

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
 Data File : BF104678.D
 Acq On : 20 Apr 2018 17:00
 Operator : JU/SJ
 Sample : J2475-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-02

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-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	493	497	507	rBV	85903	107567	4.72%	0.540%
2	5.422	563	567	576	rBV	2154297	2057189	90.21%	10.329%
3	6.445	736	741	752	rBV	2116916	2012089	88.23%	10.102%
4	6.575	759	763	766	rBV	2340995	2102191	92.18%	10.555%
5	6.804	799	802	806	rBV	842211	645583	28.31%	3.241%
6	6.963	825	829	832	rBV	1858840	1685533	73.91%	8.463%
7	7.369	894	898	901	rBV	1447907	1205764	52.87%	6.054%
8	8.086	1017	1020	1025	rBV	919821	802651	35.20%	4.030%
9	9.163	1199	1203	1213	rBV	2615103	2280499	100.00%	11.450%
10	9.557	1267	1270	1278	rBV	133378	118845	5.21%	0.597%
11	9.769	1302	1306	1310	rBV	64788	50236	2.20%	0.252%
12	9.845	1315	1319	1328	rBV	964370	841555	36.90%	4.225%
13	10.269	1388	1391	1394	rVB	81129	61124	2.68%	0.307%
14	10.633	1450	1453	1465	rVB	1283119	1236430	54.22%	6.208%
15	10.739	1469	1471	1476	rBV	71120	65598	2.88%	0.329%
16	11.192	1545	1548	1550	rBV	32920	28248	1.24%	0.142%
17	11.333	1568	1572	1575	rBV	880148	762217	33.42%	3.827%
18	11.357	1575	1576	1583	rVB	40886	29806	1.31%	0.150%
19	12.545	1775	1778	1782	rVB	92476	81107	3.56%	0.407%
20	12.774	1812	1817	1822	rBV	79594	86476	3.79%	0.434%
21	12.921	1837	1842	1845	rBV	2094539	1899176	83.28%	9.535%
22	13.345	1909	1914	1918	rBV5	48042	56062	2.46%	0.281%
23	13.774	1982	1987	1990	rBV	163517	192172	8.43%	0.965%
24	13.810	1990	1993	1998	rVB2	92875	96419	4.23%	0.484%
25	13.980	2017	2022	2025	rBV	690692	696548	30.54%	3.497%
26	14.821	2163	2165	2168	rVB	54106	52488	2.30%	0.264%
27	15.021	2196	2199	2203	rBV	42597	69134	3.03%	0.347%
28	15.451	2267	2272	2283	rVB	424851	594511	26.07%	2.985%

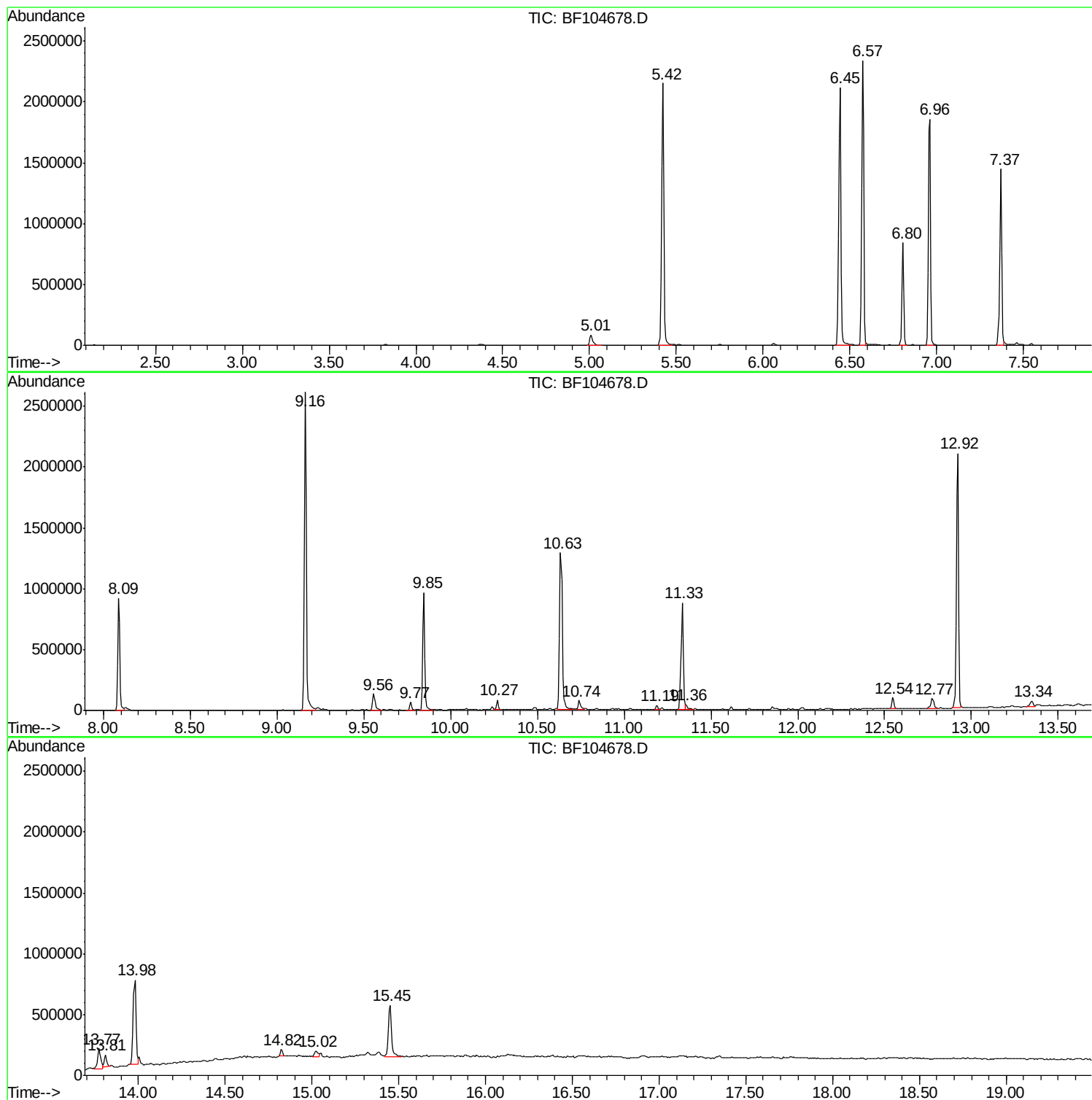
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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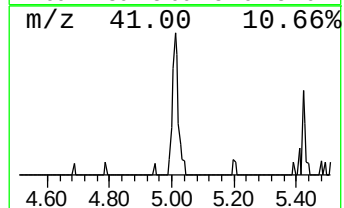
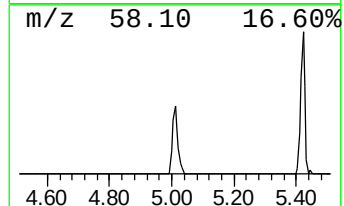
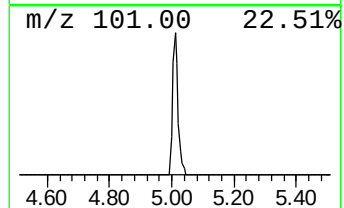
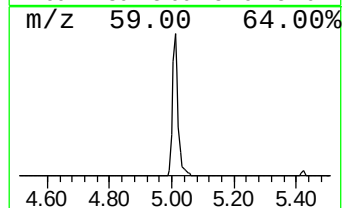
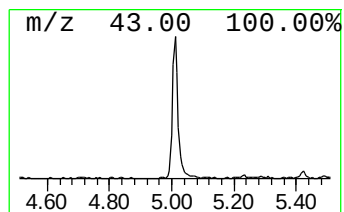
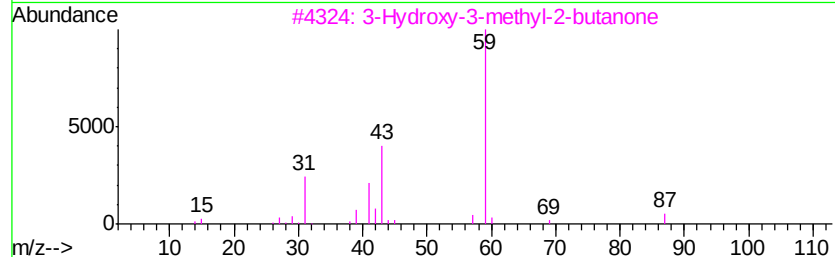
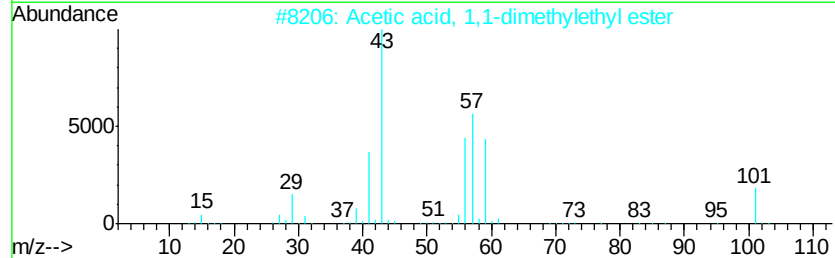
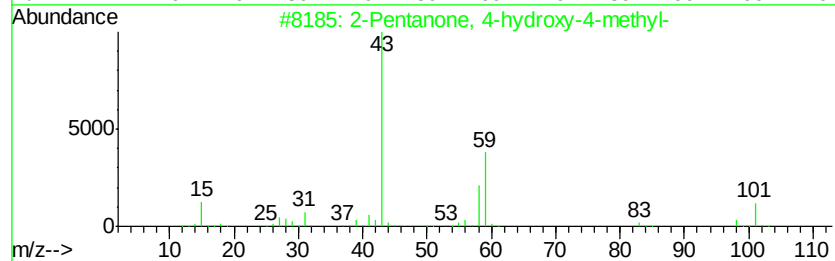
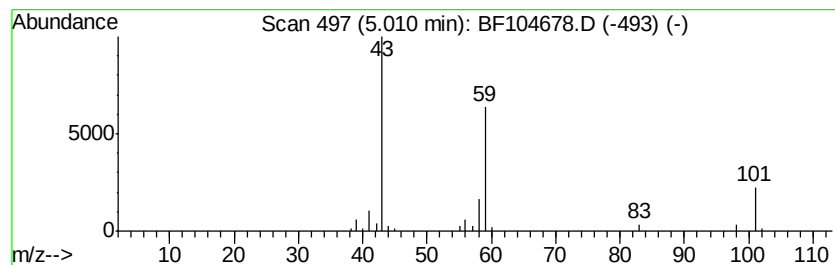
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.01	3.33 ng	107567	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			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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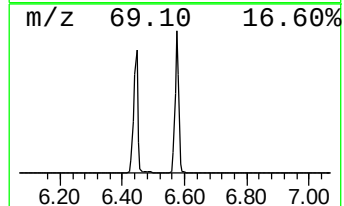
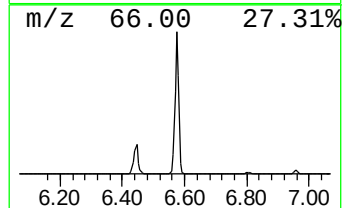
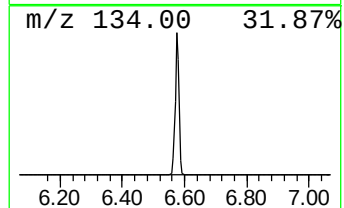
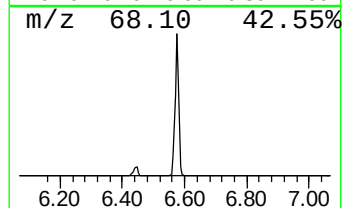
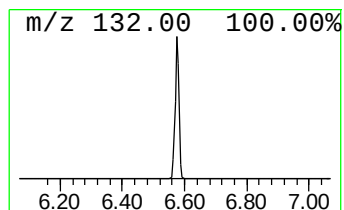
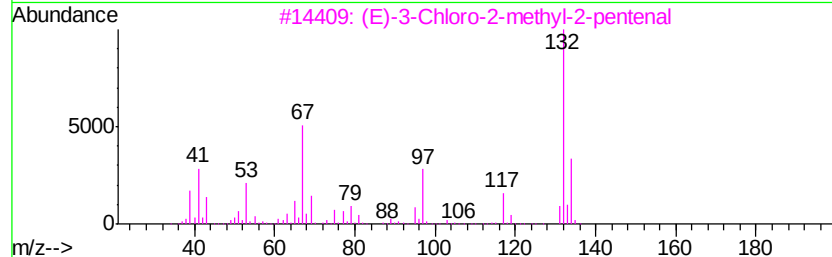
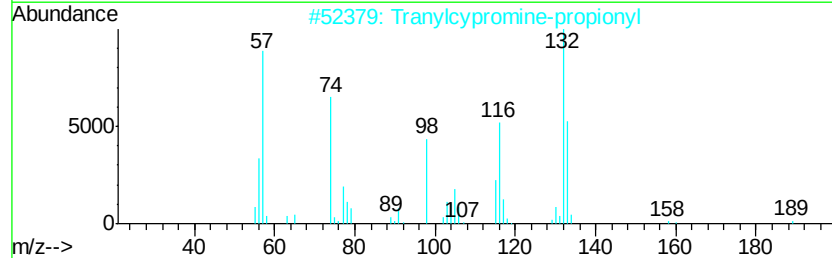
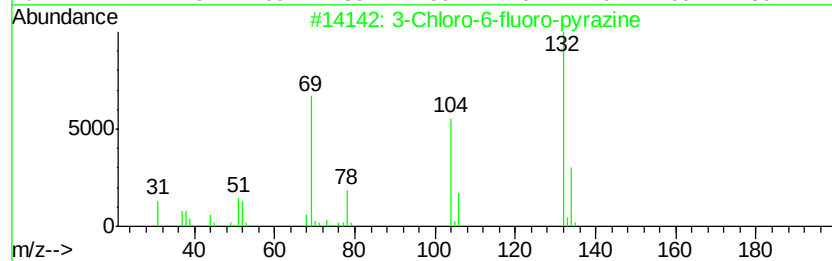
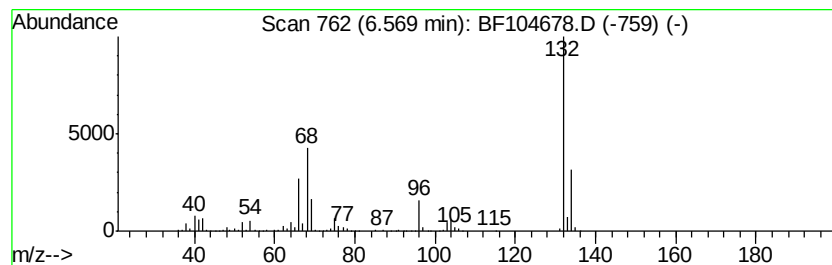
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	65.13 ng	2102190	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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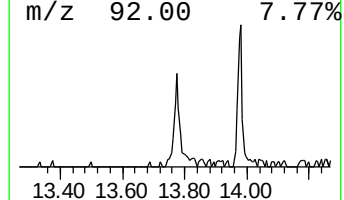
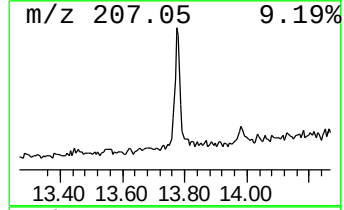
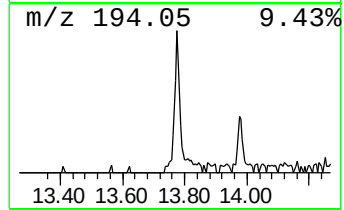
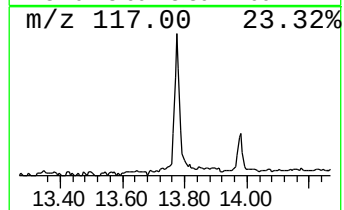
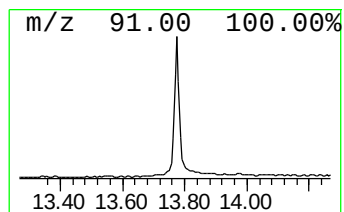
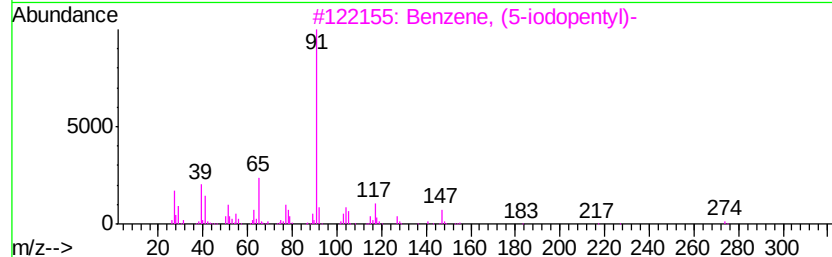
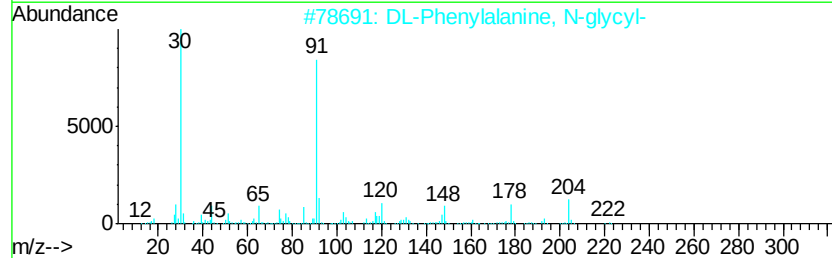
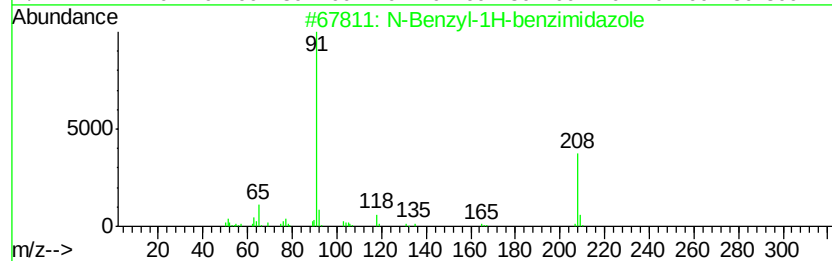
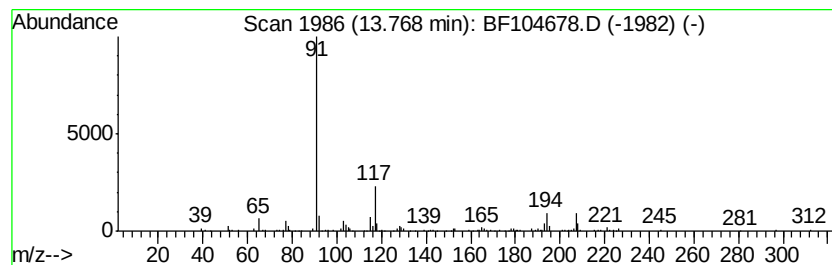
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Peak Number 6 unknown13.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	5.52 ng	192172	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-Benzyl-1H-benzimidazole	208	C14H12N2	004981-92-4	27
2		DL-Phenylalanine, N-glycyl-	222	C11H14N2O3	000721-66-4	22
3		Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
4		Isoxazole, 3-phenyl-5-[(phenylme...]	267	C16H13NOS	028884-17-5	14
5		1-Benzylamino-6-benzylloxyhexane	297	C20H27NO	060058-25-5	10



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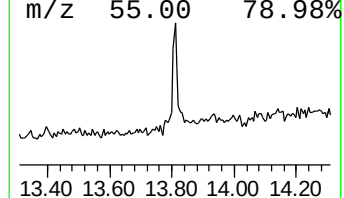
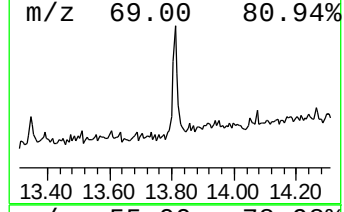
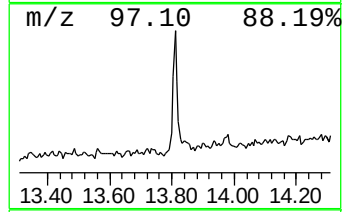
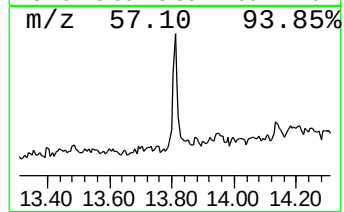
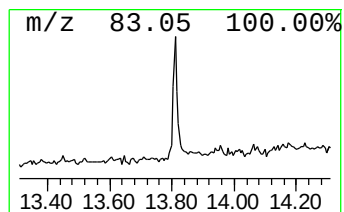
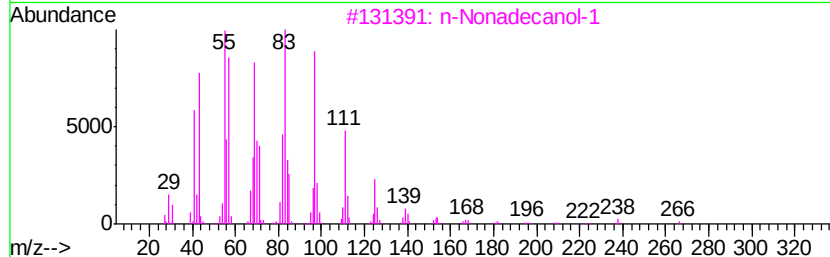
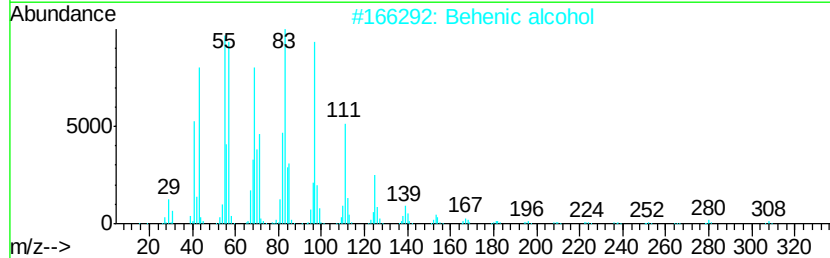
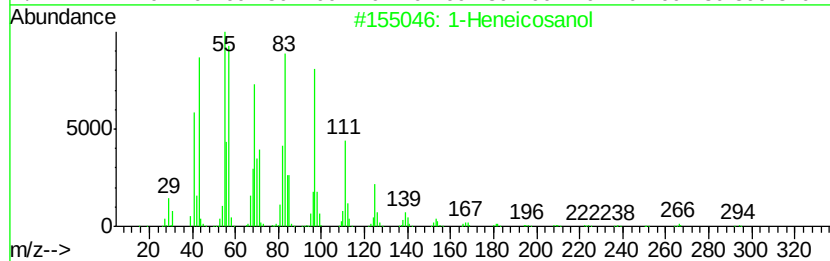
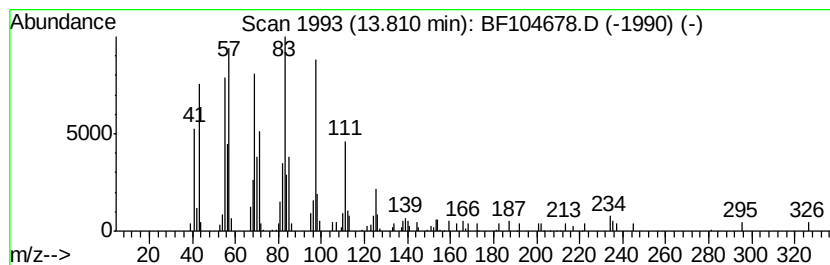
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Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.77 ng	96419	Chrysene-d12	13.98

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	94
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	92



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	3.3	ng	107567	1	6.80	645583	20.0
unknown6.57	6.57	65.1	ng	2102190	1	6.80	645583	20.0
unknown13.77	13.77	5.5	ng	192172	5	13.98	696548	20.0
1-Heneicosanol	13.81	2.8	ng	96419	5	13.98	696548	20.0