

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
 Data File : BF091559.D
 Acq On : 13 Dec 2016 17:40
 Operator : UM/SJ
 Sample : H5972-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1M-WBF-EME-05

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-BF120916.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	4.304	192	194	201	rVB2	32902	78618	1.11%	0.118%
2	4.990	251	254	257	rBV	1996489	2921494	41.24%	4.383%
3	5.424	289	292	294	rBV	6692256	7084261	100.00%	10.628%
4	6.453	379	382	385	rVB	5817648	6229366	87.93%	9.346%
5	6.579	391	393	396	rBV	5536654	6623304	93.49%	9.937%
6	6.807	411	413	416	rBV	1536123	1734838	24.49%	2.603%
7	6.967	425	427	430	rBV	5423565	5028742	70.98%	7.545%
8	7.379	460	463	465	rBV	4561726	4818883	68.02%	7.230%
9	7.482	469	472	479	rVB	65197	123435	1.74%	0.185%
10	8.099	523	526	528	rBV	2652360	2414995	34.09%	3.623%
11	9.173	617	620	623	rBV	6995677	6724496	94.92%	10.089%
12	9.573	652	655	657	rBV	2267300	2212636	31.23%	3.320%
13	9.848	677	679	682	rVB	2902599	2495484	35.23%	3.744%
14	10.293	714	718	719	rBV2	142738	214371	3.03%	0.322%
15	10.511	734	737	740	rBV	78846	134135	1.89%	0.201%
16	10.636	745	748	750	rBV	4363393	4221359	59.59%	6.333%
17	10.762	757	759	766	rBV	276470	342812	4.84%	0.514%
18	11.208	796	798	799	rBV	193418	161091	2.27%	0.242%
19	11.333	806	809	811	rBV	2043069	2349622	33.17%	3.525%
20	11.562	826	829	833	rBV	71209	85371	1.21%	0.128%
21	11.871	854	856	858	rBV	188941	287185	4.05%	0.431%
22	12.648	922	924	926	rBV	62056	72550	1.02%	0.109%
23	12.911	945	947	950	rBV	4394155	5230960	73.84%	7.848%
24	13.814	1024	1026	1032	rBV	337338	409948	5.79%	0.615%
25	13.962	1036	1039	1041	rBV	1637847	1794189	25.33%	2.692%
26	14.442	1079	1081	1083	rBV2	74907	113714	1.61%	0.171%
27	15.060	1133	1135	1138	rVB	86761	99232	1.40%	0.149%
28	15.368	1160	1162	1165	rBV	1123136	1635465	23.09%	2.454%
29	15.425	1165	1167	1173	rVB	117444	219449	3.10%	0.329%
30	15.825	1200	1202	1205	rBV	118703	186492	2.63%	0.280%
31	16.305	1241	1244	1250	rVB2	125935	297315	4.20%	0.446%
32	16.854	1290	1292	1295	rVB	84476	150312	2.12%	0.226%
33	17.505	1347	1349	1354	rVB	65475	158006	2.23%	0.237%

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ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId :
1M-WBF-EME-05

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-BF120916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

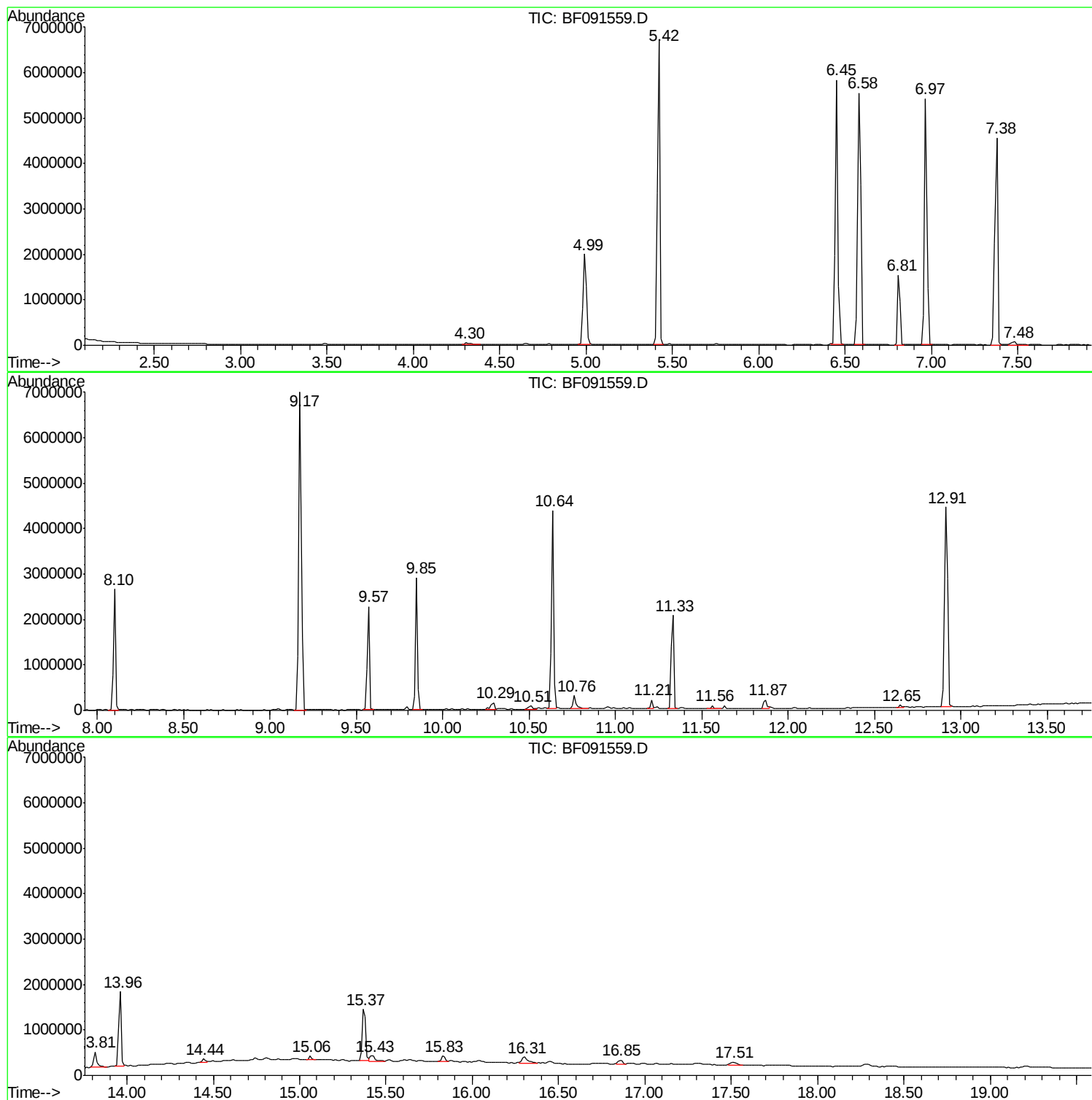
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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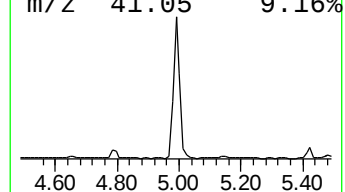
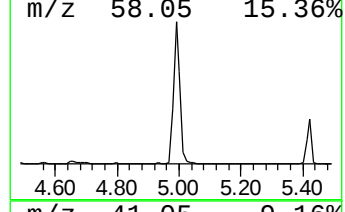
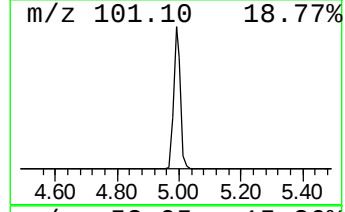
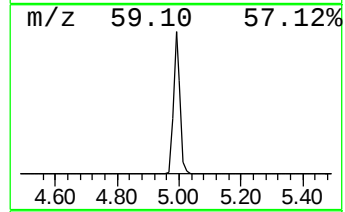
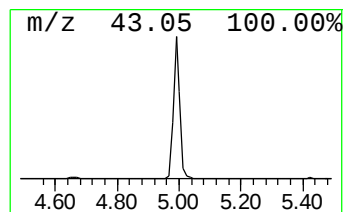
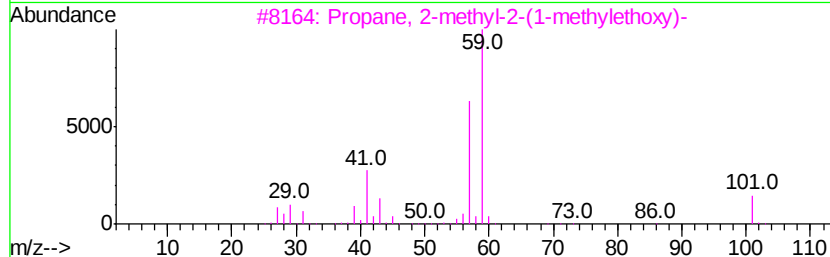
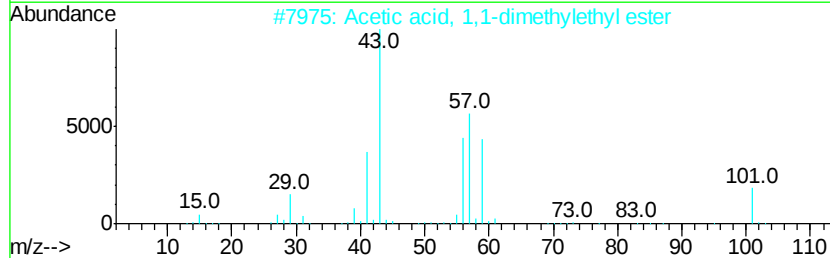
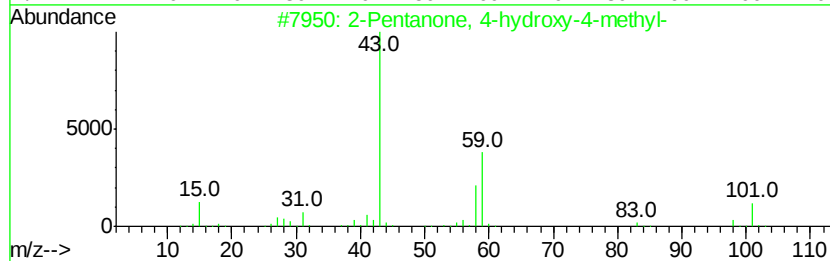
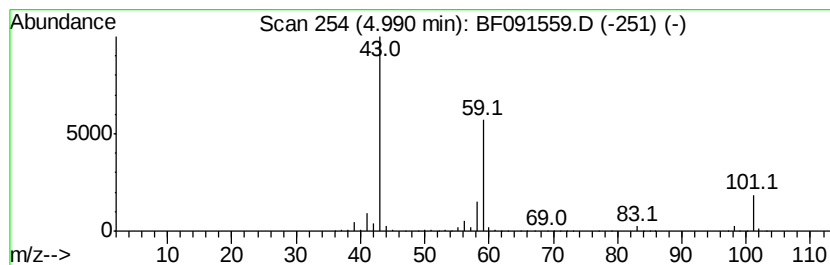
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	33.68 ng	2921490	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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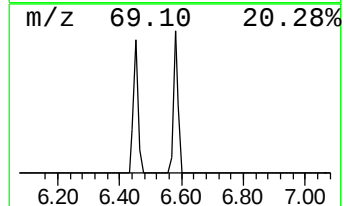
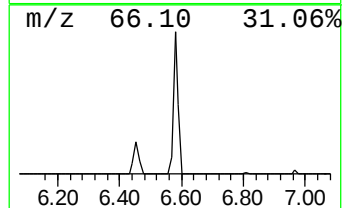
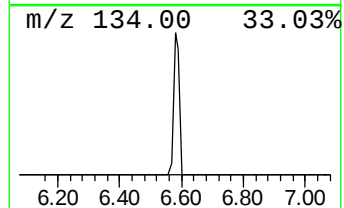
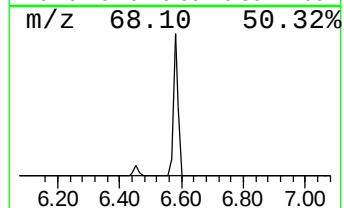
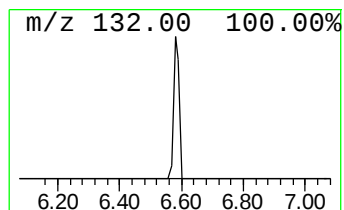
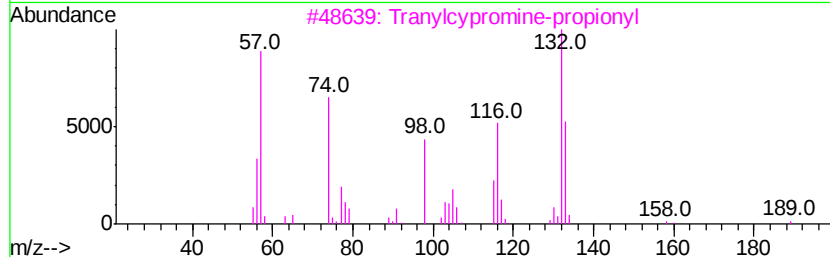
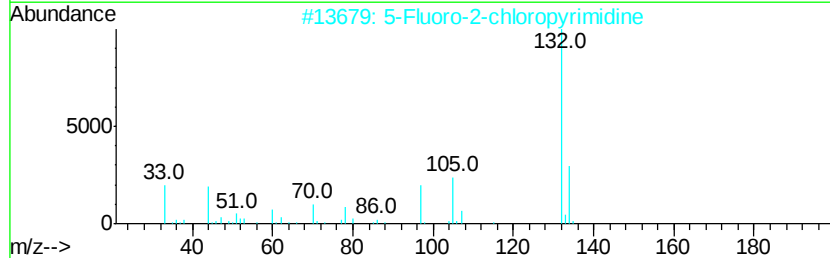
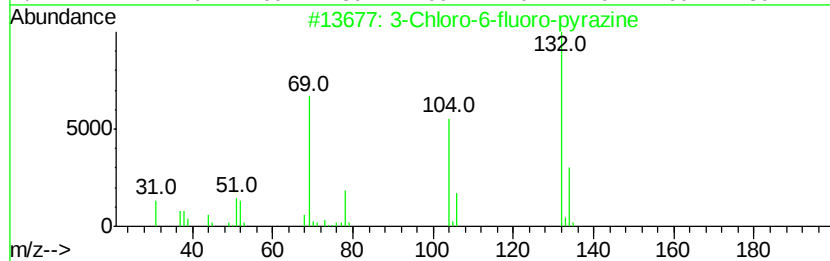
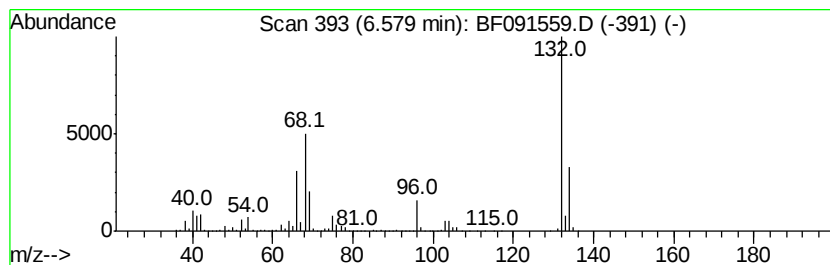
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	76.36 ng	6623300	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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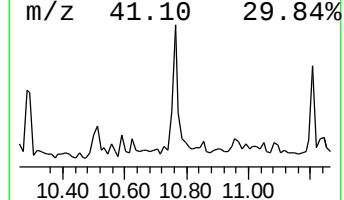
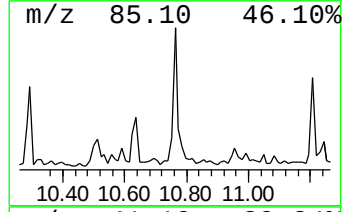
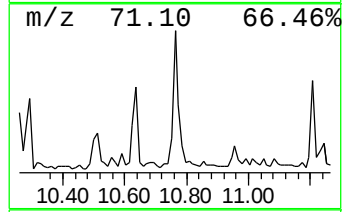
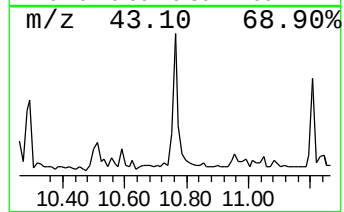
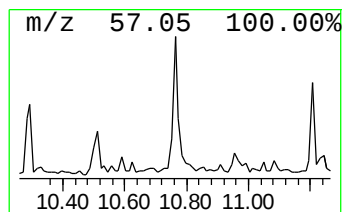
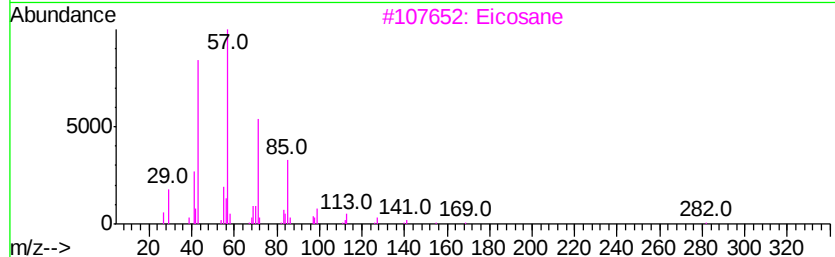
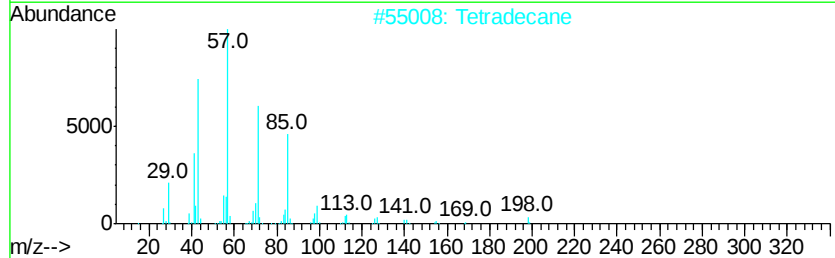
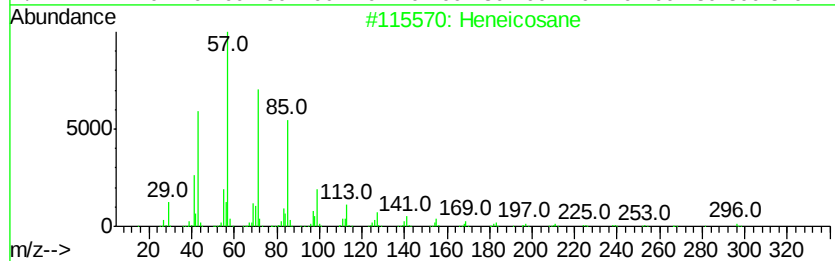
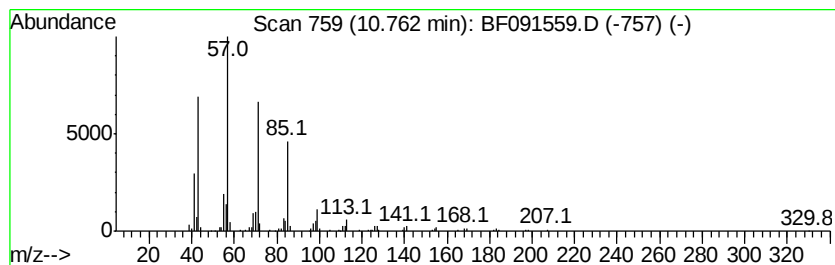
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.92 ng	342812	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Tetradecane		198	C14H30	000629-59-4	86
3	Eicosane		282	C20H42	000112-95-8	83
4	Hexadecane		226	C16H34	000544-76-3	80
5	Dodecane, 4-methyl-		184	C13H28	006117-97-1	72



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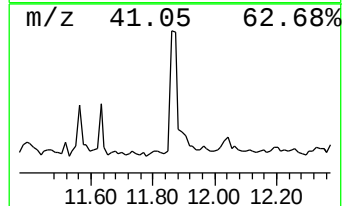
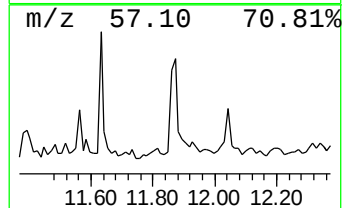
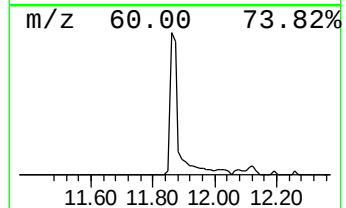
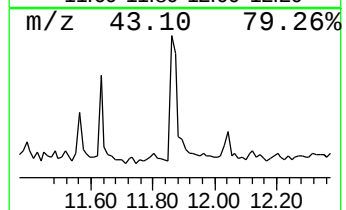
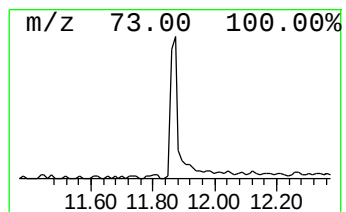
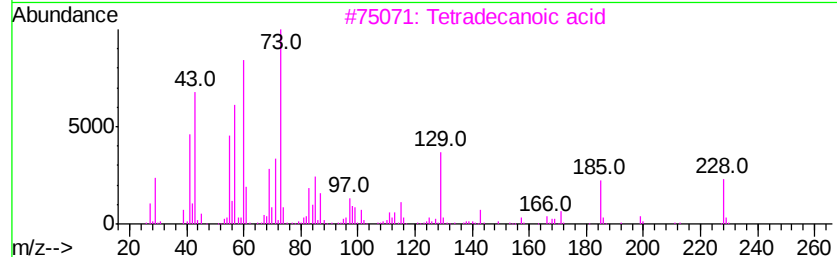
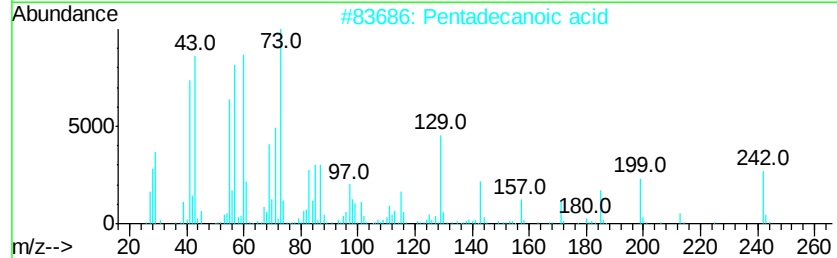
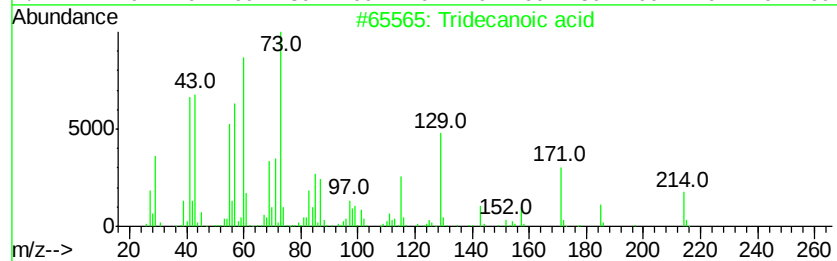
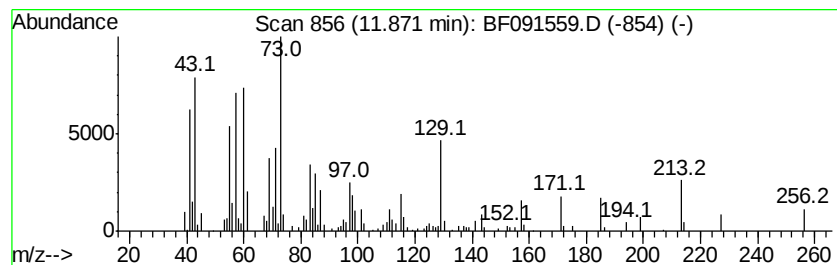
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.44 ng	287185	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	89
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	49
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



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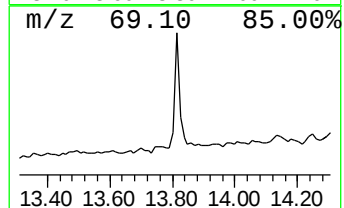
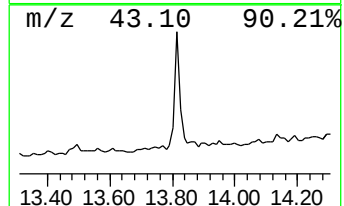
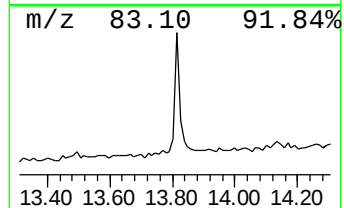
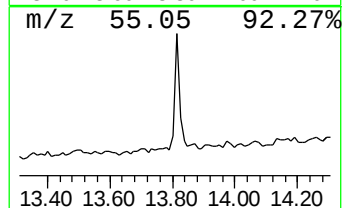
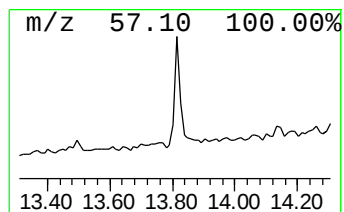
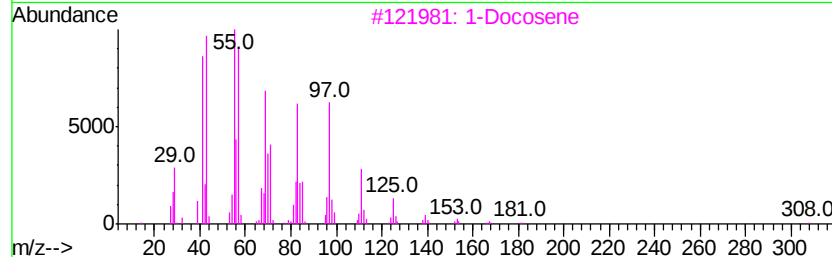
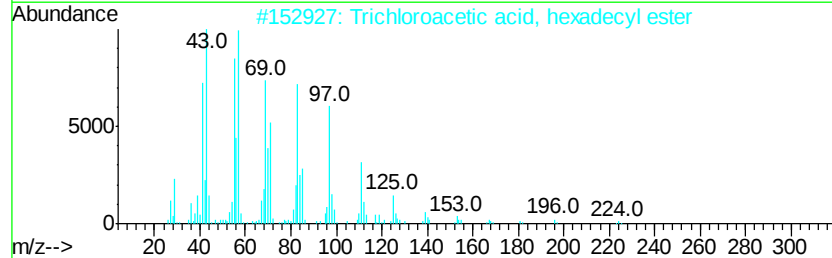
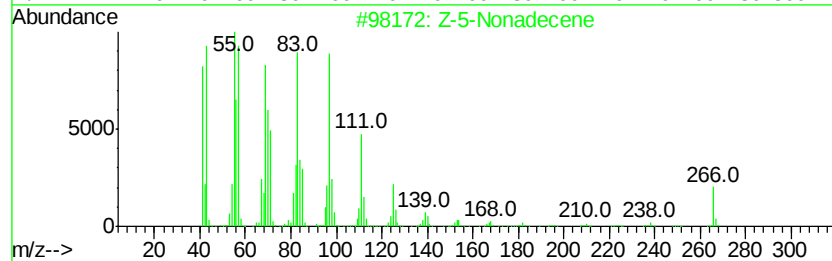
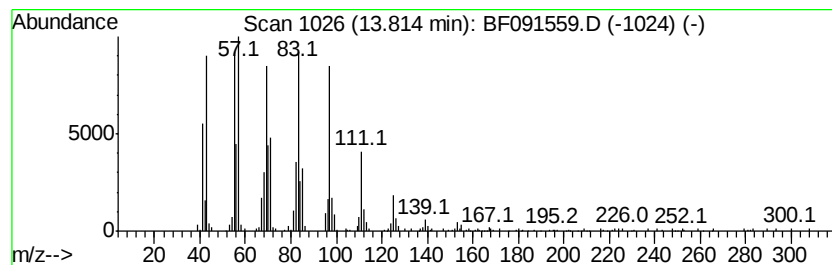
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Z-5-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	4.57 ng	409948	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3	1-Docosene	308	C22H44	001599-67-3	91
4	Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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1M-WBF-EME-05

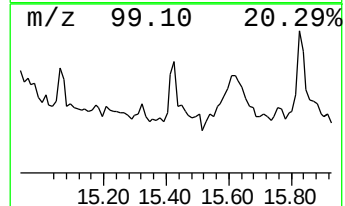
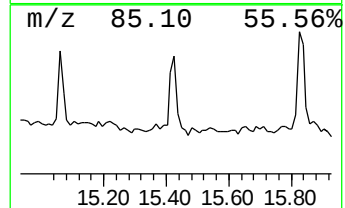
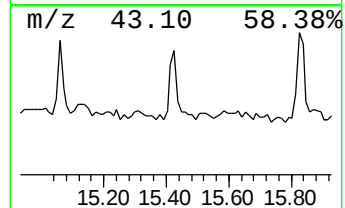
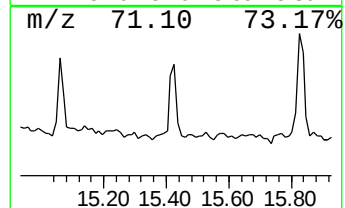
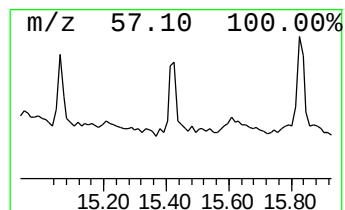
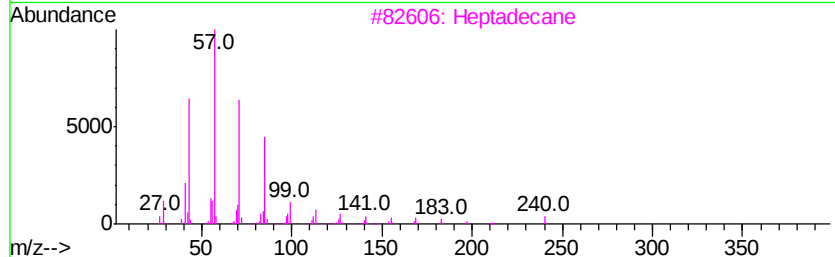
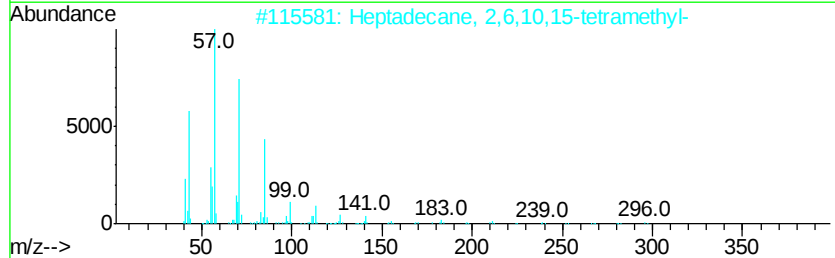
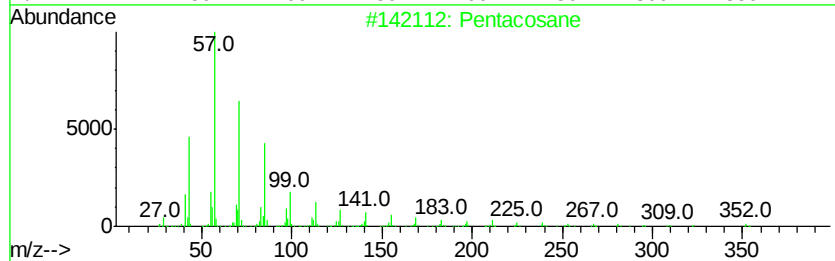
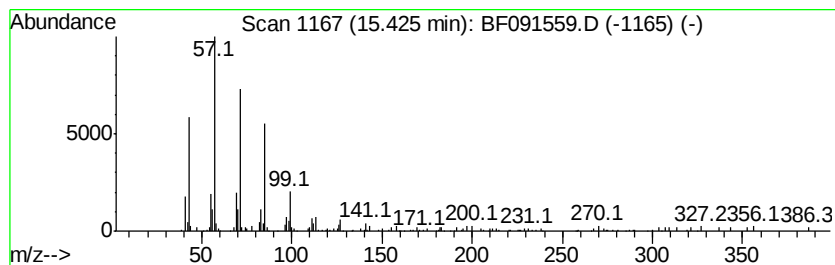
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	2.68 ng	219449	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	90
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
3		Heptadecane	240	C17H36	000629-78-7	80
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	78
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121316\
Data File : BF091559.D
Acq On : 13 Dec 2016 17:40
Operator : UM/SJ
Sample : H5972-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1M-WBF-EME-05

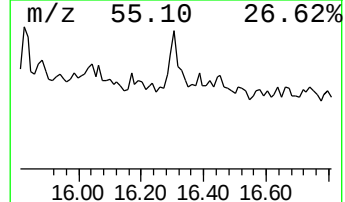
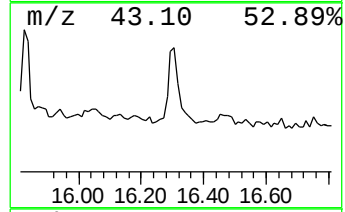
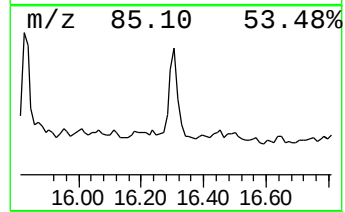
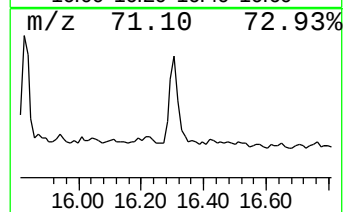
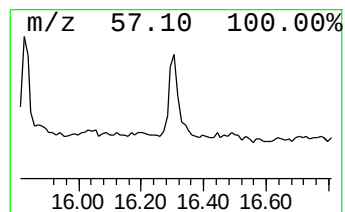
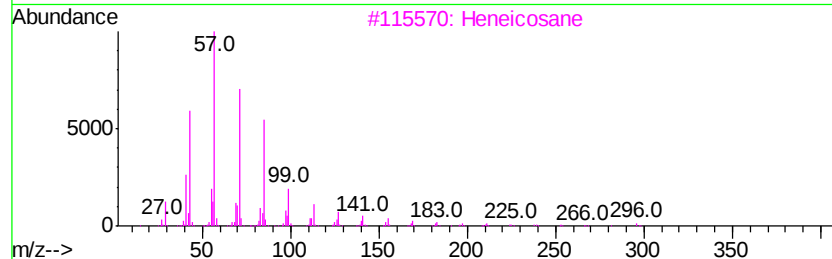
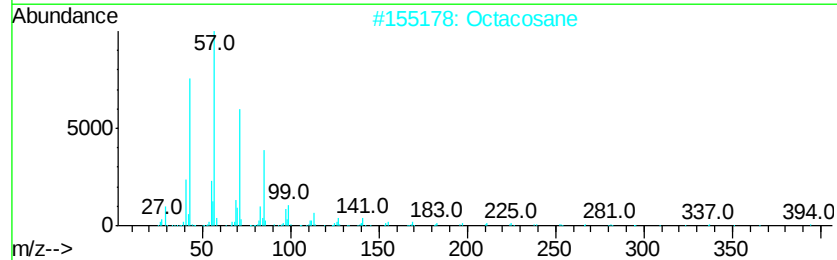
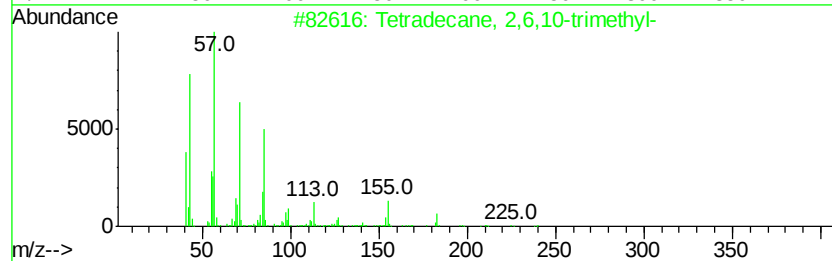
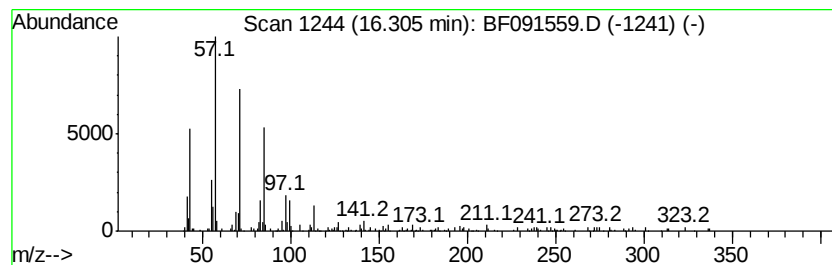
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetradecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	3.64 ng	297315	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Heneicosane	296	C21H44	000629-94-7	86
4		Hexadecane	226	C16H34	000544-76-3	83
5		Tetradecane	198	C14H30	000629-59-4	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121316\
Data File : BF091559.D
Acq On : 13 Dec 2016 17:40
Operator : UM/SJ
Sample : H5972-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1M-WBF-EME-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	33.7	ng	2921490	1	6.81	1734840	20.0
unknown6.58	6.58	76.4	ng	6623300	1	6.81	1734840	20.0
Heneicosane	10.76	2.9	ng	342812	4	11.33	2349620	20.0
Tridecanoic acid	11.87	2.4	ng	287185	4	11.33	2349620	20.0
Z-5-Nonadecene	13.81	4.6	ng	409948	5	13.96	1794190	20.0
Pentacosane	15.43	2.7	ng	219449	6	15.37	1635470	20.0
Tetradecane, 2,6,...	16.31	3.6	ng	297315	6	15.37	1635470	20.0