

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
 Data File : BF095326.D
 Acq On : 22 May 2017 21:38
 Operator : SJ/MA
 Sample : I3278-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-2669

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	5.119	537	541	564	rBV2	61556	165418	9.38%	1.032%
2	5.731	641	645	668	rBV	581714	1443490	81.85%	9.007%
3	7.301	908	912	929	rBV	650579	1409641	79.93%	8.796%
4	7.425	929	933	958	rVB	1036667	1737880	98.55%	10.844%
5	7.760	986	990	1004	rVB	361104	463306	26.27%	2.891%
6	7.995	1025	1030	1047	rBV	989763	1276359	72.38%	7.964%
7	8.660	1139	1143	1176	rBV	470593	936968	53.13%	5.846%
8	9.778	1329	1333	1354	rBV	349871	643425	36.49%	4.015%
9	11.548	1629	1634	1655	rBV	1158189	1763498	100.00%	11.004%
10	12.254	1750	1754	1763	rBV	82216	142928	8.10%	0.892%
11	12.613	1810	1815	1833	rBV2	379712	645583	36.61%	4.028%
12	13.442	1951	1956	1961	rVB	18221	21672	1.23%	0.135%
13	13.907	2031	2035	2058	rBV	428055	799647	45.34%	4.990%
14	14.213	2082	2087	2097	rBV2	17729	28418	1.61%	0.177%
15	15.013	2219	2223	2227	rBV	346975	464332	26.33%	2.897%
16	15.048	2227	2229	2243	rVV	95934	182011	10.32%	1.136%
17	15.854	2362	2366	2375	rVB	13910	20941	1.19%	0.131%
18	15.965	2379	2385	2396	rVV5	32620	81553	4.62%	0.509%
19	16.795	2522	2526	2537	rBV	216445	295480	16.76%	1.844%
20	17.095	2573	2577	2586	rVB	219776	286716	16.26%	1.789%
21	17.324	2612	2616	2627	rBV	811309	983558	55.77%	6.137%
22	17.418	2627	2632	2639	rVB4	12051	26116	1.48%	0.163%
23	17.565	2653	2657	2661	rVB	20403	27079	1.54%	0.169%
24	17.654	2668	2672	2675	rBV	15326	19457	1.10%	0.121%
25	17.707	2675	2681	2686	rBV4	20798	39078	2.22%	0.244%
26	18.371	2791	2794	2796	rBV	15208	18357	1.04%	0.115%
27	18.395	2796	2798	2802	rVV2	19986	18770	1.06%	0.117%
28	18.571	2825	2828	2830	rBV3	16083	20862	1.18%	0.130%
29	18.683	2842	2847	2851	rBV2	453096	664303	37.67%	4.145%
30	18.718	2851	2853	2860	rVB	118425	167159	9.48%	1.043%
31	18.812	2866	2869	2874	rVB2	25128	31980	1.81%	0.200%
32	18.971	2893	2896	2902	rVB5	12509	19674	1.12%	0.123%
33	19.195	2931	2934	2938	rVB2	15832	22152	1.26%	0.138%
34	19.348	2957	2960	2968	rVB6	14064	31276	1.77%	0.195%

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35	19.801	3032	3037	3044	rBV3	55431	72215	4.09%	0.451%
36	19.959	3059	3064	3067	rBV	117558	182111	10.33%	1.136%
37	20.077	3081	3084	3090	rVB4	26735	34492	1.96%	0.215%
38	20.248	3110	3113	3120	rBV	84747	111599	6.33%	0.696%
39	20.306	3120	3123	3128	rVV	92900	112665	6.39%	0.703%
40	20.359	3128	3132	3141	rBV	315855	464282	26.33%	2.897%
41	20.777	3199	3203	3205	rBV4	15689	25762	1.46%	0.161%
42	20.806	3206	3208	3213	rVB5	20628	28377	1.61%	0.177%
43	21.712	3359	3362	3372	rVB4	25307	59251	3.36%	0.370%
44	22.106	3424	3429	3432	rBV2	17308	36616	2.08%	0.228%

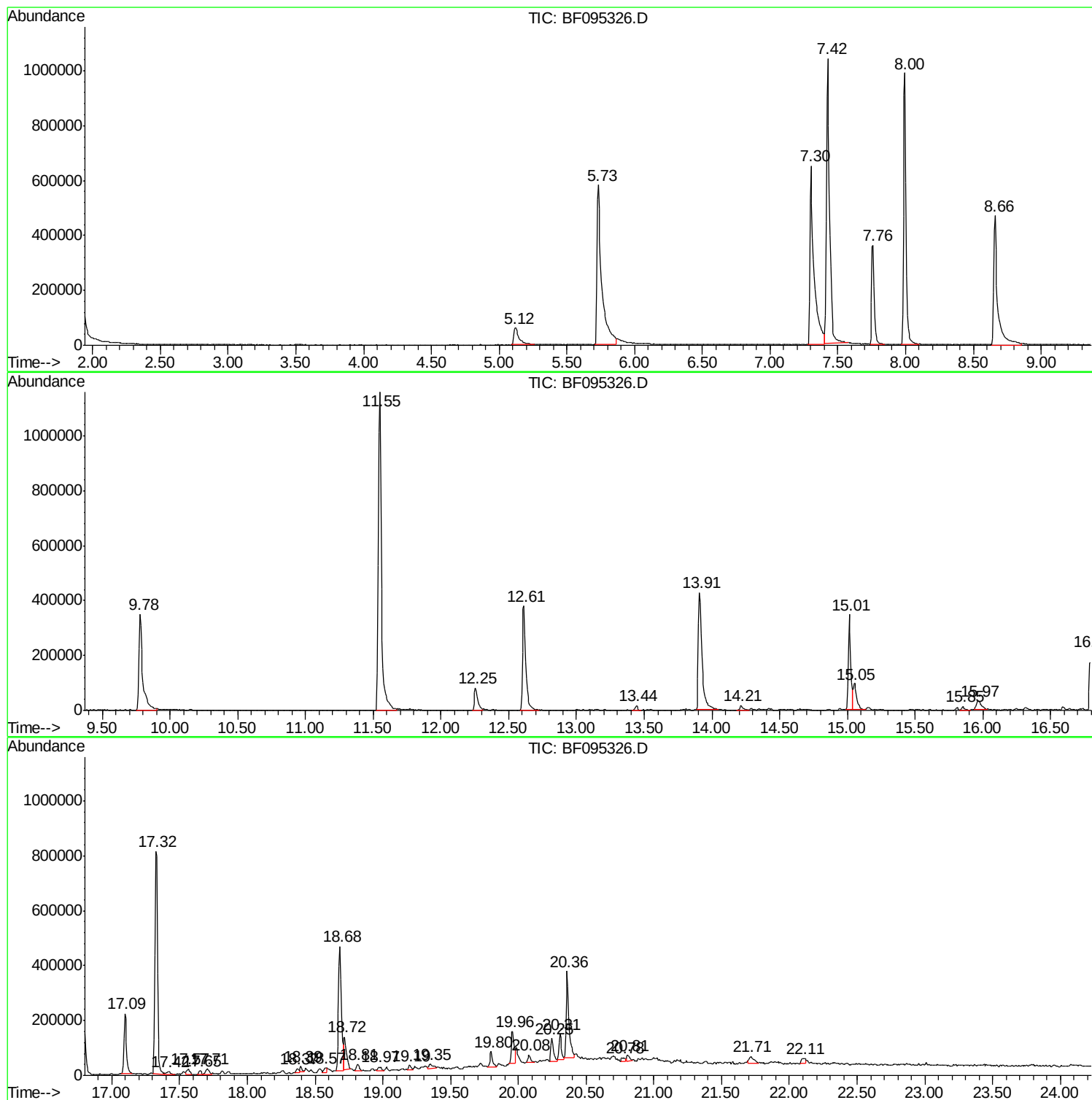
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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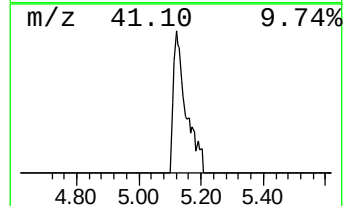
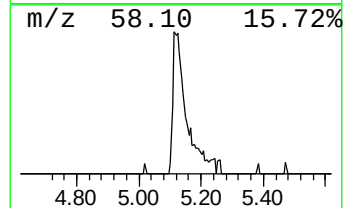
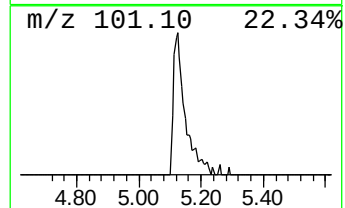
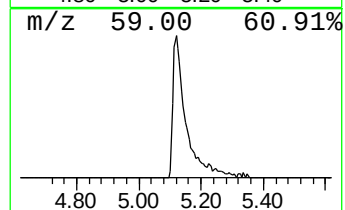
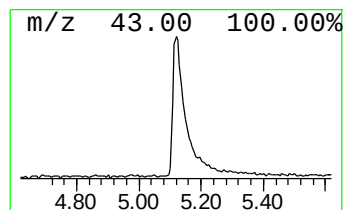
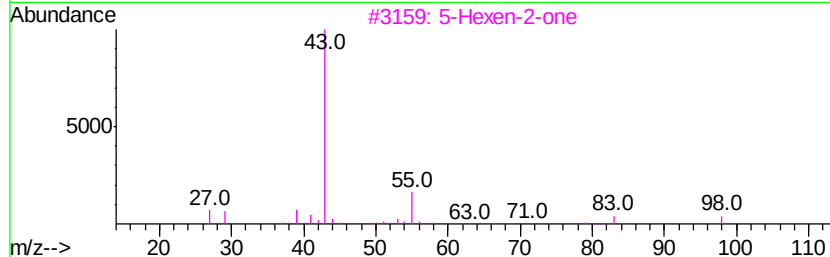
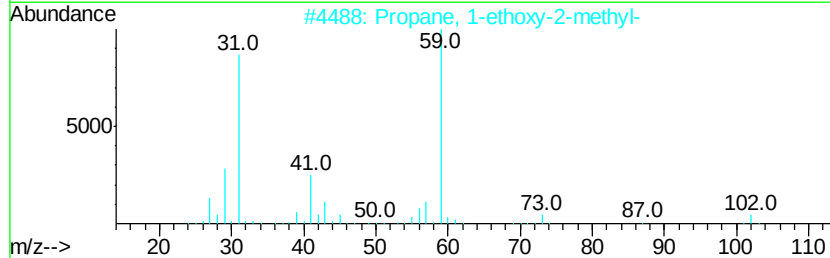
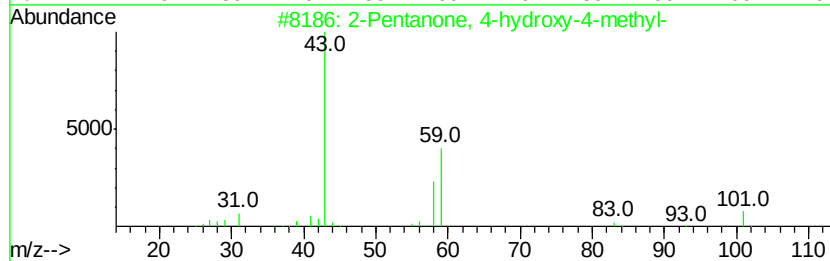
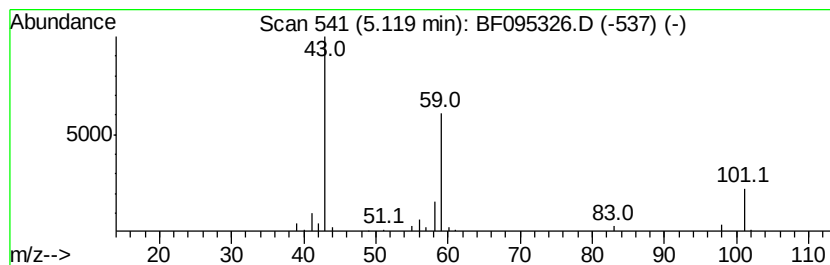
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	7.14 ng	165418	1,4-Dichlorobenzene-d4	7.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3			5-Hexen-2-one	98	C6H10O	000109-49-9	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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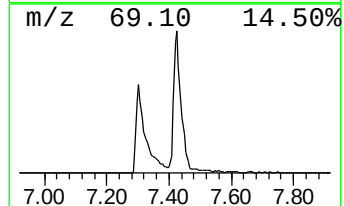
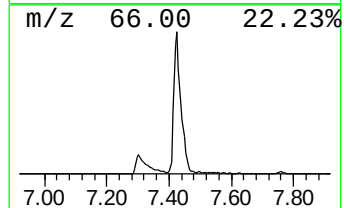
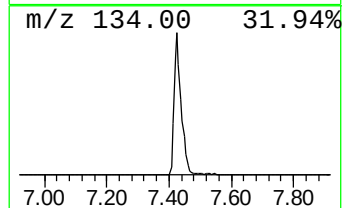
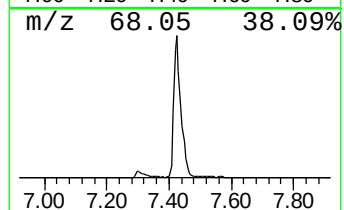
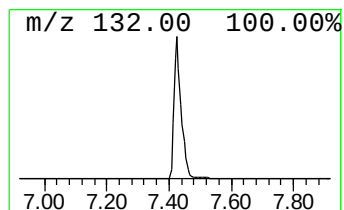
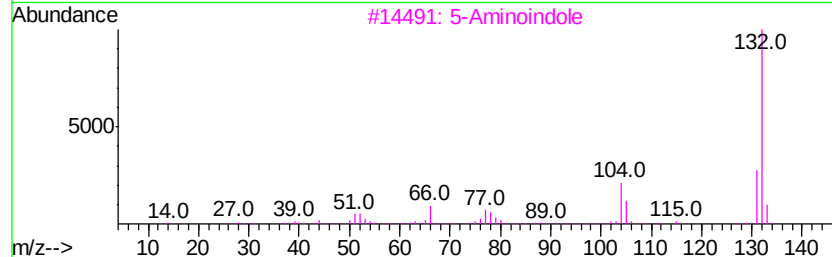
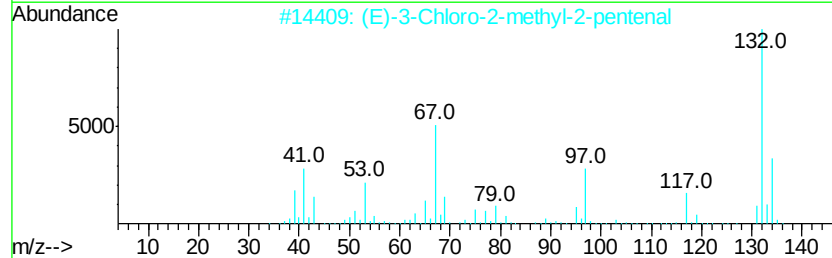
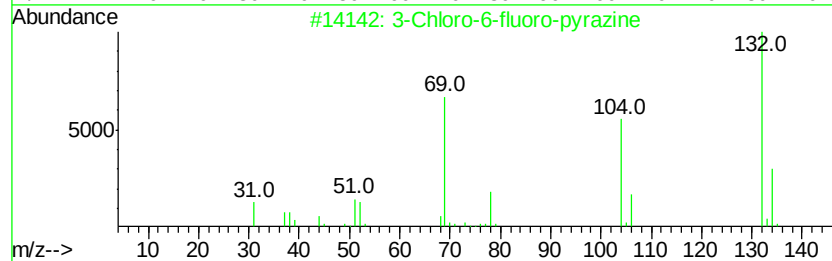
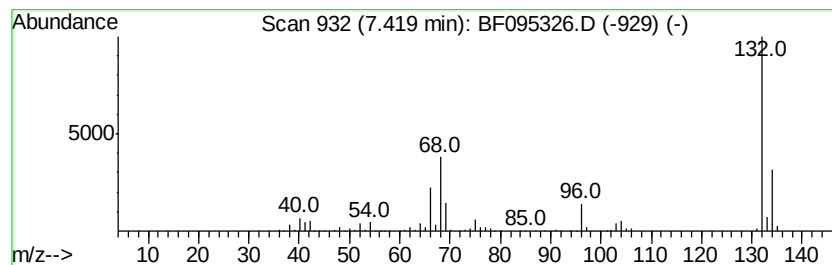
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	75.02 ng	1737880	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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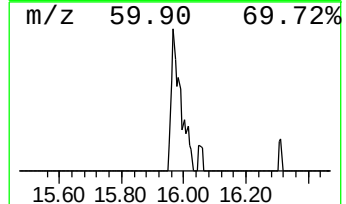
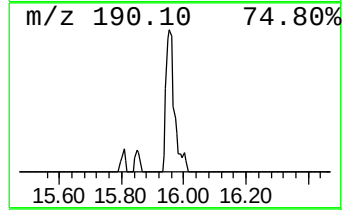
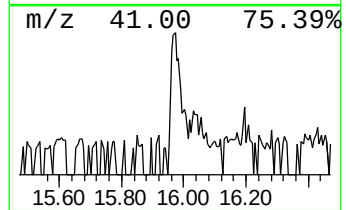
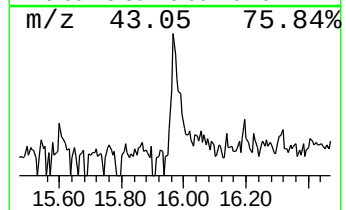
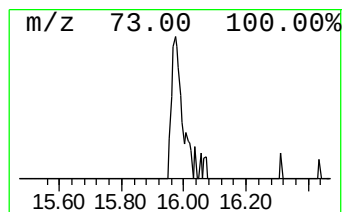
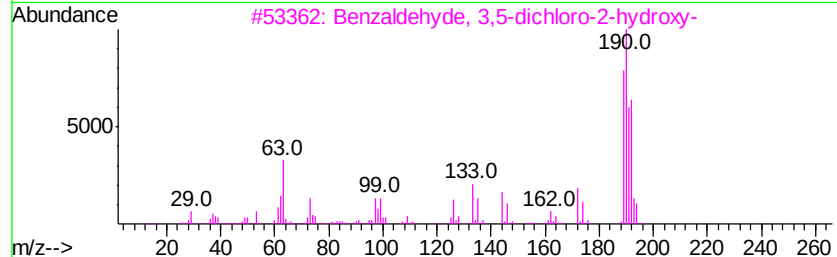
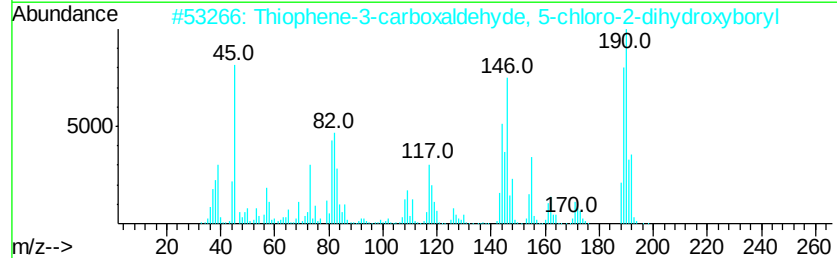
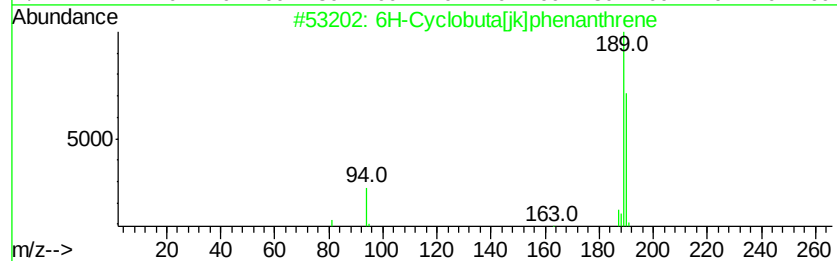
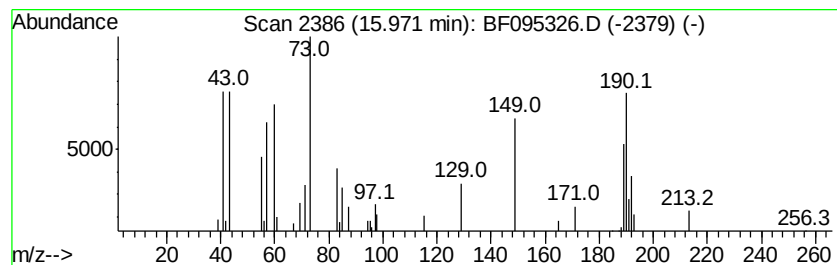
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown15.97 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.97	3.51 ng	81553	Phenanthrene-d10	15.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	38
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	35
3	Benzaldehyde, 3,5-dichloro-2-hvd...	190	C7H4Cl2O2	000090-60-8	32
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	27
5	Methyl 6-O-[1-methylpropyl]-.bet...	250	C11H22O6	1000126-15-7	22



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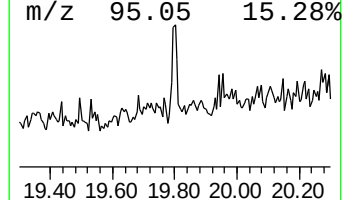
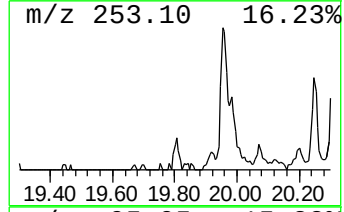
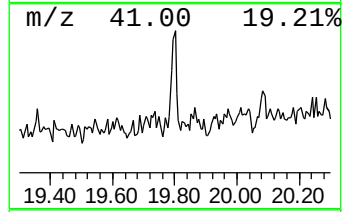
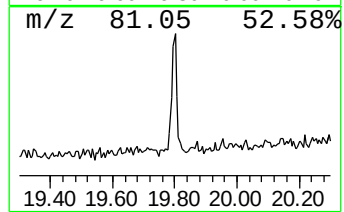
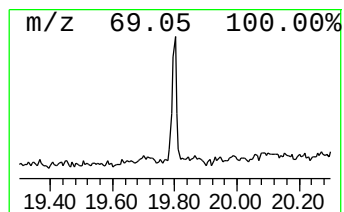
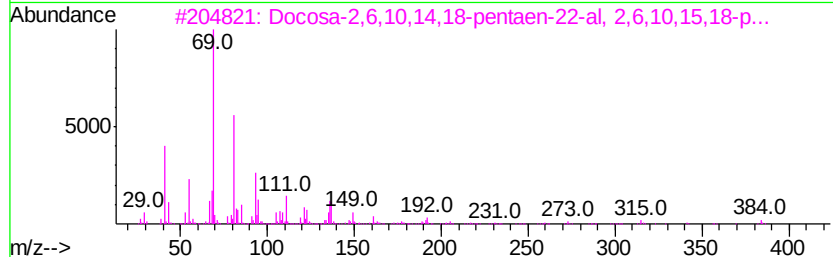
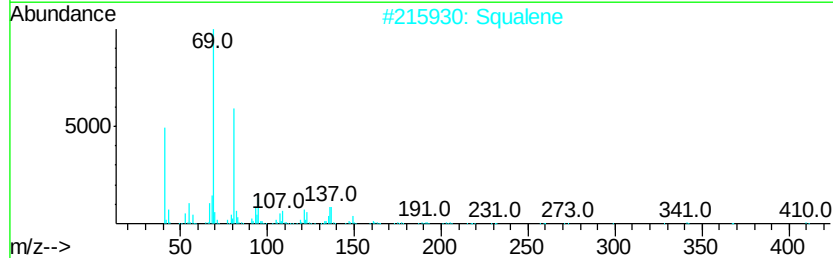
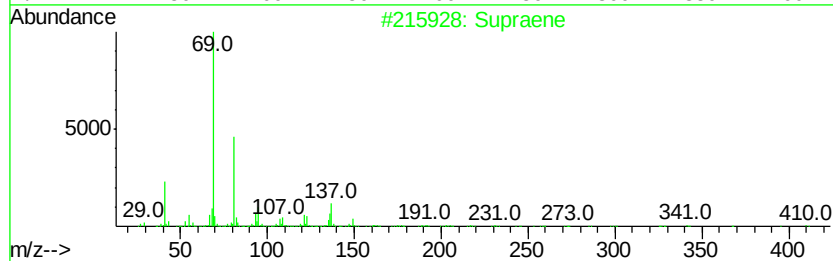
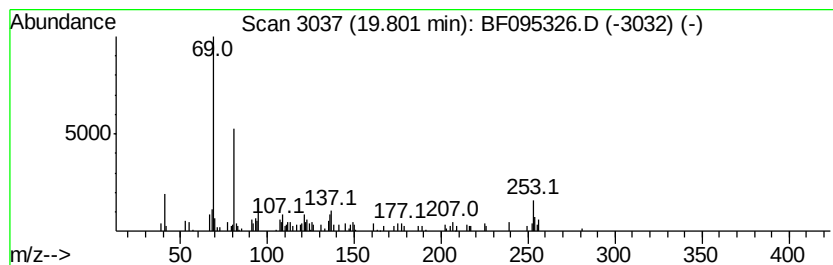
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Peak Number 5 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.80	3.11 ng	72215	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	68
2		Squalene	410	C30H50	000111-02-4	68
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
5		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	7.1	ng	165418	1	7.76	463306	20.0
unknown7.42	7.42	75.0	ng	1737880	1	7.76	463306	20.0
unknown15.97	15.97	3.5	ng	81553	4	15.01	464332	20.0
Supraene	19.80	3.1	ng	72215	6	20.36	464282	20.0