

Data Path : Z:\HPCHEM1\BNA F\Data\BF051017\
 Data File : BF095058.D
 Acq On : 10 May 2017 16:21
 Operator : SJ/MA
 Sample : PB98833BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98833BL

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-BF050217.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	5.031	522	526	550	rBV	153369	324419	10.18%	1.330%
2	5.660	628	633	663	rBV	1620726	2630916	82.58%	10.785%
3	7.254	899	904	919	rBV	1643815	2441151	76.63%	10.007%
4	7.372	919	924	935	rVB	2059794	2744132	86.14%	11.249%
5	7.707	977	981	995	rVB	419683	509519	15.99%	2.089%
6	7.948	1017	1022	1036	rBV	1746143	2069670	64.96%	8.484%
7	8.607	1129	1134	1158	rBV	1073005	1597075	50.13%	6.547%
8	9.730	1320	1325	1341	rBV	454196	688515	21.61%	2.822%
9	11.501	1620	1626	1647	rBV	2539162	3185830	100.00%	13.060%
10	12.560	1801	1806	1818	rBV2	508995	772917	24.26%	3.168%
11	13.854	2021	2026	2043	rBV	1160474	1757262	55.16%	7.204%
12	14.960	2210	2214	2232	rBV2	499374	778704	24.44%	3.192%
13	15.630	2324	2328	2337	rBV	85153	95528	3.00%	0.392%
14	15.930	2375	2379	2386	rBV	71811	81643	2.56%	0.335%
15	16.648	2496	2501	2507	rBV2	22439	38272	1.20%	0.157%
16	17.206	2591	2596	2601	rBV	30034	36410	1.14%	0.149%
17	17.289	2604	2610	2621	rVV	2594995	3185098	99.98%	13.057%
18	18.630	2834	2838	2853	rBV	560752	784152	24.61%	3.215%
19	20.300	3117	3122	3134	rBV	348994	564723	17.73%	2.315%
20	20.818	3205	3210	3221	rBV3	40388	72218	2.27%	0.296%
21	20.977	3234	3237	3244	rVB9	23588	35892	1.13%	0.147%

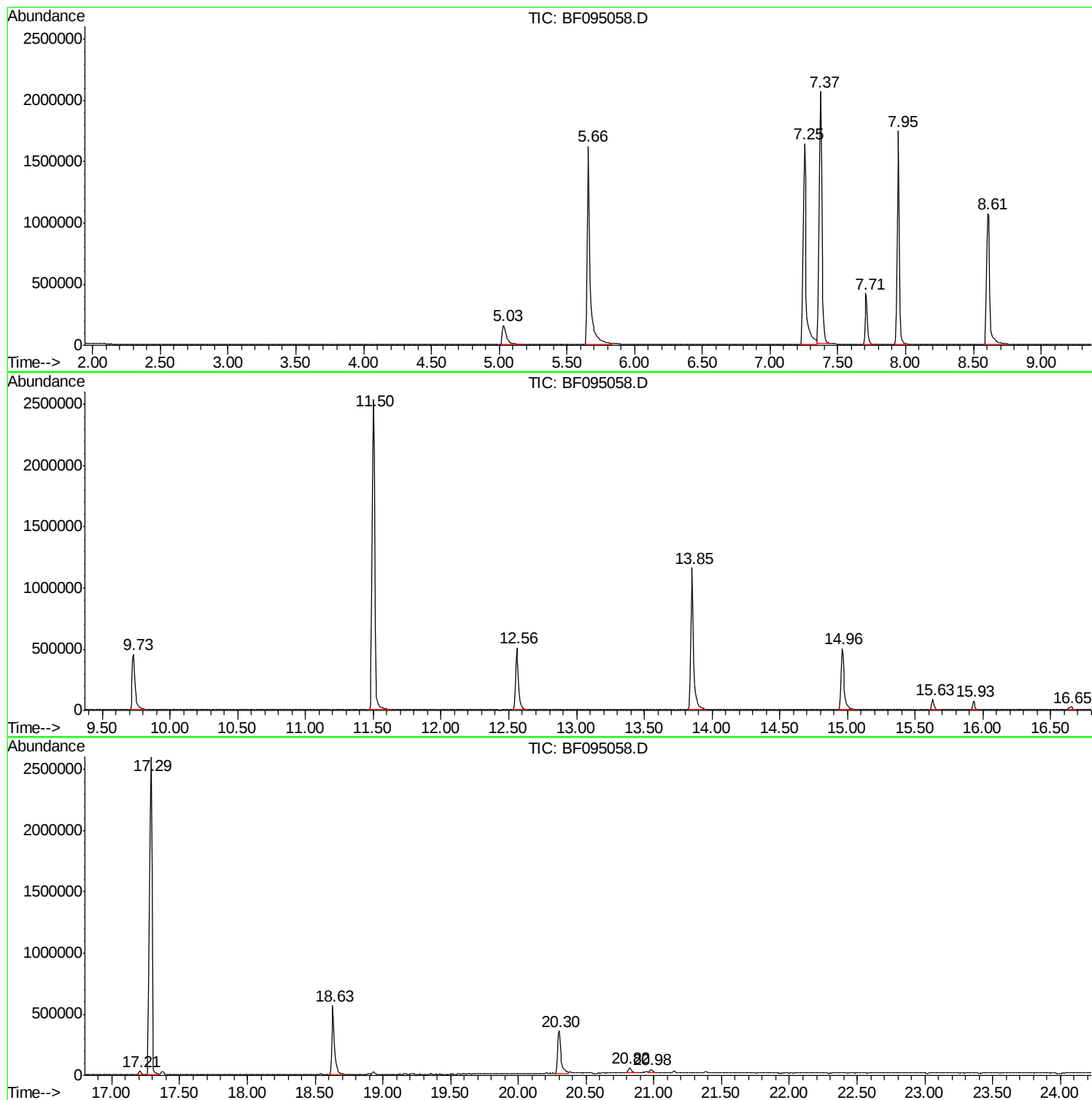
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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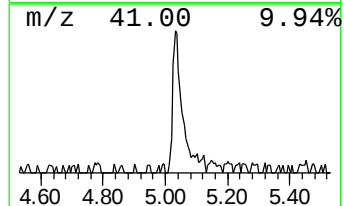
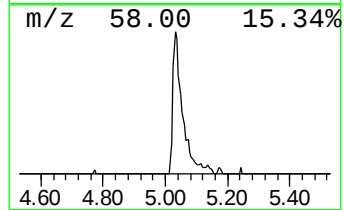
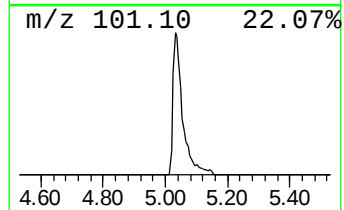
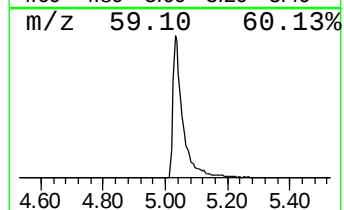
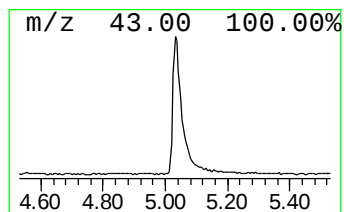
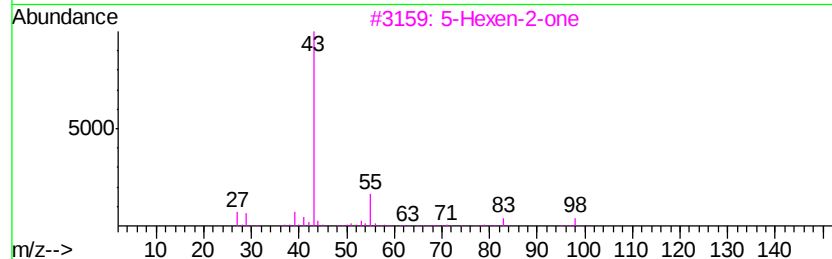
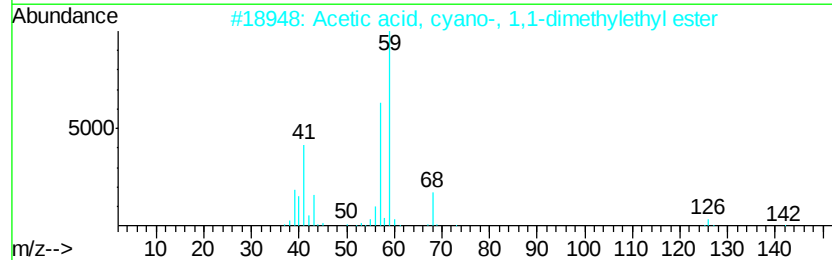
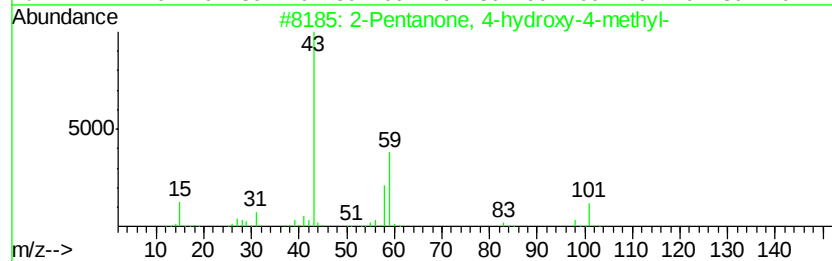
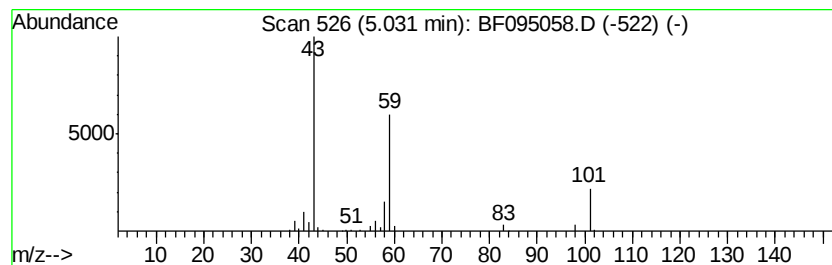
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	12.73 ng	324419	1,4-Dichlorobenzene-d4	7.71

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	25
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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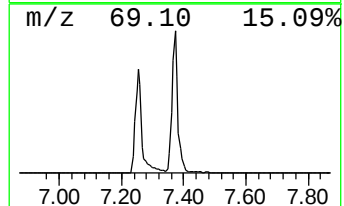
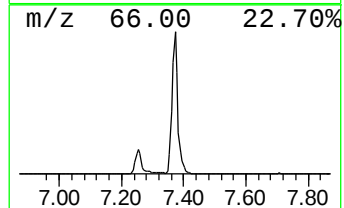
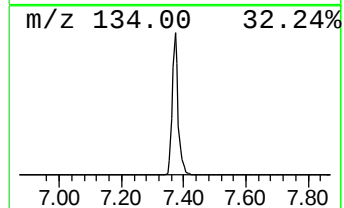
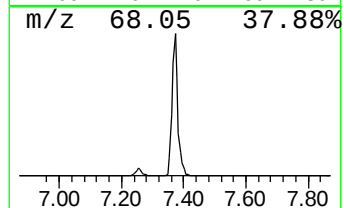
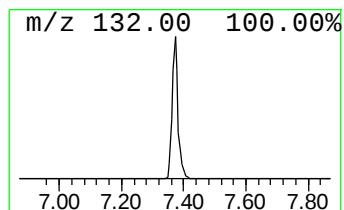
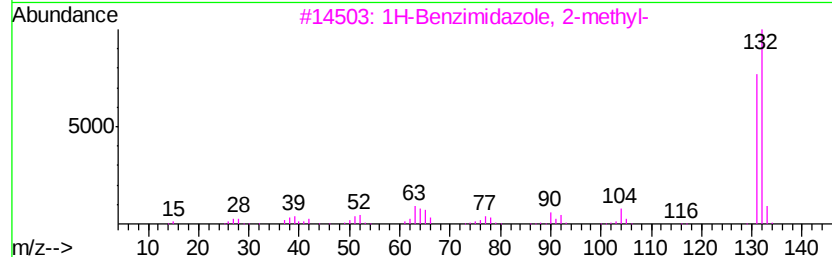
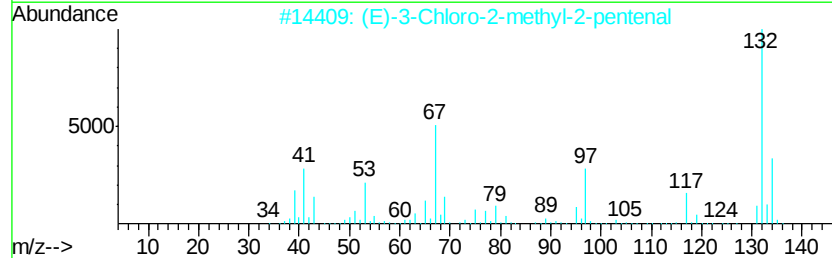
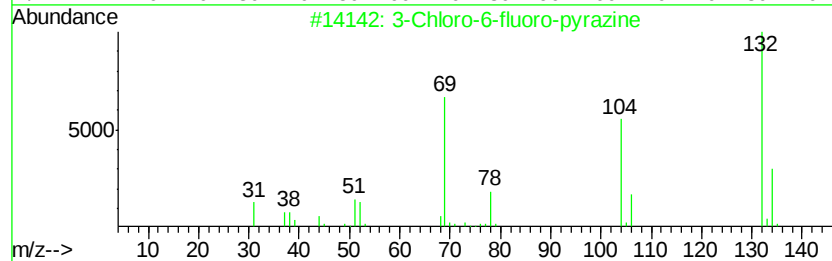
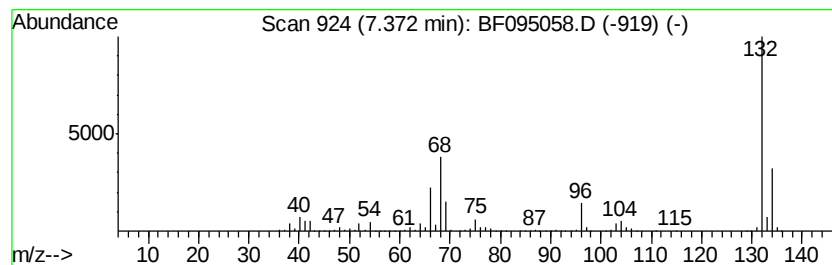
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Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	107.72 ng	2744130	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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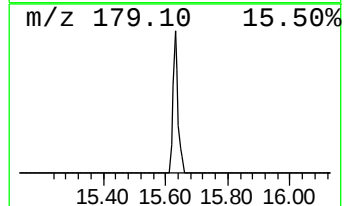
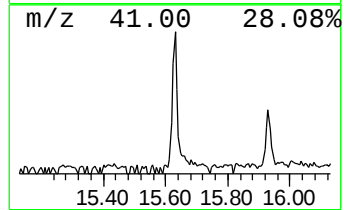
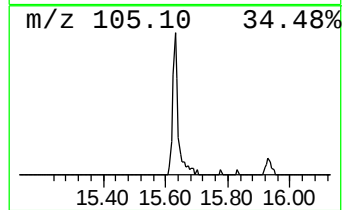
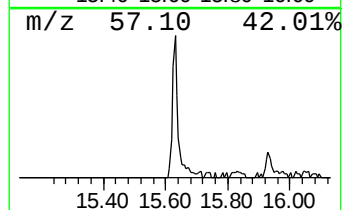
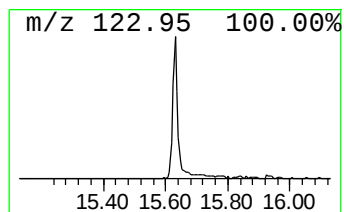
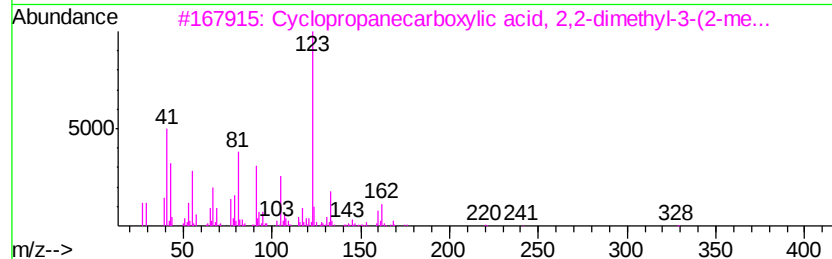
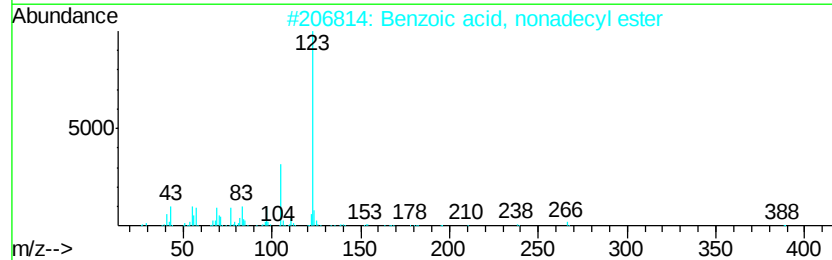
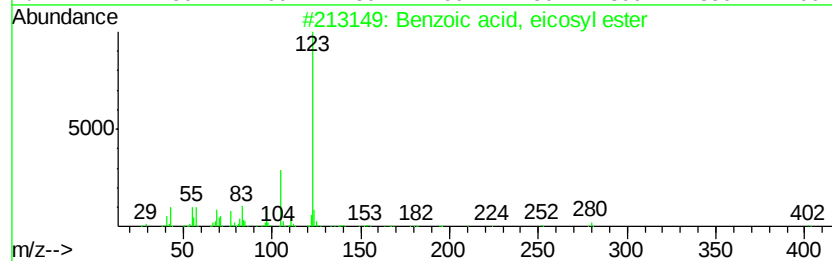
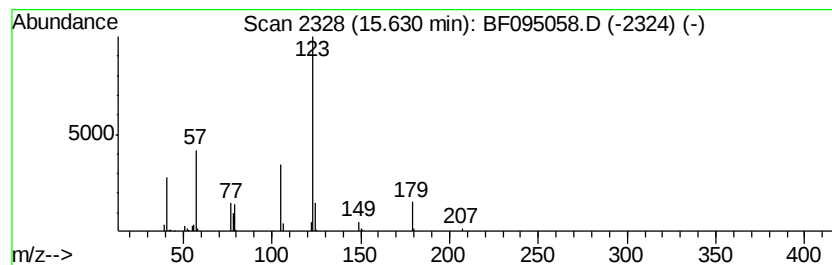
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Peak Number 4 unknown15.63 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.45 ng	95528	Phenanthrene-d10	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, eicosyl ester	402	C27H46O2	1000340-23-3	45
2		Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	45
3		Cyclopropanecarboxylic acid, 2,2...	328	C21H28O3	000121-21-1	38
4		Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	38
5		Furan, 2-(1,1-dimethylethyl)-4-m...	138	C9H14O	006141-68-0	36



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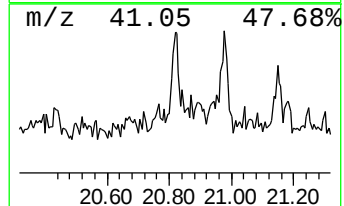
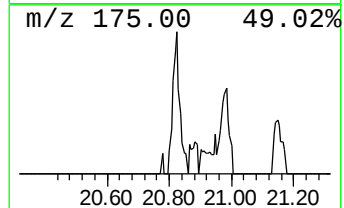
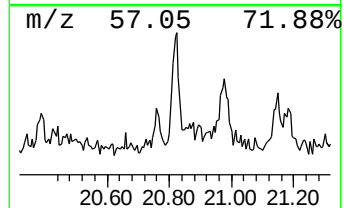
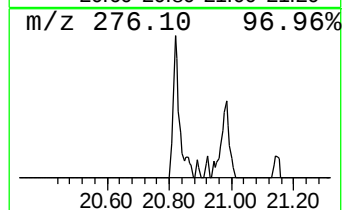
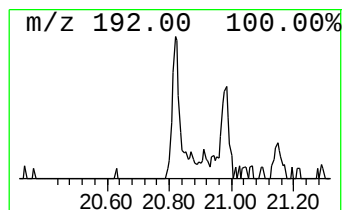
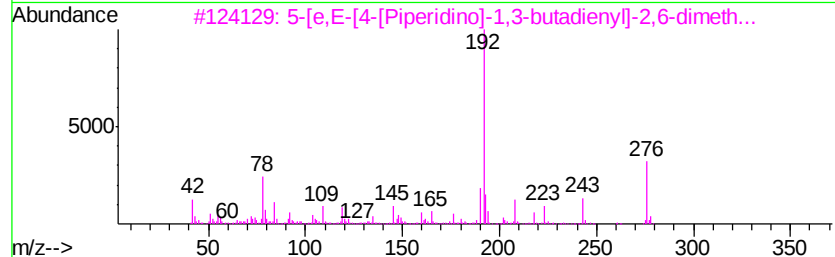
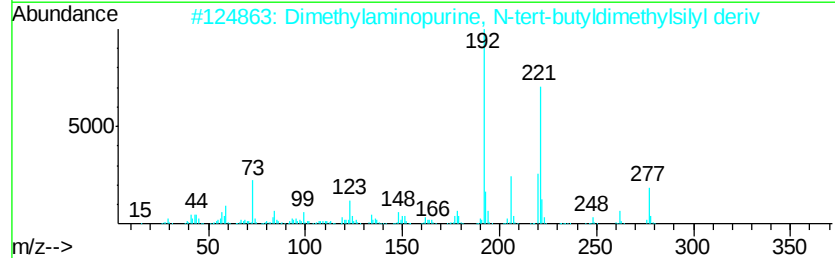
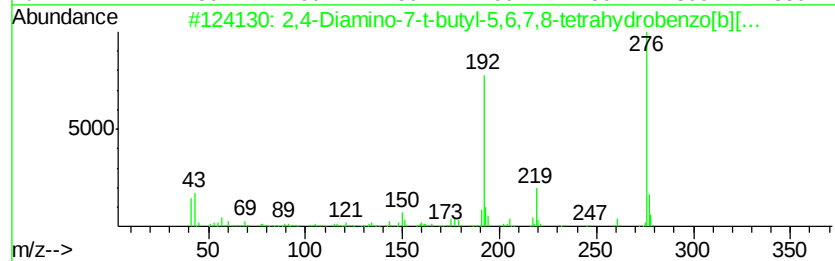
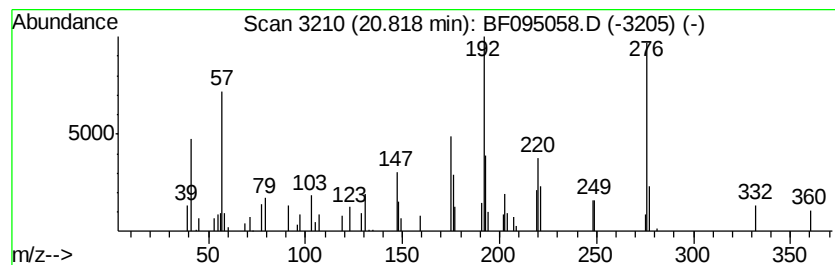
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Peak Number 5 unknown20.82 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	2.56 ng	72218	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Diamino-7-t-butyl-5,6,7,8-te...	276	C14H20N4S	049620-43-1	46
2		Dimethylaminopurine, N-tert-butyl...	277	C13H23N5Si	1000364-71-6	38
3		5-[e,E-[4-[Piperidino]-1,3-butadienyl]-2,6-dimethyl-5,6,7,8-tetrahydrobenzo[b][1,2,4]triazol-2-yl]-2-methylpropane-1-thiol	276	C14H20N4S	1000212-30-3	38
4		Pyrazole-5-carboxylic acid, 4-bromo-	218	C6H7BrN2O2	1000272-87-8	35
5		Bicyclo[2.2.1]hept-2-ene, 2-iodo-	220	C7H9I	058426-15-6	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	12.7	ng	324419	1	7.71	509519	20.0
unknown7.37	7.37	107.7	ng	2744130	1	7.71	509519	20.0
unknown15.63	15.63	2.5	ng	95528	4	14.96	778704	20.0
unknown20.82	20.82	2.6	ng	72218	6	20.30	564723	20.0