

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061317\
 Data File : BF095899.D
 Acq On : 13 Jun 2017 18:01
 Operator : SJ/MA
 Sample : I3614-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-5

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-BF060517.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	4.551	499	504	521	rBV	308999	586711	33.44%	5.300%
2	5.322	632	635	654	rBV	28357	103101	5.88%	0.931%
3	6.969	912	915	921	rBV	35402	80364	4.58%	0.726%
4	7.022	921	924	940	rVB	168632	414198	23.60%	3.741%
5	7.351	976	980	990	rBV	261528	372850	21.25%	3.368%
6	7.439	990	995	1002	rVB2	18323	25091	1.43%	0.227%
7	7.581	1015	1019	1034	rBV	721489	1024031	58.36%	9.250%
8	7.822	1053	1060	1064	rBV	20978	36180	2.06%	0.327%
9	7.957	1077	1083	1087	rBV2	22460	33323	1.90%	0.301%
10	8.092	1098	1106	1109	rBV2	13333	23114	1.32%	0.209%
11	8.263	1131	1135	1152	rBV	512316	822770	46.89%	7.432%
12	8.981	1252	1257	1261	rBV	59740	83303	4.75%	0.752%
13	9.381	1320	1325	1339	rBV	366323	552289	31.47%	4.989%
14	11.086	1609	1615	1620	rVB2	24871	32295	1.84%	0.292%
15	11.157	1620	1627	1639	rBV	1283800	1754748	100.00%	15.851%
16	11.857	1741	1746	1757	rBV	313362	411962	23.48%	3.721%
17	12.198	1799	1804	1810	rBV2	460556	622291	35.46%	5.621%
18	12.245	1810	1812	1820	rVB4	16613	27277	1.55%	0.246%
19	13.057	1943	1950	1955	rVB2	25214	31463	1.79%	0.284%
20	13.504	2021	2026	2037	rBV	176135	298656	17.02%	2.698%
21	13.598	2037	2042	2051	rVB5	10899	22193	1.26%	0.200%
22	13.827	2075	2081	2088	rBV2	30591	50796	2.89%	0.459%
23	14.557	2202	2205	2208	rBV	16546	20430	1.16%	0.185%
24	14.592	2208	2211	2221	rVB	419961	595786	33.95%	5.382%
25	15.621	2375	2386	2401	rBV2	125415	212575	12.11%	1.920%
26	16.721	2567	2573	2580	rBV3	142119	187965	10.71%	1.698%
27	16.780	2580	2583	2589	rVB2	26389	34371	1.96%	0.310%
28	16.974	2610	2616	2621	rBV	1391078	1650492	94.06%	14.909%
29	18.227	2824	2829	2838	rBV3	53220	83171	4.74%	0.751%
30	18.315	2840	2844	2853	rBV	398566	476331	27.15%	4.303%
31	19.456	3034	3038	3042	rVB	41546	49706	2.83%	0.449%
32	19.986	3124	3128	3140	rBV	233324	350699	19.99%	3.168%

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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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

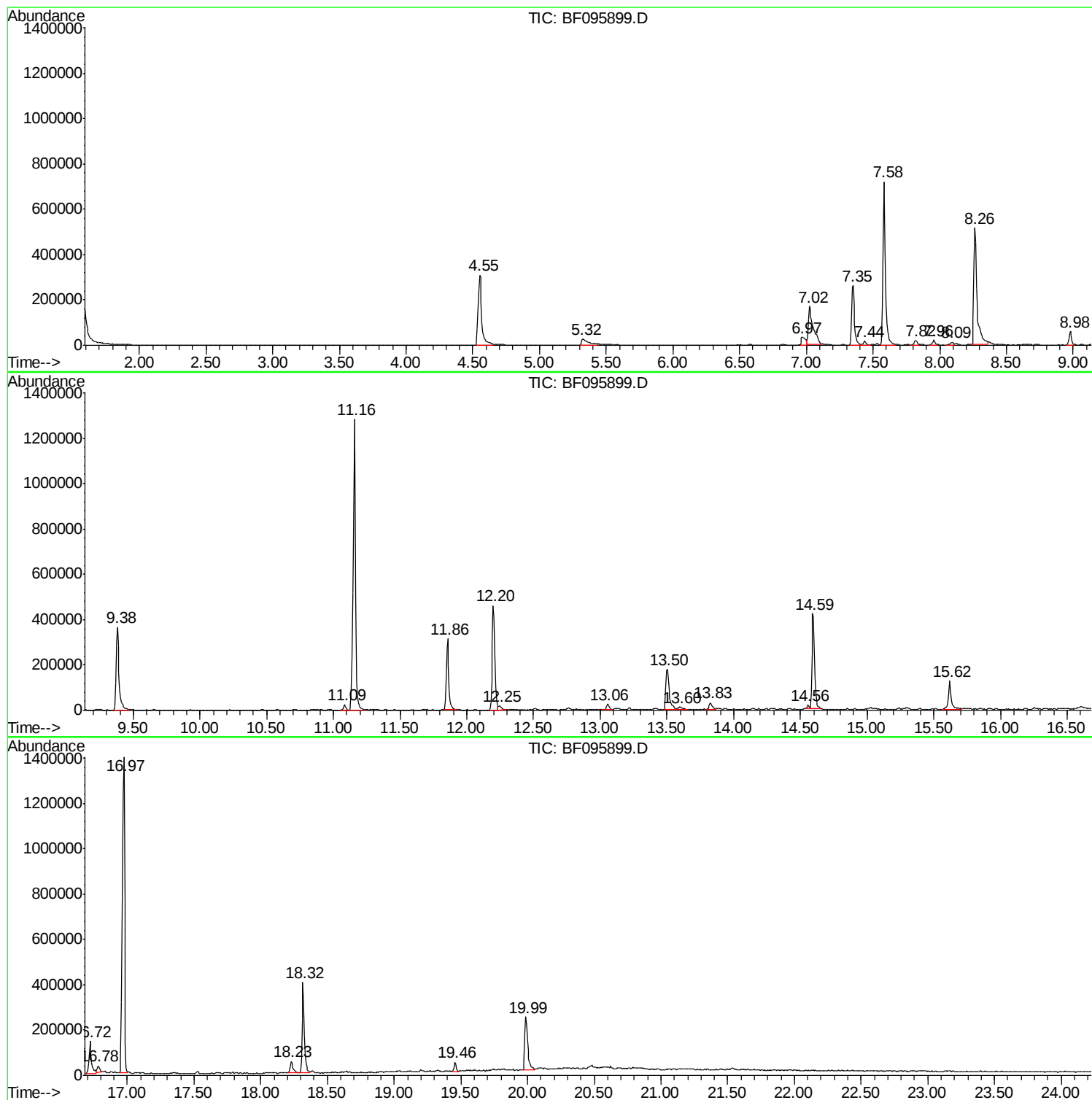
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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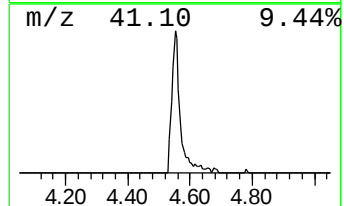
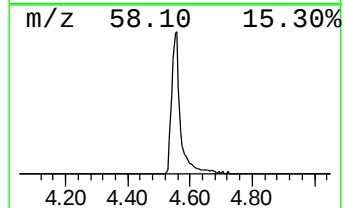
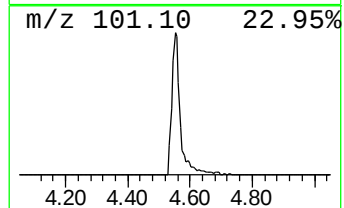
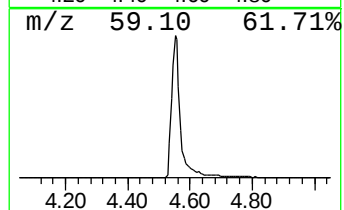
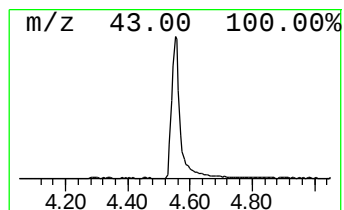
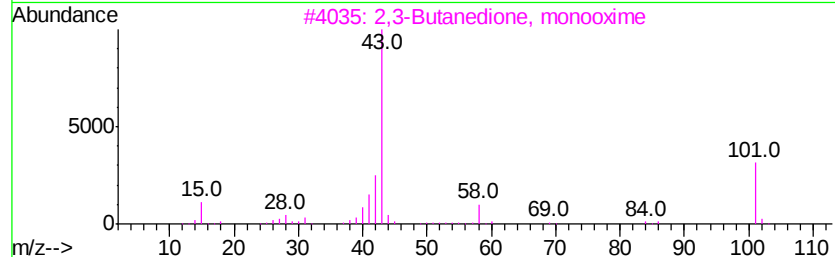
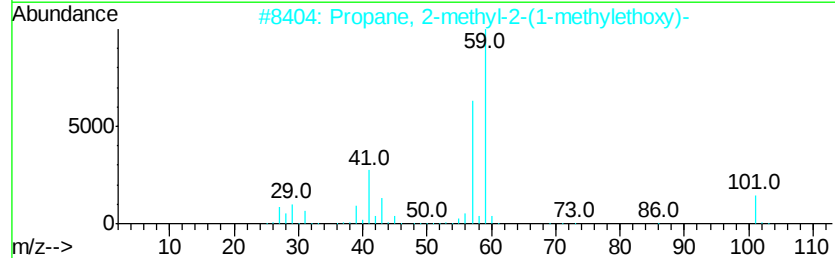
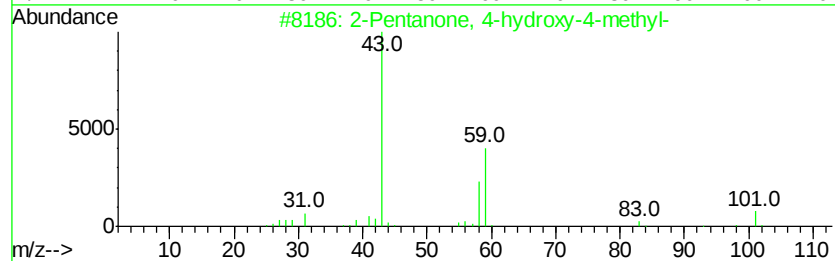
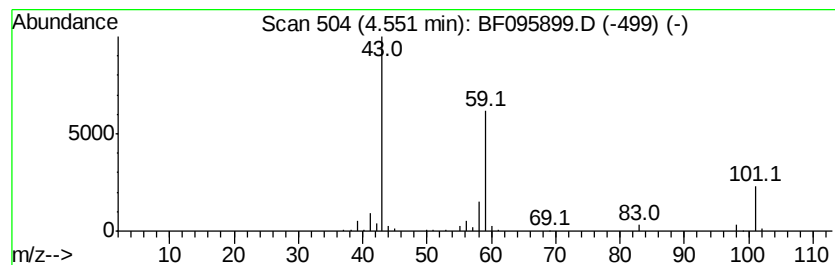
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	31.47 ng	586711	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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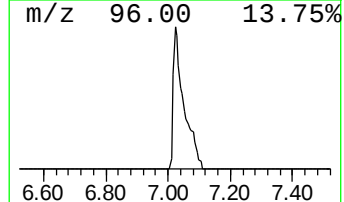
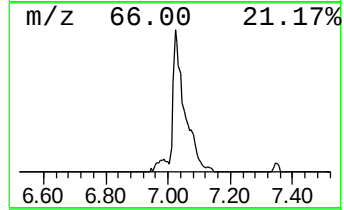
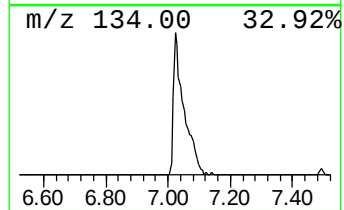
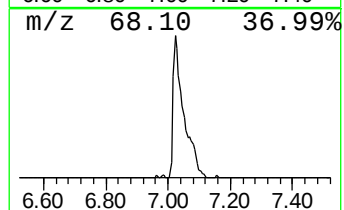
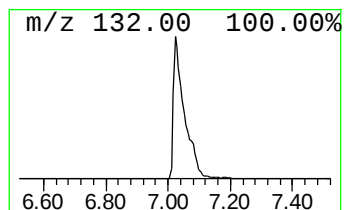
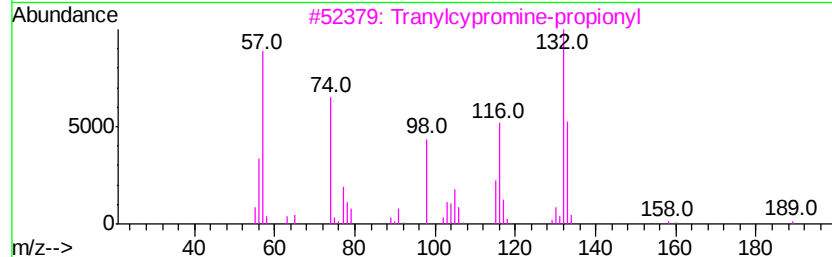
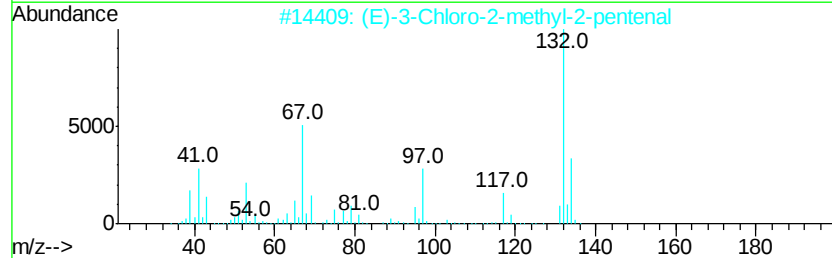
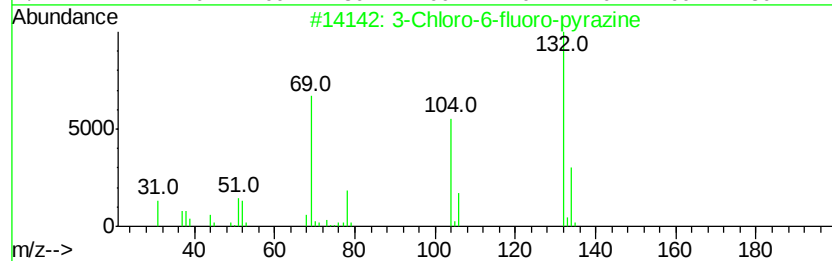
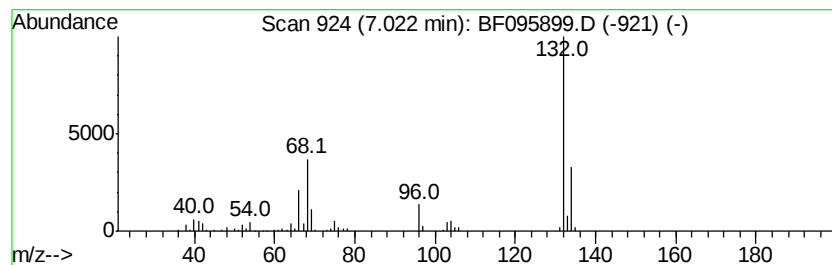
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	22.22 ng	414198	1,4-Dichlorobenzene-d4	7.35

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10



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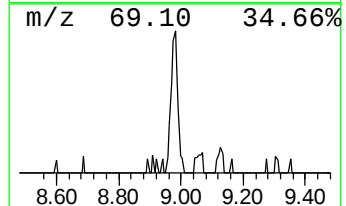
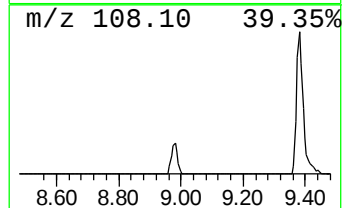
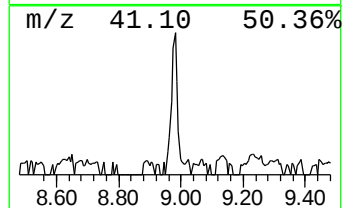
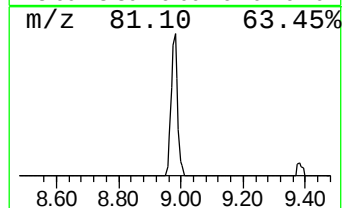
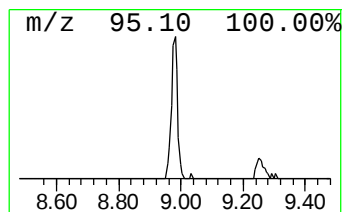
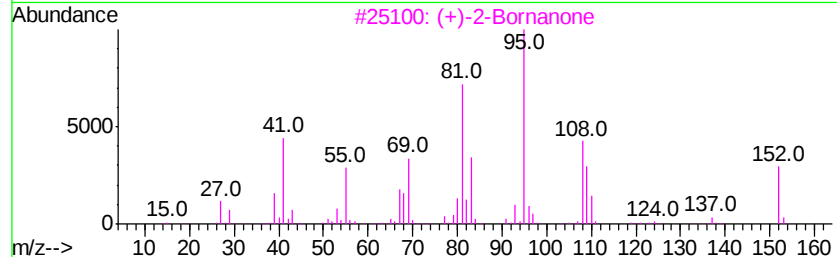
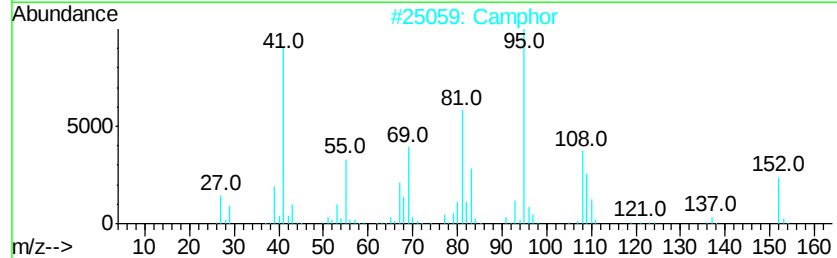
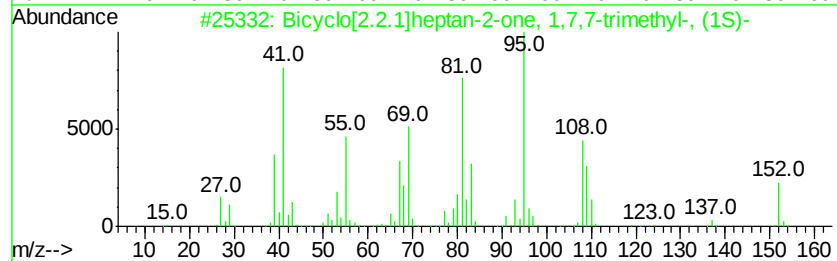
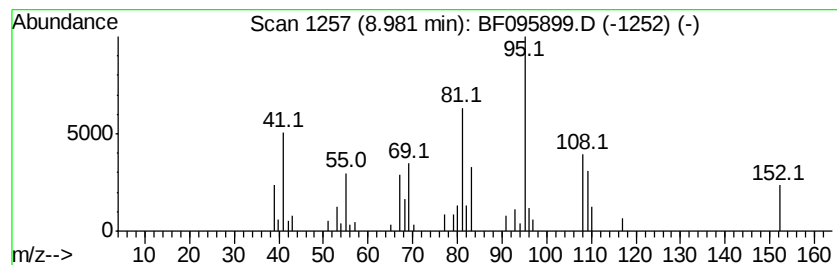
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	3.02 ng	83303	Napthalene-d8	9.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2		Camphor	152	C10H16O	000076-22-2	96
3		(+)-2-Bornanone	152	C10H16O	000464-49-3	96
4		4-(1,2-Dimethyl-cyclopent-2-enyl)...	166	C11H18O	075698-06-5	43
5		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	43



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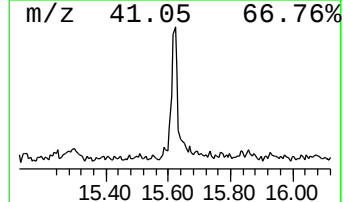
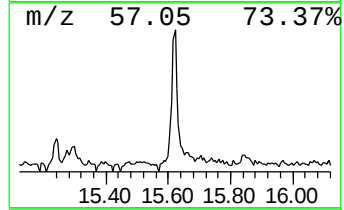
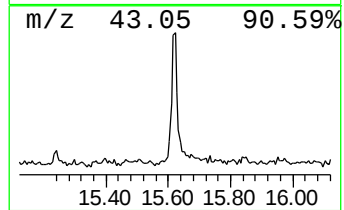
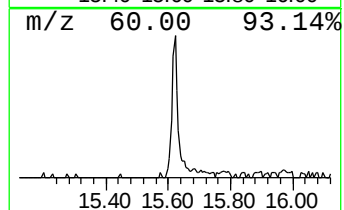
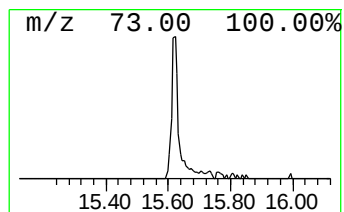
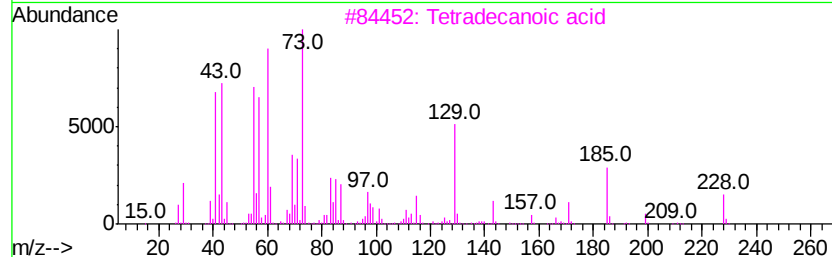
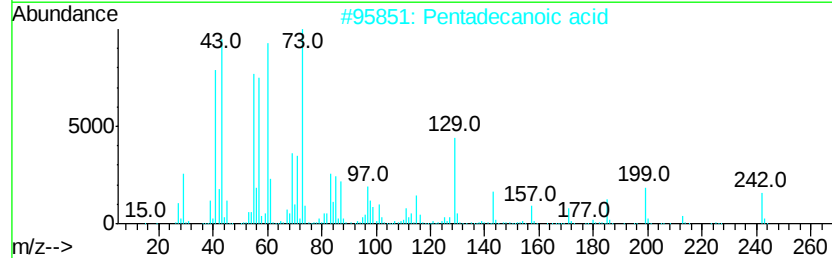
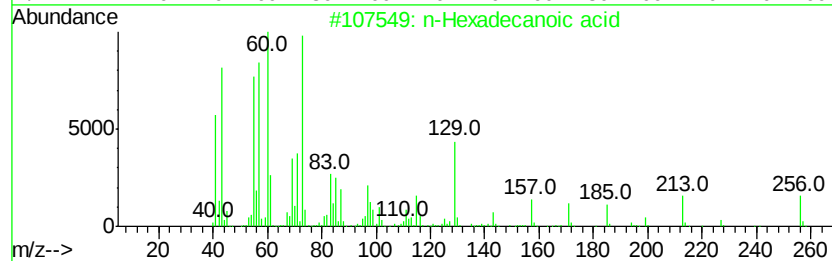
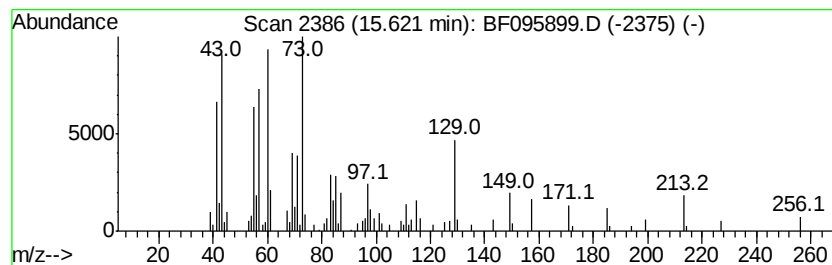
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	7.14 ng	212575	Phenanthrene-d10	14.59

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Undecanoic acid	186	C11H22O2	000112-37-8	68



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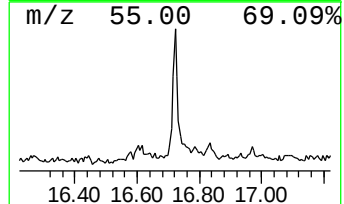
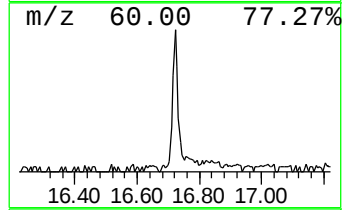
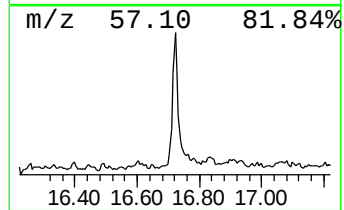
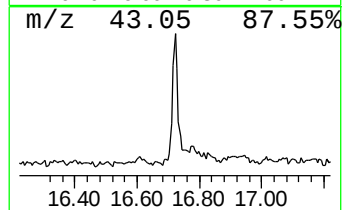
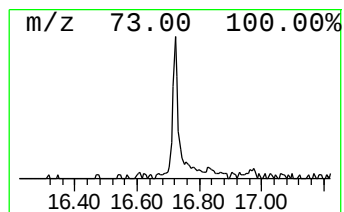
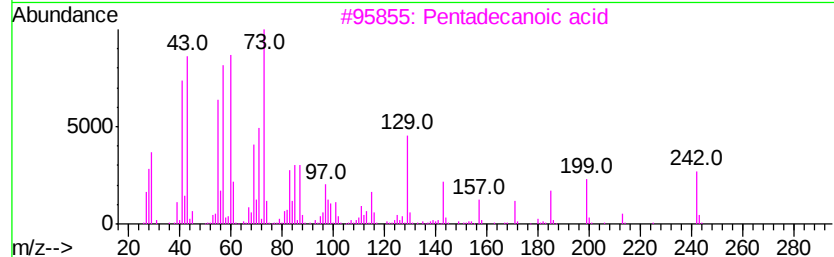
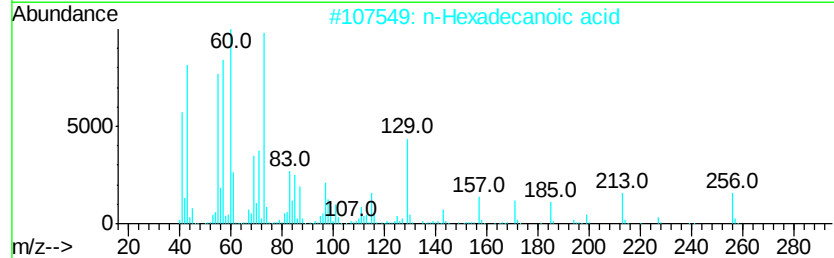
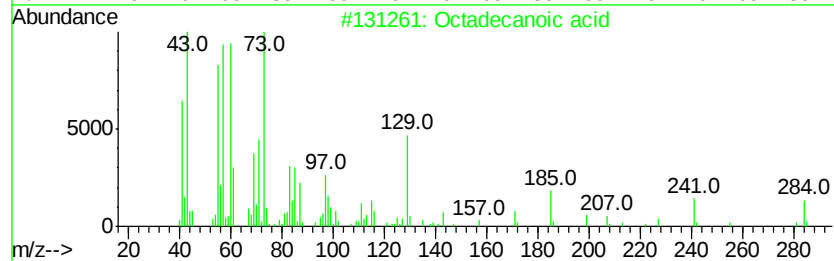
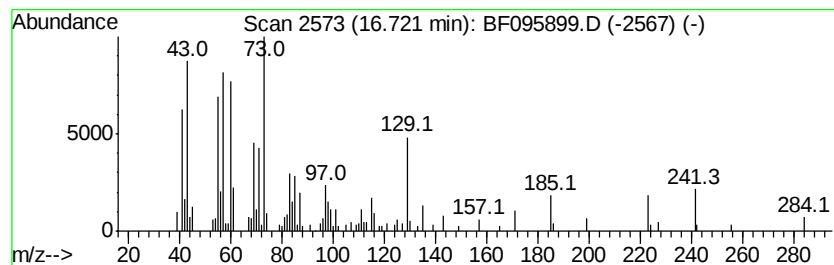
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.72	7.89 ng	187965	Chrysene-d12		18.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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ClientSampleId :
MW-5

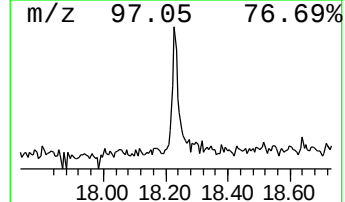
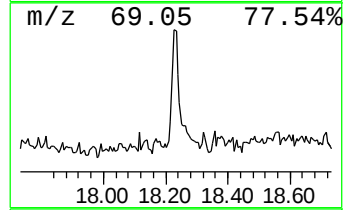
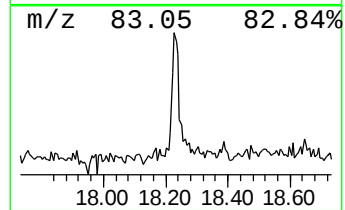
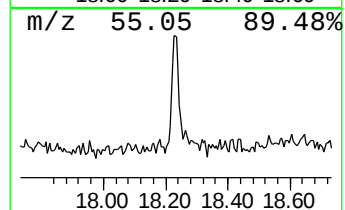
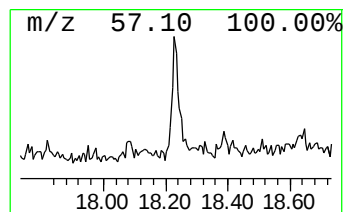
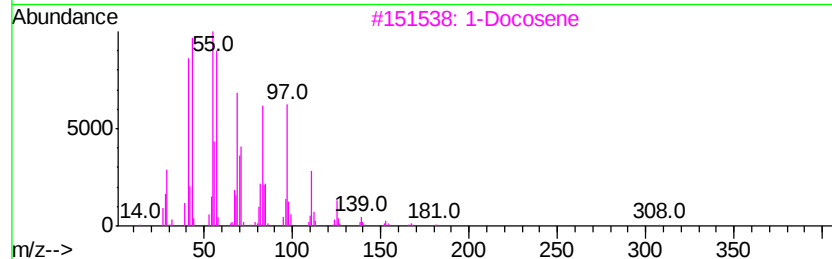
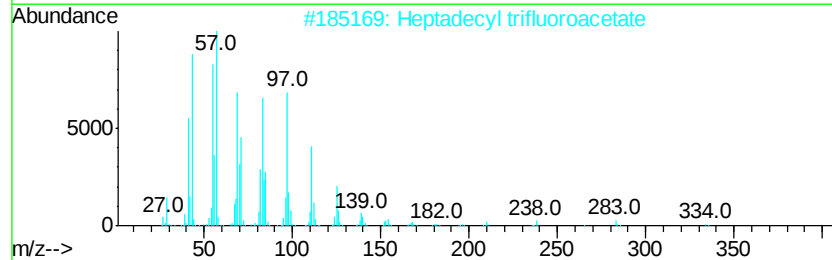
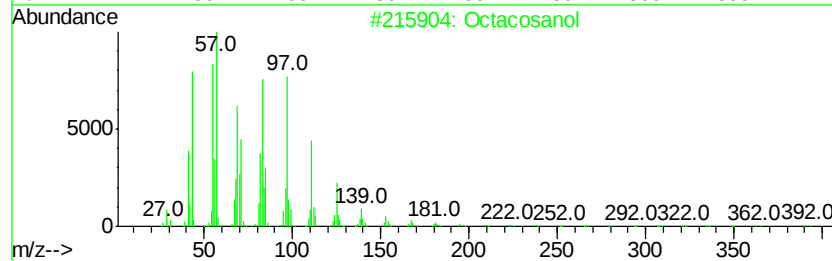
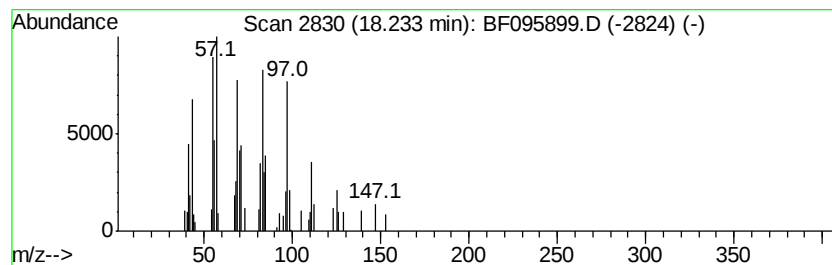
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	3.49 ng	83171	Chrysene-d12	18.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	87
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
3		1-Docosene	308	C22H44	001599-67-3	83
4		1-Nonadecene	266	C19H38	018435-45-5	83
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061317\
Data File : BF095899.D
Acq On : 13 Jun 2017 18:01
Operator : SJ/MA
Sample : I3614-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

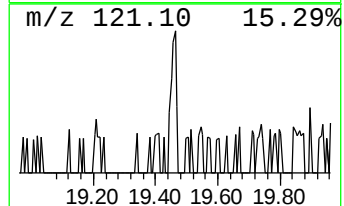
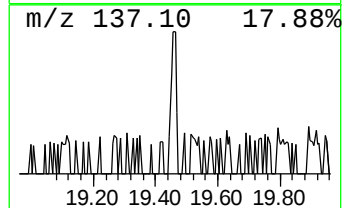
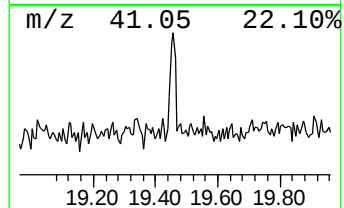
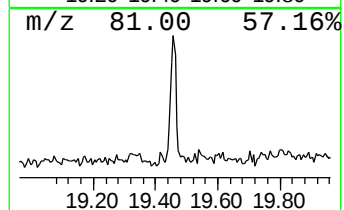
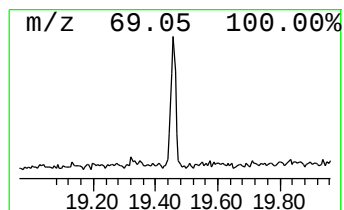
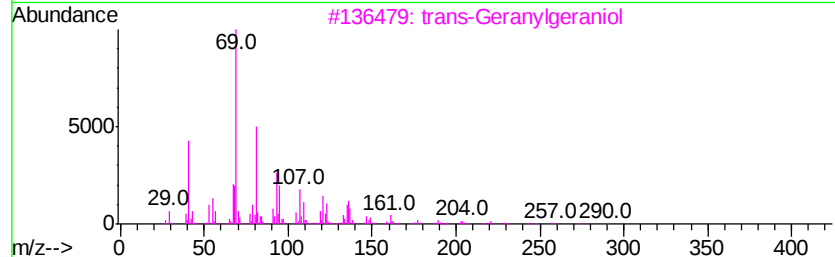
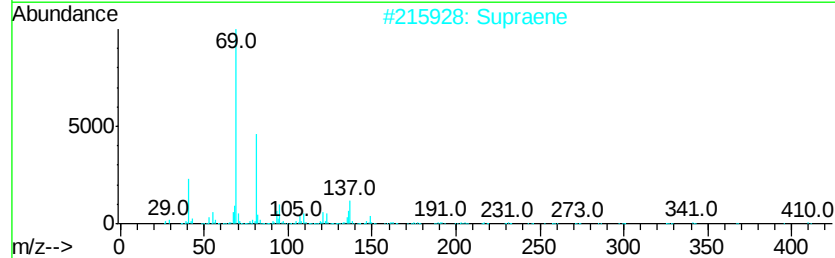
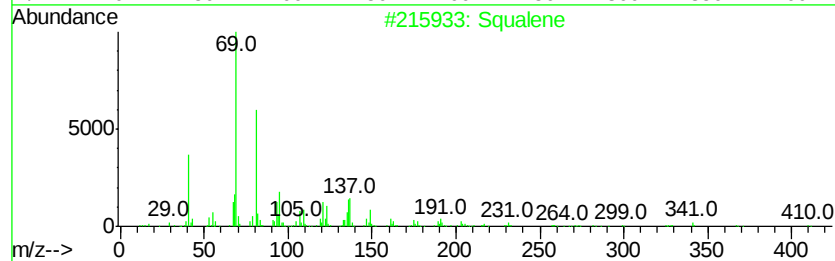
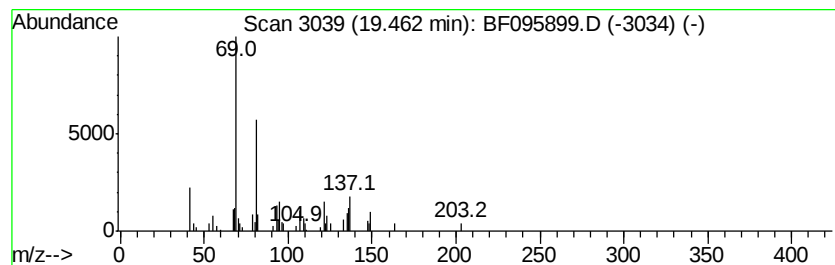
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.46	2.83 ng	49706	Perylene-d12	19.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		Supraene	410	C30H50	007683-64-9	86
3		trans-Geranylgeraniol	290	C20H34O	024034-73-9	59
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	53
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061317\
Data File : BF095899.D
Acq On : 13 Jun 2017 18:01
Operator : SJ/MA
Sample : I3614-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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
2-Pentanone, 4-hy...	4.55	31.5	ng	586711	1	7.35	372850	20.0
unknown7.02	7.02	22.2	ng	414198	1	7.35	372850	20.0
Bicyclo[2.2.1]hep...	8.98	3.0	ng	83303	2	9.38	552289	20.0
n-Hexadecanoic acid	15.62	7.1	ng	212575	4	14.59	595786	20.0
Octadecanoic acid	16.72	7.9	ng	187965	5	18.32	476331	20.0
Octacosanol	18.23	3.5	ng	83171	5	18.32	476331	20.0
Squalene	19.46	2.8	ng	49706	6	19.99	350699	20.0