

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051617\
 Data File : BF095183.D
 Acq On : 17 May 2017 6:10
 Operator : SJ/MA
 Sample : I3153-08
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DS-4-6

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	1.972	4	6	21	rVB2	70558	106229	3.43%	0.452%
2	3.507	256	267	286	rBV	407765	859893	27.76%	3.658%
3	5.148	541	546	564	rBV	216300	485917	15.69%	2.067%
4	5.754	644	649	683	rBV	1496386	2796840	90.29%	11.899%
5	6.907	841	845	849	rBV	51862	57978	1.87%	0.247%
6	7.325	911	916	931	rBV	1566031	2300261	74.26%	9.786%
7	7.442	931	936	954	rVB	1856032	2648105	85.49%	11.266%
8	7.777	989	993	1005	rVB	418469	476492	15.38%	2.027%
9	8.013	1028	1033	1048	rBV	1593220	2035439	65.71%	8.660%
10	8.677	1140	1146	1161	rBV	1076673	1449310	46.79%	6.166%
11	9.789	1331	1335	1353	rBV	448414	605842	19.56%	2.577%
12	11.565	1631	1637	1650	rBV	2361628	3097533	100.00%	13.178%
13	12.083	1720	1725	1730	rVB3	36146	43015	1.39%	0.183%
14	12.254	1750	1754	1766	rBV	214484	333649	10.77%	1.419%
15	12.395	1774	1778	1783	rBV2	46175	60545	1.95%	0.258%
16	12.477	1787	1792	1796	rVB5	22644	41195	1.33%	0.175%
17	12.618	1811	1816	1828	rBV2	487913	722499	23.32%	3.074%
18	13.454	1955	1958	1962	rBV	52891	61273	1.98%	0.261%
19	13.918	2032	2037	2056	rBV	891068	1327819	42.87%	5.649%
20	14.230	2086	2090	2092	rBV	46488	56066	1.81%	0.239%
21	14.959	2210	2214	2218	rBV2	28456	34501	1.11%	0.147%
22	15.024	2218	2225	2230	rBV	397838	545119	17.60%	2.319%
23	15.983	2382	2388	2397	rBV8	39783	88714	2.86%	0.377%
24	16.648	2497	2501	2508	rVB3	44628	48200	1.56%	0.205%
25	16.806	2525	2528	2538	rBV	56233	77545	2.50%	0.330%
26	17.112	2576	2580	2587	rVB	66863	86359	2.79%	0.367%
27	17.342	2614	2619	2631	rBV	1717294	2009399	64.87%	8.549%
28	18.689	2843	2848	2863	rBV	328558	517153	16.70%	2.200%
29	19.965	3061	3065	3069	rBV2	34476	56835	1.83%	0.242%
30	20.259	3112	3115	3122	rBV	20308	34672	1.12%	0.148%
31	20.318	3122	3125	3129	rBV	27046	31484	1.02%	0.134%
32	20.365	3129	3133	3144	rVV	228448	337247	10.89%	1.435%
33	20.888	3217	3222	3233	rBV10	22268	71902	2.32%	0.306%

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DS-4-6

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

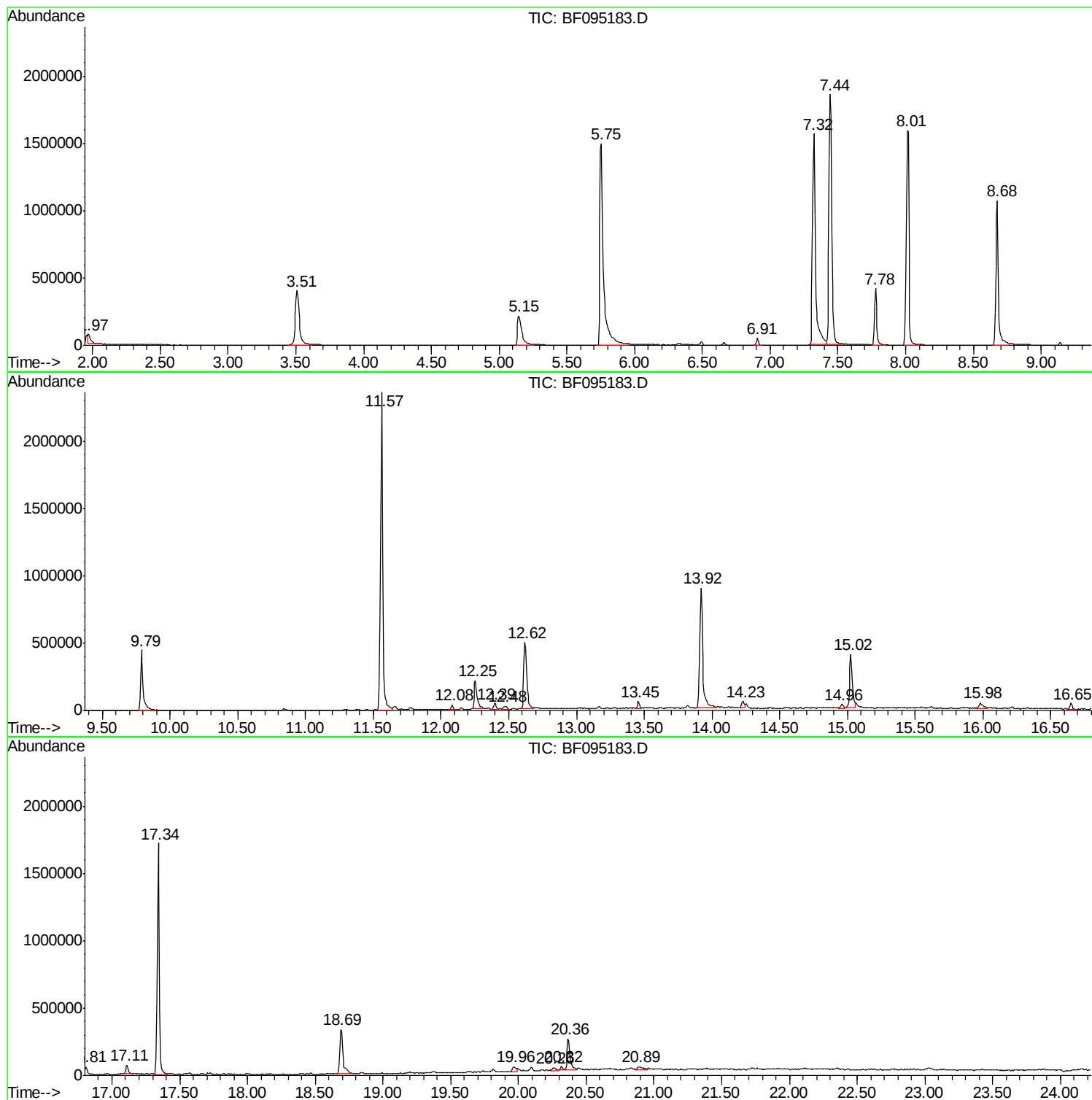
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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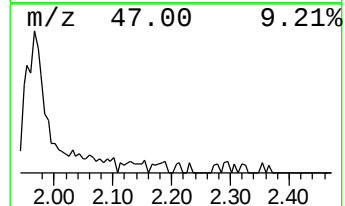
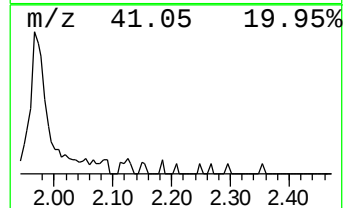
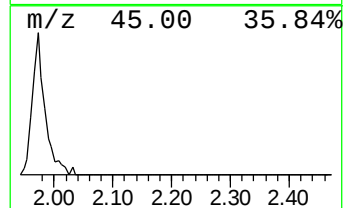
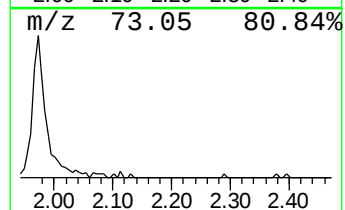
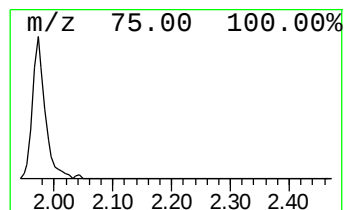
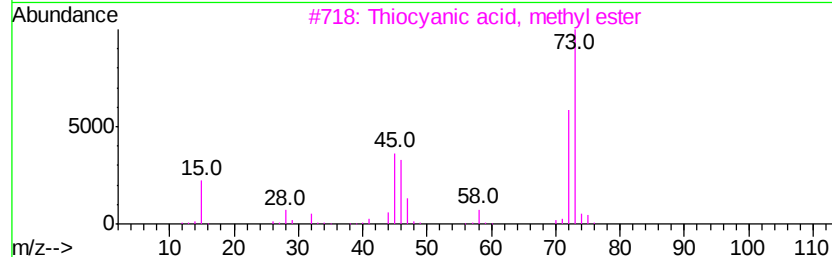
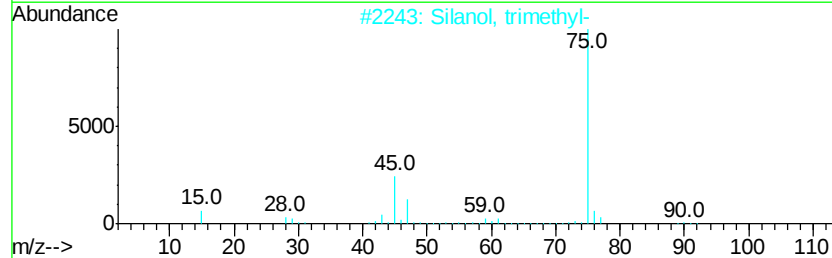
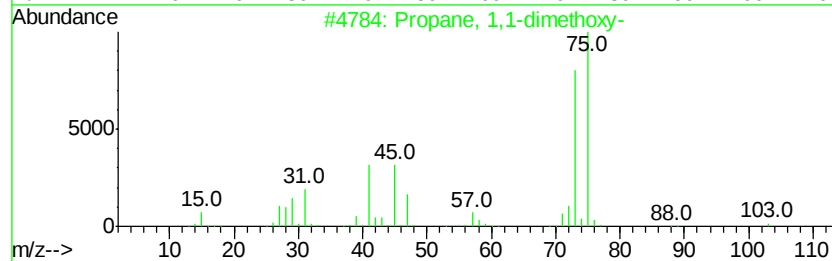
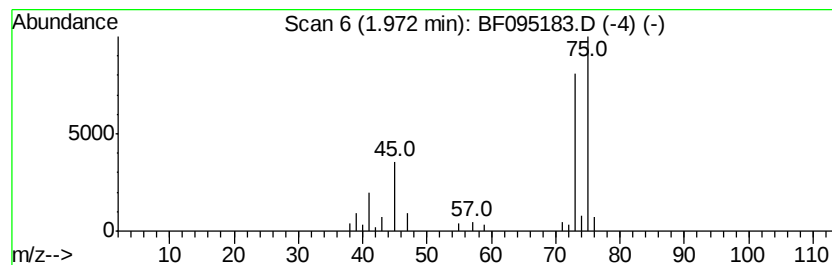
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.97 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.97	4.46 ng	106229	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
2		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	36
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	16
4		Ethyl formate	74	C3H6O2	000109-94-4	9
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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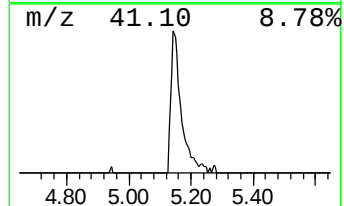
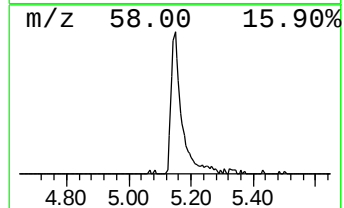
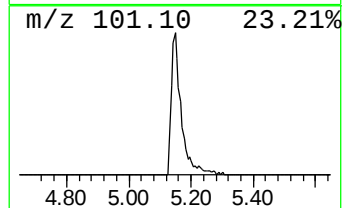
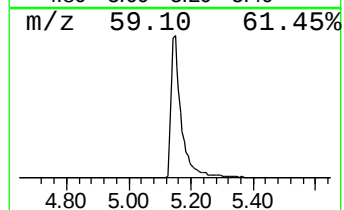
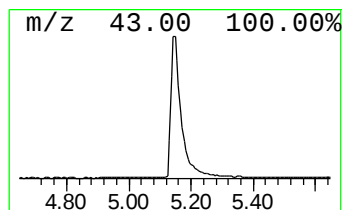
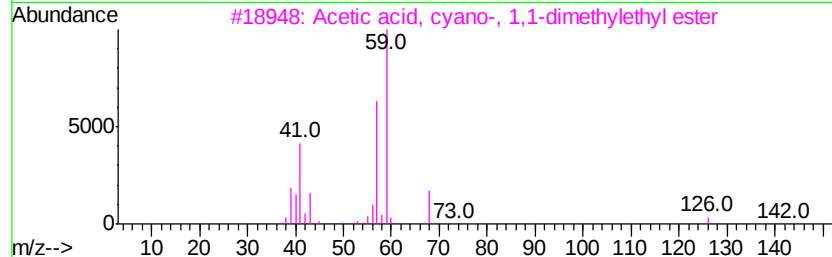
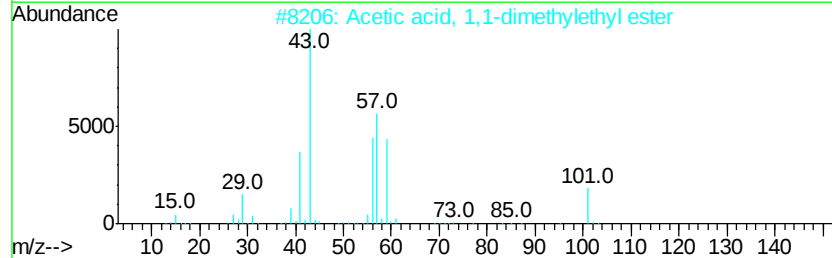
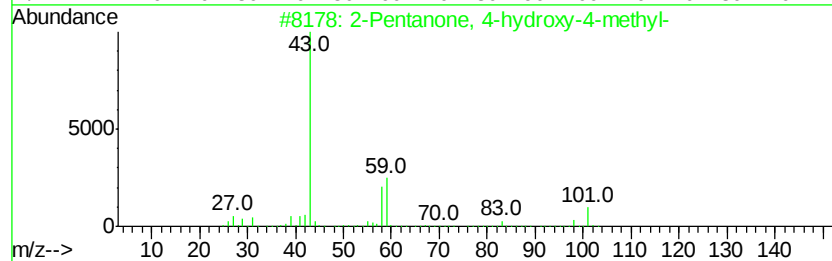
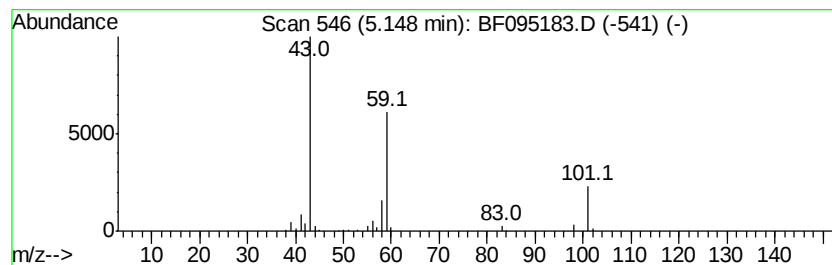
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	20.40 ng	485917	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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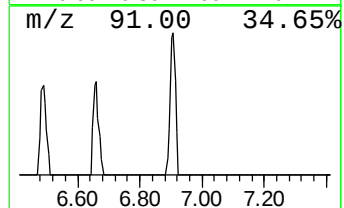
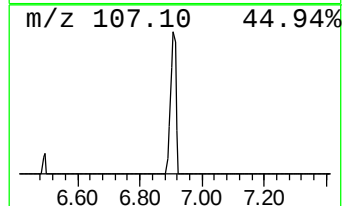
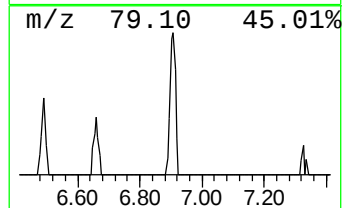
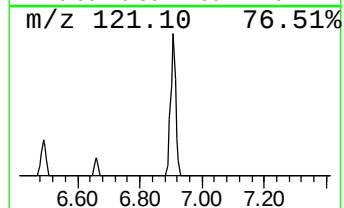
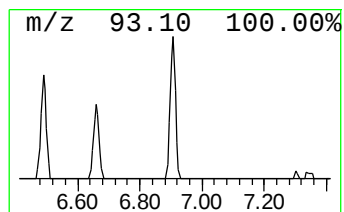
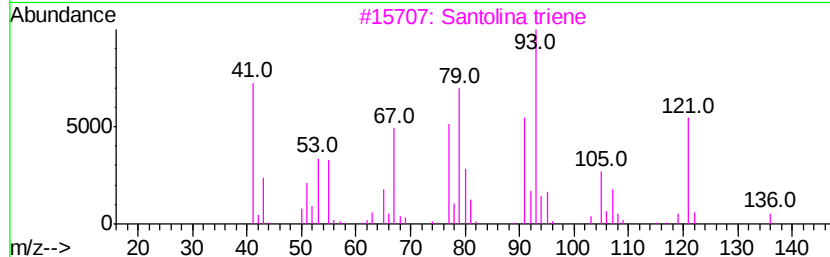
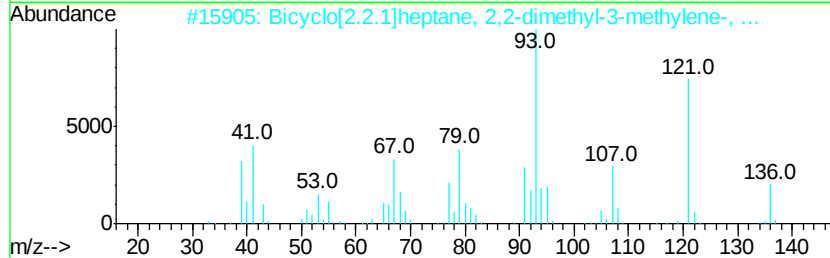
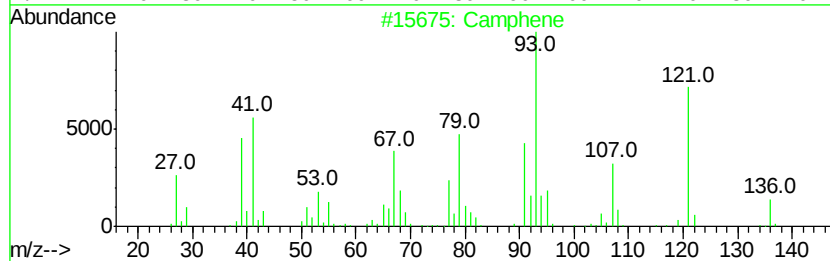
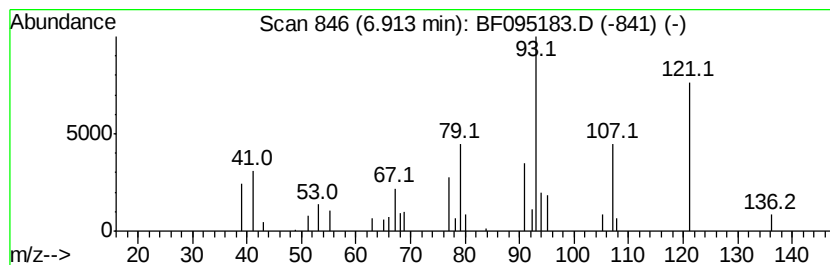
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Camphene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.91	2.43 ng	57978	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Camphene	136	C10H16	000079-92-5	96
2		Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	91
3		Santolina triene	136	C10H16	002153-66-4	91
4		Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	80
5		Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	74



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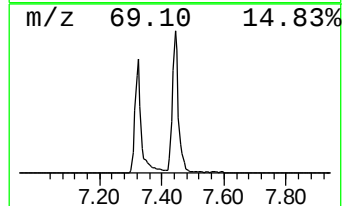
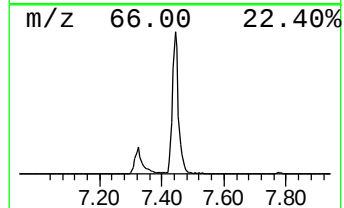
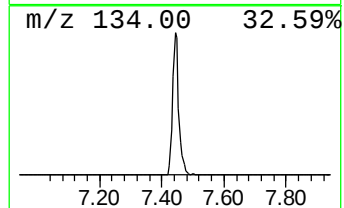
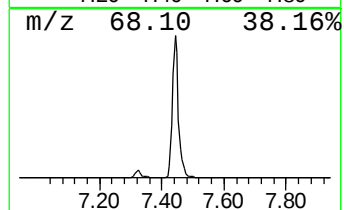
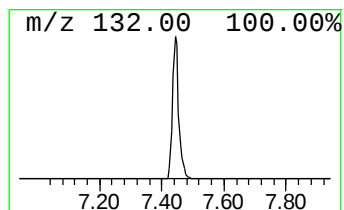
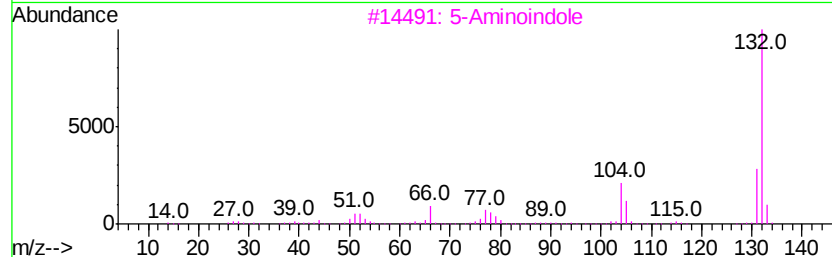
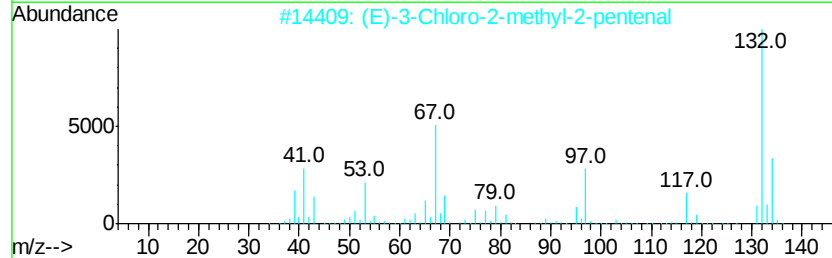
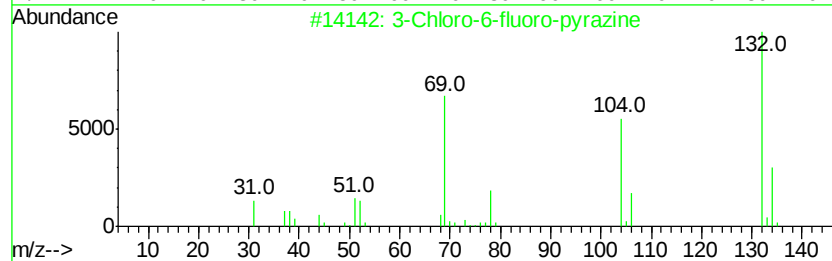
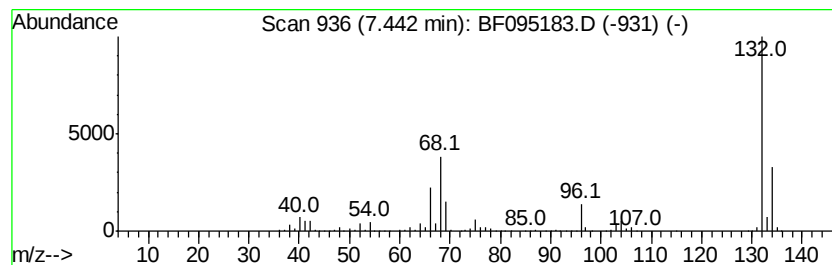
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	111.15 ng	2648110	1,4-Dichlorobenzene-d4	7.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	16
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	10



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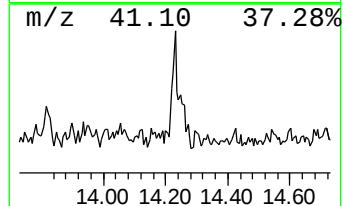
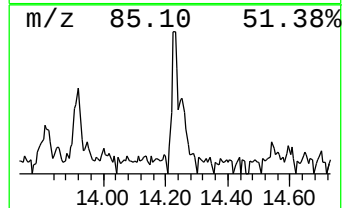
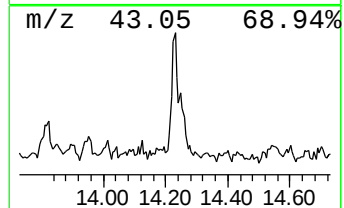
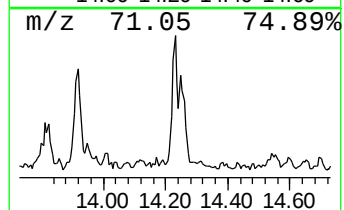
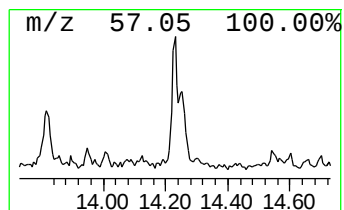
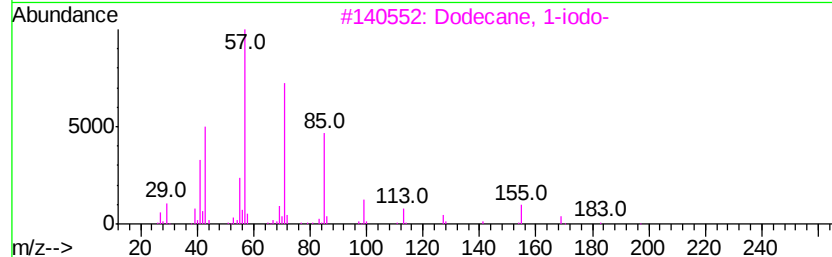
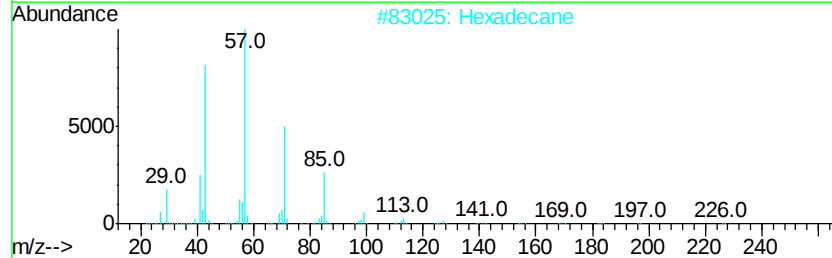
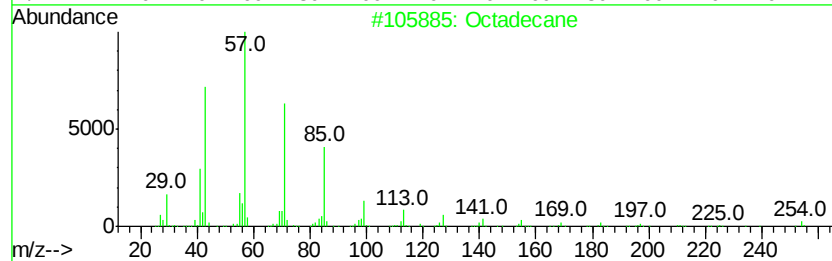
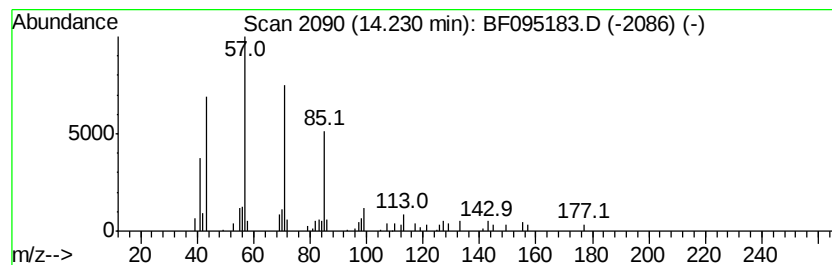
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.06 ng	56066	Phenanthrene-d10	15.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	80
2	Hexadecane		226	C16H34	000544-76-3	72
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	72
4	Tetracosane		338	C24H50	000646-31-1	64
5	Nonane, 2-methyl-5-propyl-		184	C13H28	031081-17-1	64



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ClientSampleId :
DS-4-6

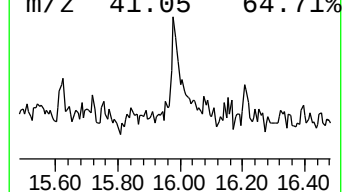
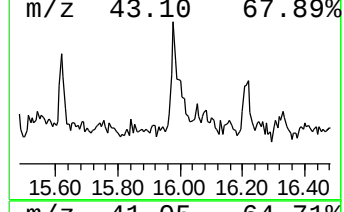
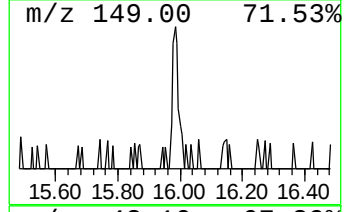
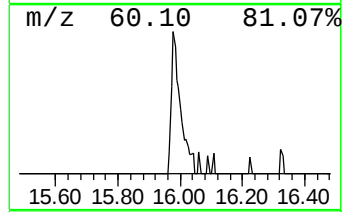
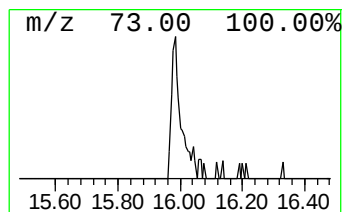
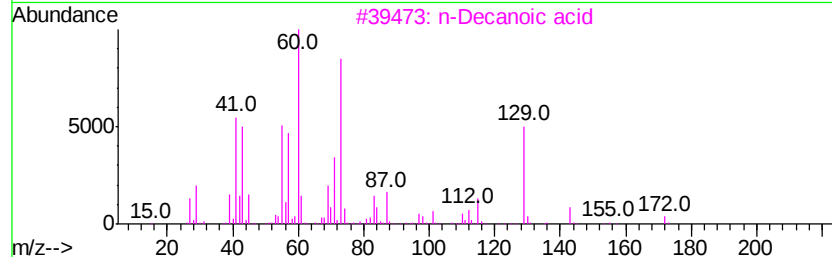
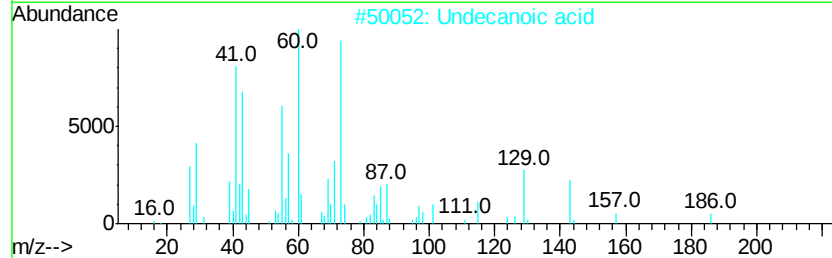
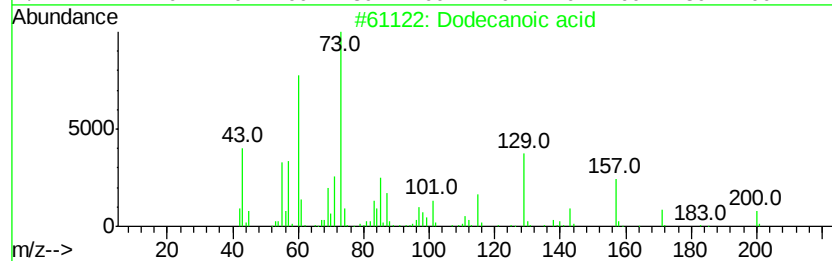
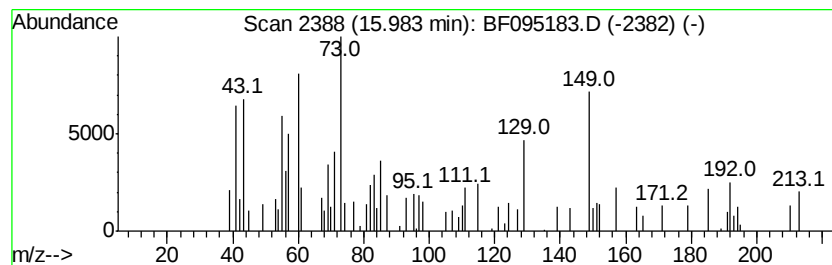
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.98 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	3.25 ng	88714	Phenanthrene-d10	15.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanoic acid	200	C12H24O2	000143-07-7	38
2		Undecanoic acid	186	C11H22O2	000112-37-8	35
3		n-Decanoic acid	172	C10H20O2	000334-48-5	27
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	25
5		Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	16



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051617\
Data File : BF095183.D
Acq On : 17 May 2017 6:10
Operator : SJ/MA
Sample : I3153-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DS-4-6

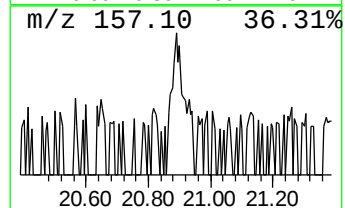
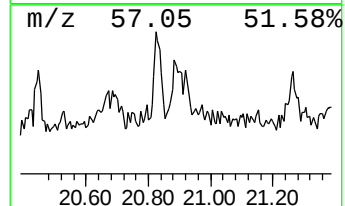
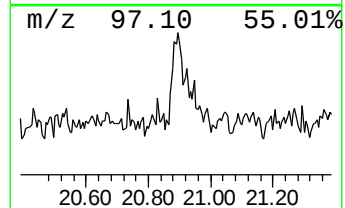
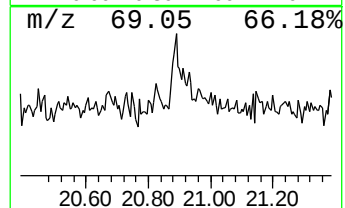
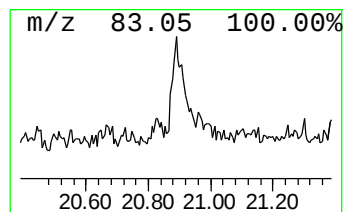
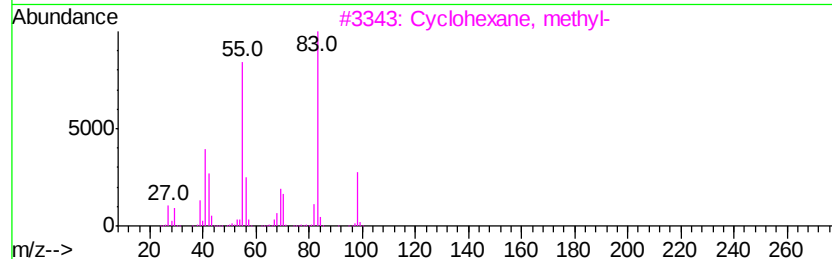
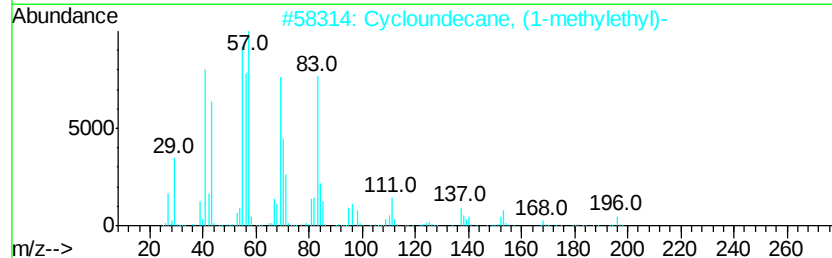
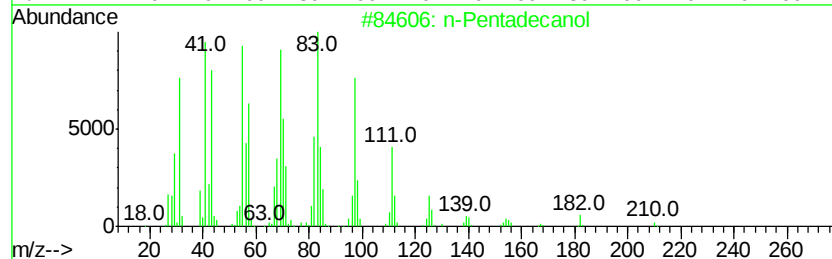
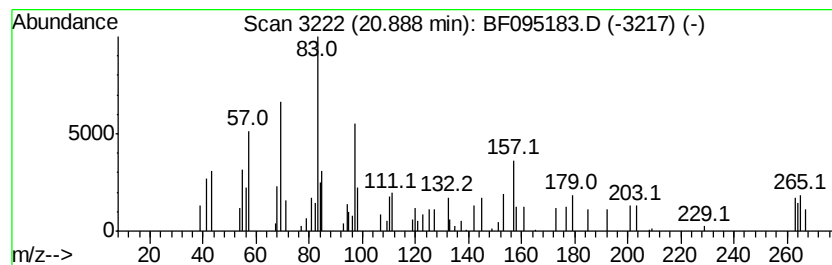
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.89	4.26 ng	71902	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Pentadecanol	228	C15H32O	000629-76-5	38
2		Cycloundecane, (1-methylethyl)-	196	C14H28	062338-56-1	35
3		Cyclohexane, methyl-	98	C7H14	000108-87-2	30
4		Cyclohexanecarboxylic acid, 4-pe...	368	C22H28N2O3	133856-87-8	27
5		7-Tetradecanol	214	C14H30O	003981-79-1	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051617\
Data File : BF095183.D
Acq On : 17 May 2017 6:10
Operator : SJ/MA
Sample : I3153-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DS-4-6

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.97	1.97	4.5	ng	106229	1	7.78	476492	20.0
2-Pentanone, 4-hy...	5.15	20.4	ng	485917	1	7.78	476492	20.0
Camphene	6.91	2.4	ng	57978	1	7.78	476492	20.0
unknown7.44	7.44	111.2	ng	2648110	1	7.78	476492	20.0
Octadecane	14.23	2.1	ng	56066	4	15.02	545119	20.0
unknown15.98	15.98	3.3	ng	88714	4	15.02	545119	20.0
unknown20.89	20.89	4.3	ng	71902	6	20.37	337247	20.0