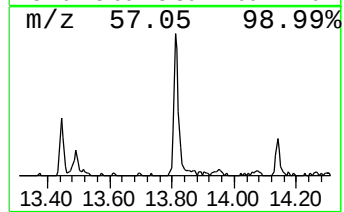
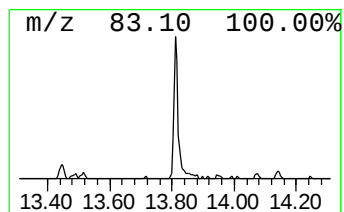
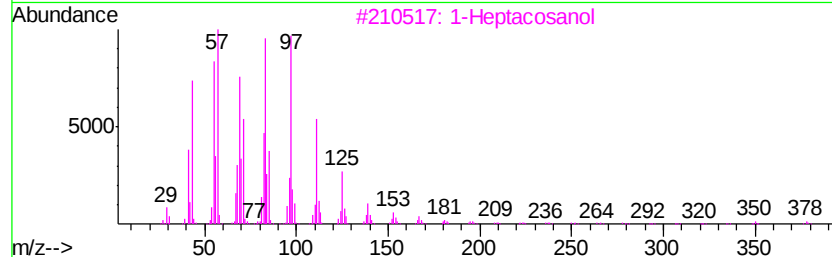
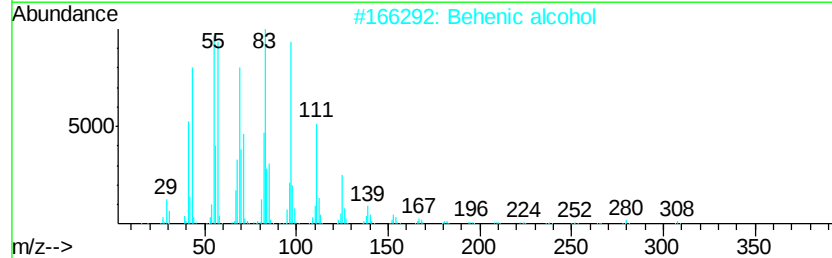
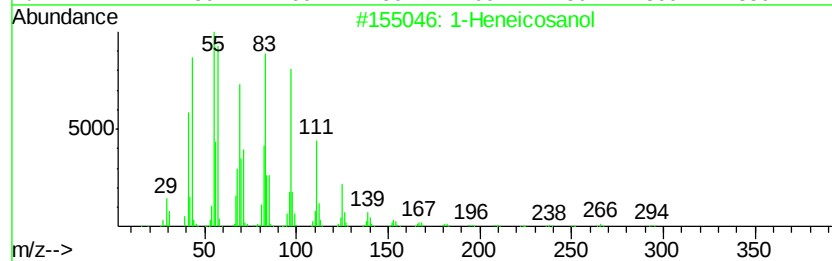
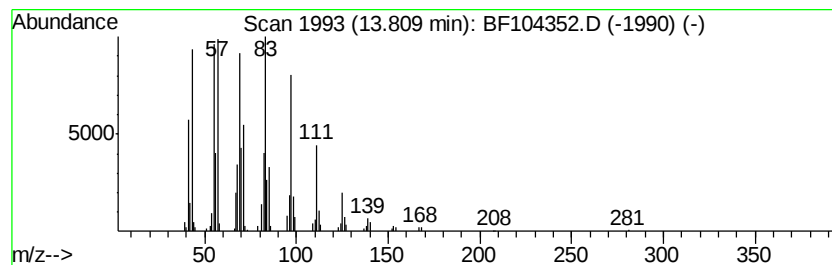
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Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.19 ng	192722	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	93
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	2.7	ng	108664	1	6.80	797718	20.0
unknown6.57	6.57	52.5	ng	2094370	1	6.80	797718	20.0
Hexadecanoic acid...	12.74	2.5	ng	91184	5	13.97	743213	20.0
1-Heneicosanol	13.81	5.2	ng	192722	5	13.97	743213	20.0