

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
 Data File : BF094699.D
 Acq On : 28 Apr 2017 22:20
 Operator : SJ/MA
 Sample : I2895-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-6.0-7.0

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-BF041717.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	2.984	173	178	184	rBV	43193	50037	1.72%	0.213%
2	3.937	336	340	349	rBV	427054	500191	17.16%	2.126%
3	4.331	403	407	421	rBV	2782658	2776520	95.24%	11.804%
4	4.713	468	472	476	rBV	31837	32751	1.12%	0.139%
5	5.401	584	589	592	rBV	2615239	2817410	96.64%	11.978%
6	5.525	605	610	613	rBV	3024017	2915275	100.00%	12.394%
7	5.766	648	651	655	rBV	643551	612826	21.02%	2.605%
8	5.948	677	682	685	rBV	2071592	1950480	66.91%	8.292%
9	6.419	757	762	765	rBV	1692549	1702051	58.38%	7.236%
10	7.260	901	905	909	rBV	920619	817314	28.04%	3.475%
11	7.819	995	1000	1006	rVB	40925	45442	1.56%	0.193%
12	8.554	1122	1125	1126	rBV	38152	33240	1.14%	0.141%
13	8.583	1126	1130	1133	rVB	2570801	2374585	81.45%	10.095%
14	9.083	1212	1215	1219	rBV	254170	229993	7.89%	0.978%
15	9.225	1235	1239	1244	rBV	25463	35834	1.23%	0.152%
16	9.395	1258	1268	1273	rBV2	850824	848103	29.09%	3.606%
17	9.989	1366	1369	1372	rVB	47893	43151	1.48%	0.183%
18	10.266	1411	1416	1419	rBV2	30831	40032	1.37%	0.170%
19	10.372	1430	1434	1444	rBV	1306460	1413035	48.47%	6.007%
20	10.577	1466	1469	1470	rBV	54027	53442	1.83%	0.227%
21	10.595	1470	1472	1476	rVB	35212	34804	1.19%	0.148%
22	11.130	1559	1563	1565	rBV	37902	41864	1.44%	0.178%
23	11.166	1566	1569	1573	rVB	38067	40910	1.40%	0.174%
24	11.219	1574	1578	1581	rBV	728139	706901	24.25%	3.005%
25	11.242	1581	1582	1585	rVB	47312	39957	1.37%	0.170%
26	11.360	1599	1602	1607	rBV6	16912	32396	1.11%	0.138%
27	11.954	1700	1703	1714	rBV3	98527	152976	5.25%	0.650%
28	12.501	1794	1796	1803	rBV5	57125	83170	2.85%	0.354%
29	12.713	1828	1832	1835	rBV	106190	120414	4.13%	0.512%
30	12.983	1875	1878	1882	rBV	108245	131248	4.50%	0.558%
31	13.195	1910	1914	1918	rVB	1640222	1737799	59.61%	7.388%
32	14.471	2127	2131	2135	rBV	565862	620892	21.30%	2.640%
33	16.101	2405	2408	2415	rVB	403403	487114	16.71%	2.071%

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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-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

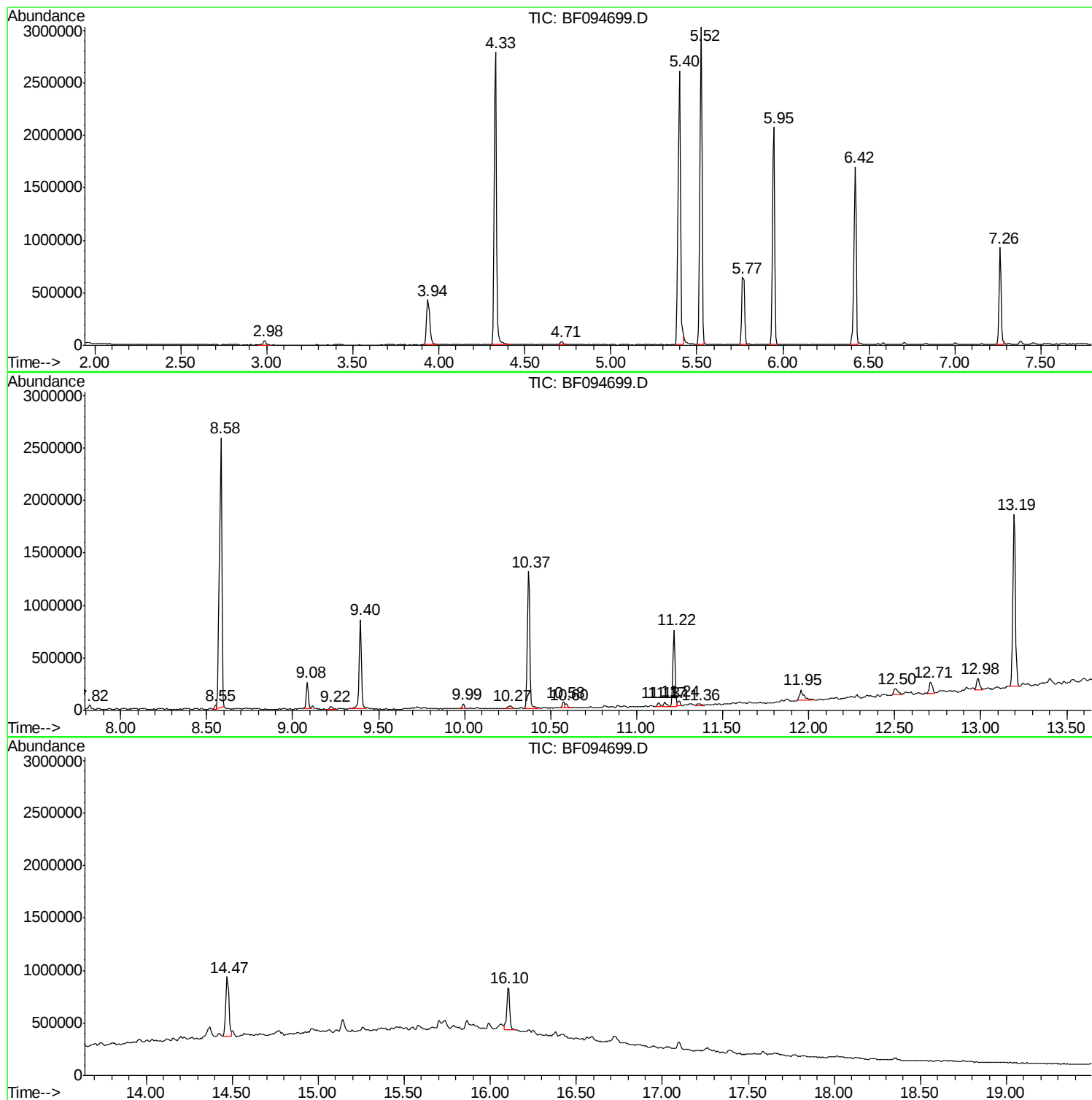
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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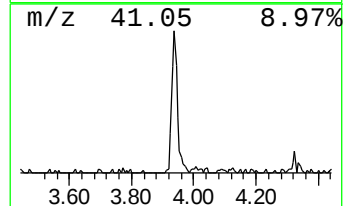
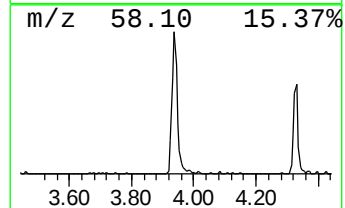
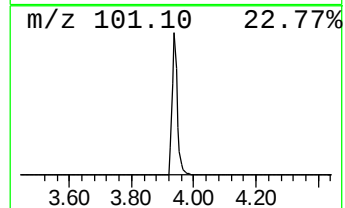
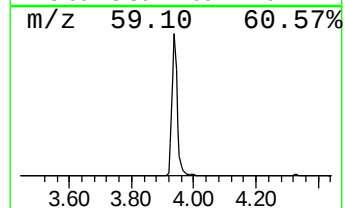
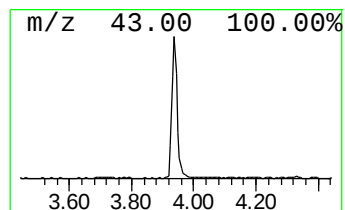
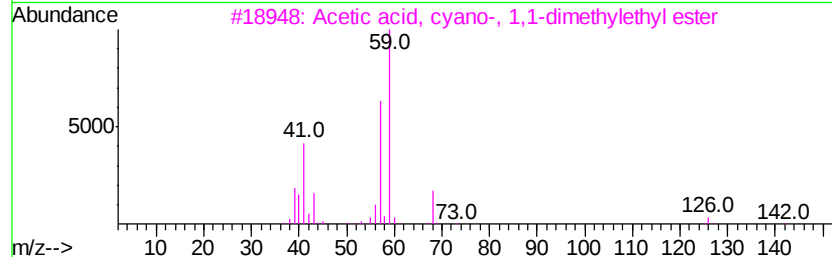
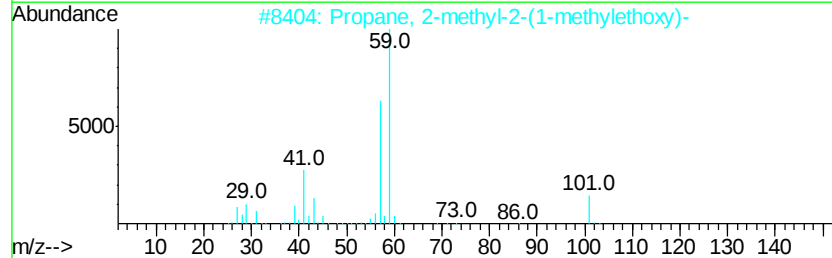
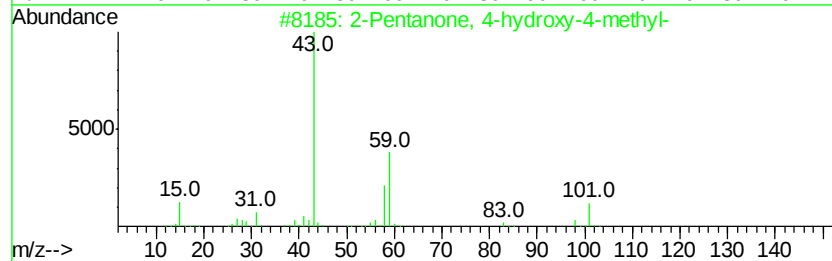
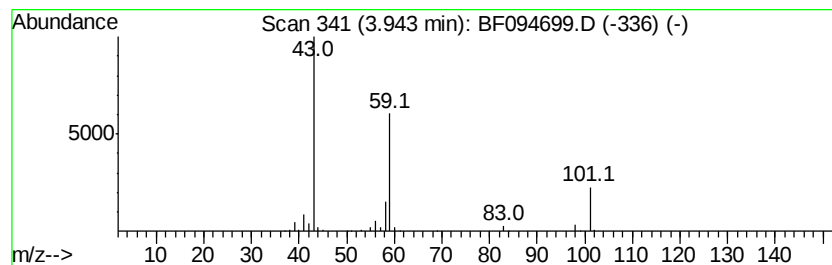
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	16.32 ng	500191	1,4-Dichlorobenzene-d4	5.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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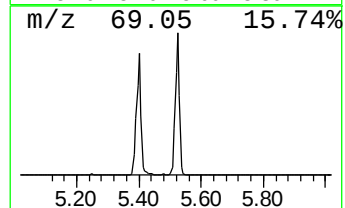
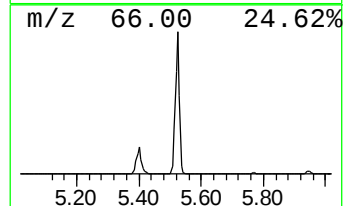
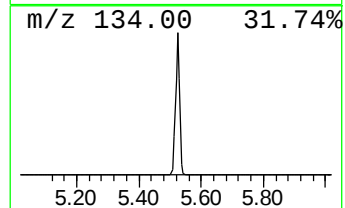
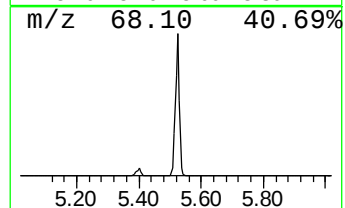
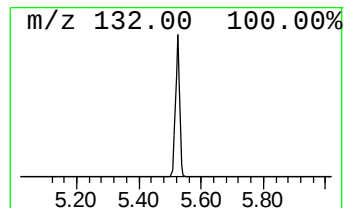
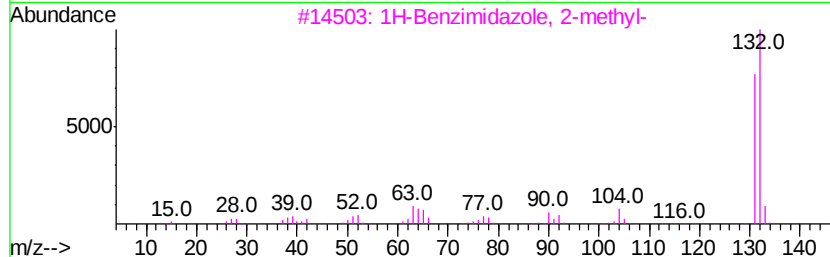
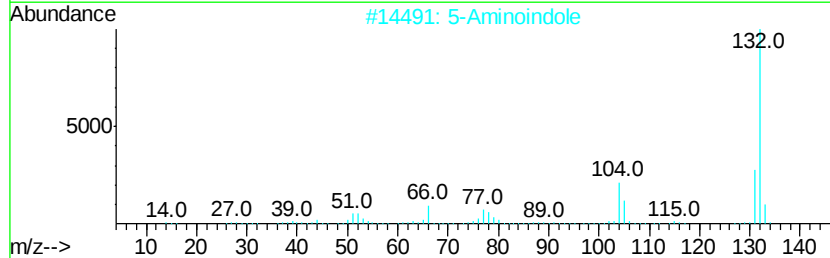
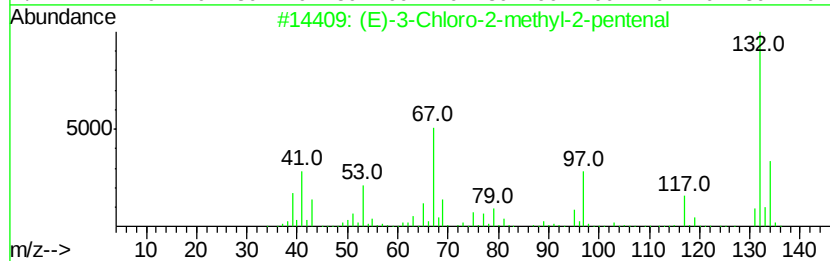
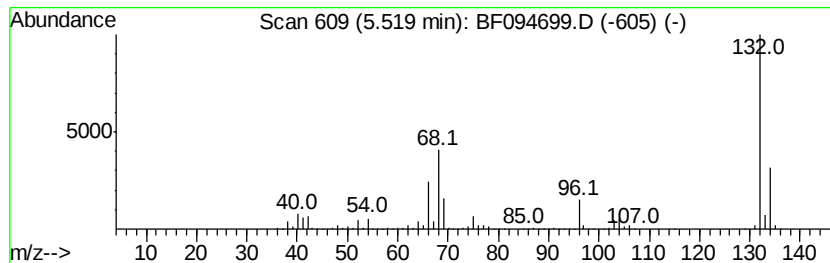
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	95.14 ng	2915280	1,4-Dichlorobenzene-d4	5.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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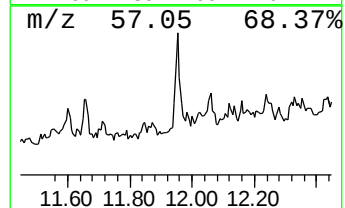
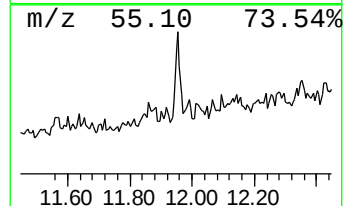
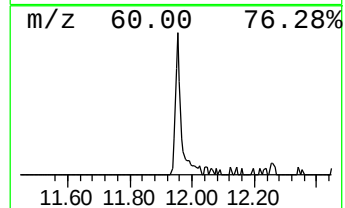
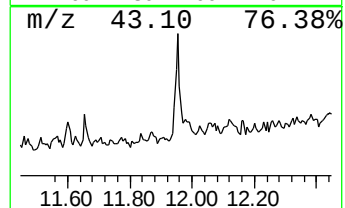
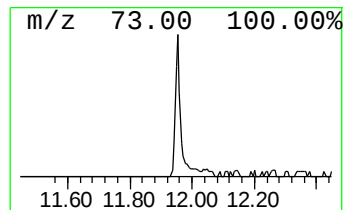
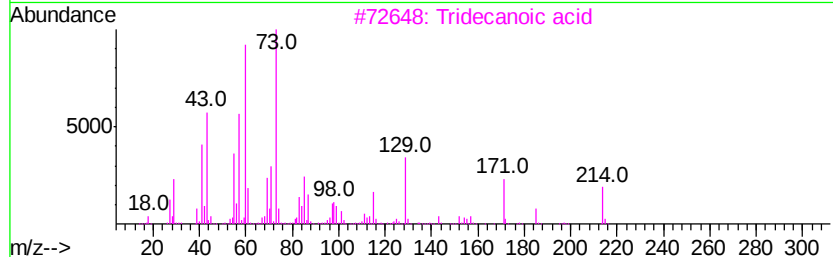
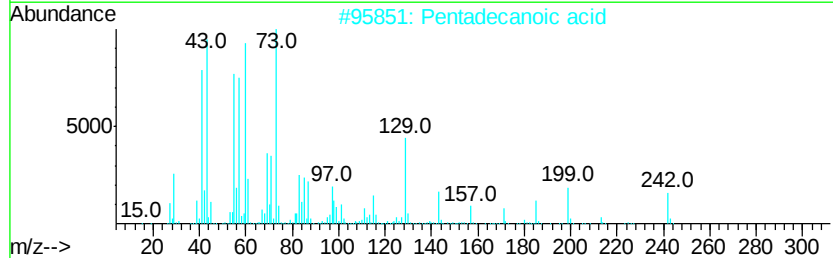
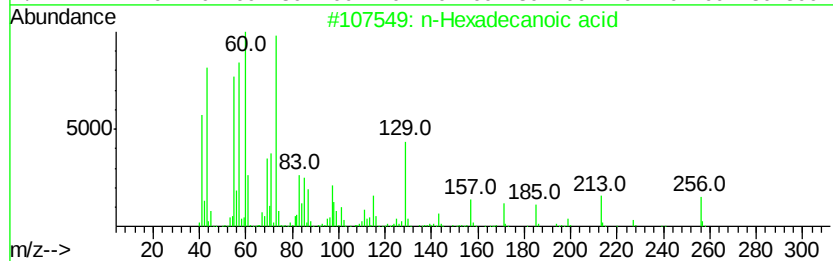
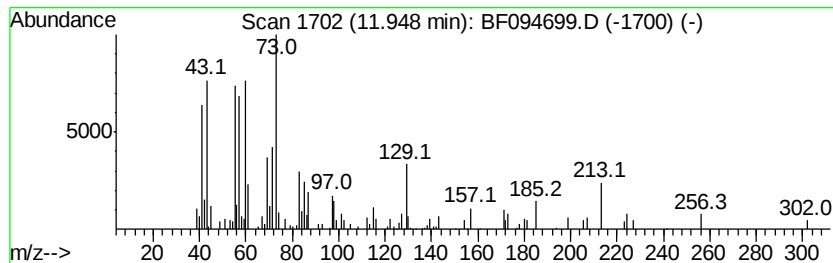
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	4.33 ng	152976	Phenanthrene-d10	11.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Undecanoic acid	186	C11H22O2	000112-37-8	47
5	.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1000157-04-9	47



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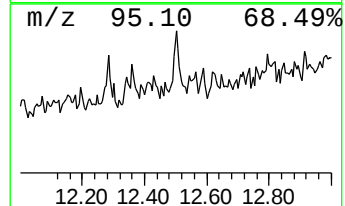
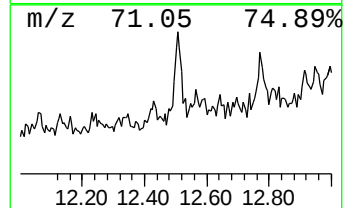
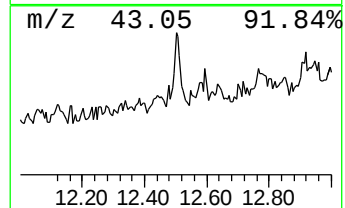
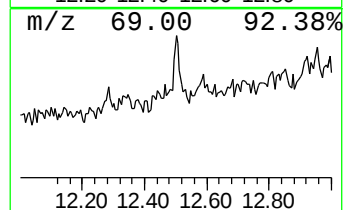
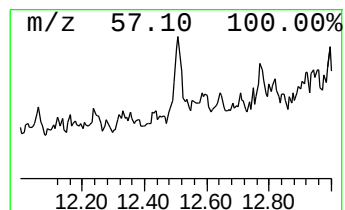
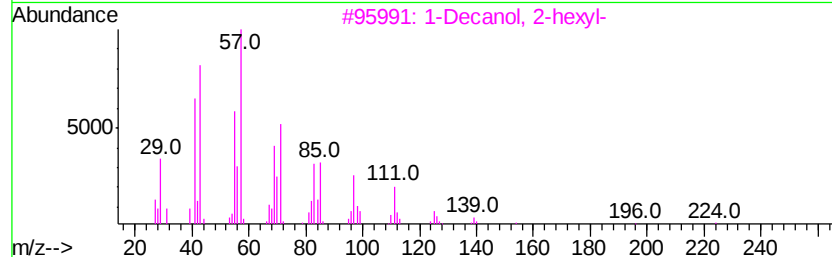
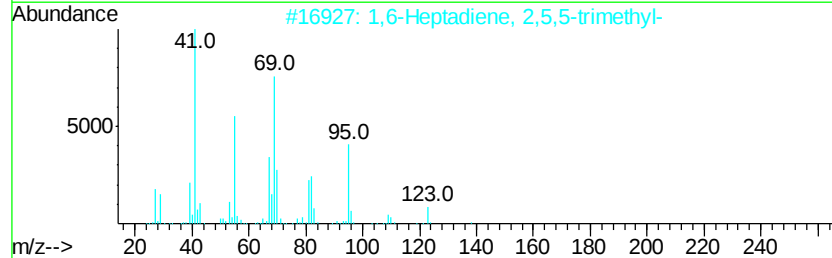
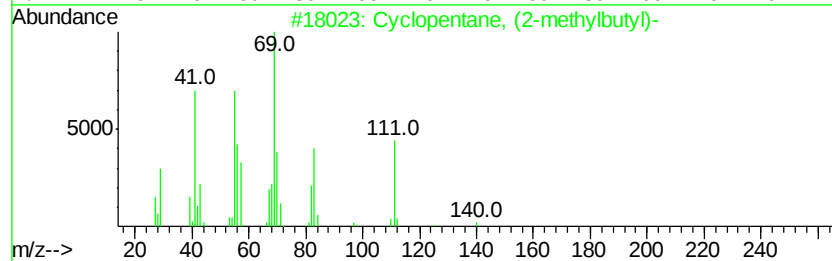
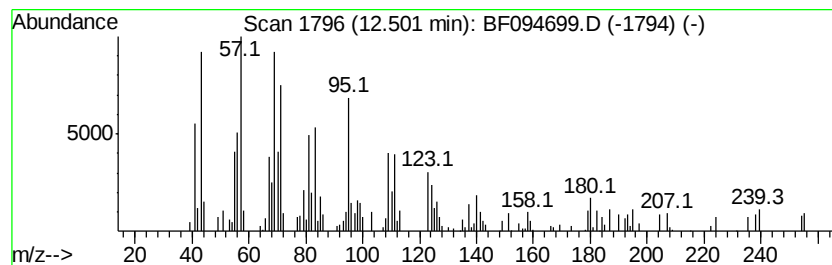
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Peak Number 5 unknown12.50 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.50	2.35 ng	83170	Phenanthrene-d10	11.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	43
2	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	41
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
4	n-Nonenylsuccinic anhydride	224	C13H20O3	028928-97-4	38
5	Cyclohexanepropanol, 2,2-dimethy...	182	C12H22O	095452-04-3	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.94	16.3	ng	500191	1	5.77	612826	20.0
unknown5.52	5.52	95.1	ng	2915280	1	5.77	612826	20.0
n-Hexadecanoic acid	11.95	4.3	ng	152976	4	11.22	706901	20.0
unknown12.50	12.50	2.4	ng	83170	4	11.22	706901	20.0