

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
 Data File : BF101480.D
 Acq On : 18 Dec 2017 15:04
 Operator : SJ/JU
 Sample : I6680-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-02-121417-A

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-BF121417.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	5.034	497	501	521	rBV	919697	1540602	34.53%	3.907%
2	5.439	565	570	586	rBV	3505272	4313005	96.68%	10.938%
3	6.451	737	742	760	rBV	3395777	4461339	100.00%	11.314%
4	6.581	760	764	767	rBV	3888628	4008056	89.84%	10.165%
5	6.804	799	802	811	rBV	1218849	1160982	26.02%	2.944%
6	6.963	825	829	843	rVB	3315271	3243751	72.71%	8.226%
7	7.380	895	900	914	rBV	2515008	2817114	63.15%	7.144%
8	7.480	914	917	924	rVB2	29933	50739	1.14%	0.129%
9	8.092	1017	1021	1038	rVB	1365715	1561903	35.01%	3.961%
10	9.163	1198	1203	1212	rBV	3908839	3920590	87.88%	9.943%
11	9.233	1212	1215	1218	rVB	72756	61847	1.39%	0.157%
12	9.504	1254	1261	1264	rBV4	27753	48635	1.09%	0.123%
13	9.557	1264	1270	1276	rBV	399742	415163	9.31%	1.053%
14	9.710	1291	1296	1300	rBV	44092	57082	1.28%	0.145%
15	9.763	1302	1305	1308	rVB	169633	125904	2.82%	0.319%
16	9.845	1315	1319	1323	rBV	1577700	1392610	31.22%	3.532%
17	9.874	1323	1324	1332	rVB	43338	50281	1.13%	0.128%
18	10.239	1382	1386	1388	rBV	141462	140958	3.16%	0.357%
19	10.263	1388	1390	1393	rVB	210464	157353	3.53%	0.399%
20	10.480	1421	1427	1429	rBV	73210	85335	1.91%	0.216%
21	10.639	1450	1454	1463	rBV	2068023	2104901	47.18%	5.338%
22	10.733	1467	1470	1479	rVB	209938	245229	5.50%	0.622%
23	11.180	1543	1546	1549	rBV	138386	121282	2.72%	0.308%
24	11.333	1569	1572	1575	rBV	1252635	1213389	27.20%	3.077%
25	11.357	1575	1576	1581	rVV	205616	176360	3.95%	0.447%
26	11.610	1616	1619	1625	rVB	108682	91853	2.06%	0.233%
27	11.851	1655	1660	1667	rBV4	141276	243268	5.45%	0.617%
28	11.951	1674	1677	1680	rBV2	48006	55984	1.25%	0.142%
29	12.015	1685	1688	1690	rBV	76016	57611	1.29%	0.146%
30	12.404	1748	1754	1759	rBV4	74210	154436	3.46%	0.392%
31	12.551	1776	1779	1784	rBV	188908	196016	4.39%	0.497%
32	12.639	1791	1794	1799	rVB4	38319	55080	1.23%	0.140%
33	12.780	1815	1818	1825	rVB	181405	240718	5.40%	0.610%
34	12.921	1837	1842	1845	rBV	2857763	2623019	58.79%	6.652%

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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 >
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35	13.804	1988	1992	1996	rBV	392752	474796	10.64%	1.204%
36	13.986	2019	2023	2026	rBV	1028703	987075	22.13%	2.503%
37	15.456	2270	2273	2281	rVB	589024	777037	17.42%	1.971%

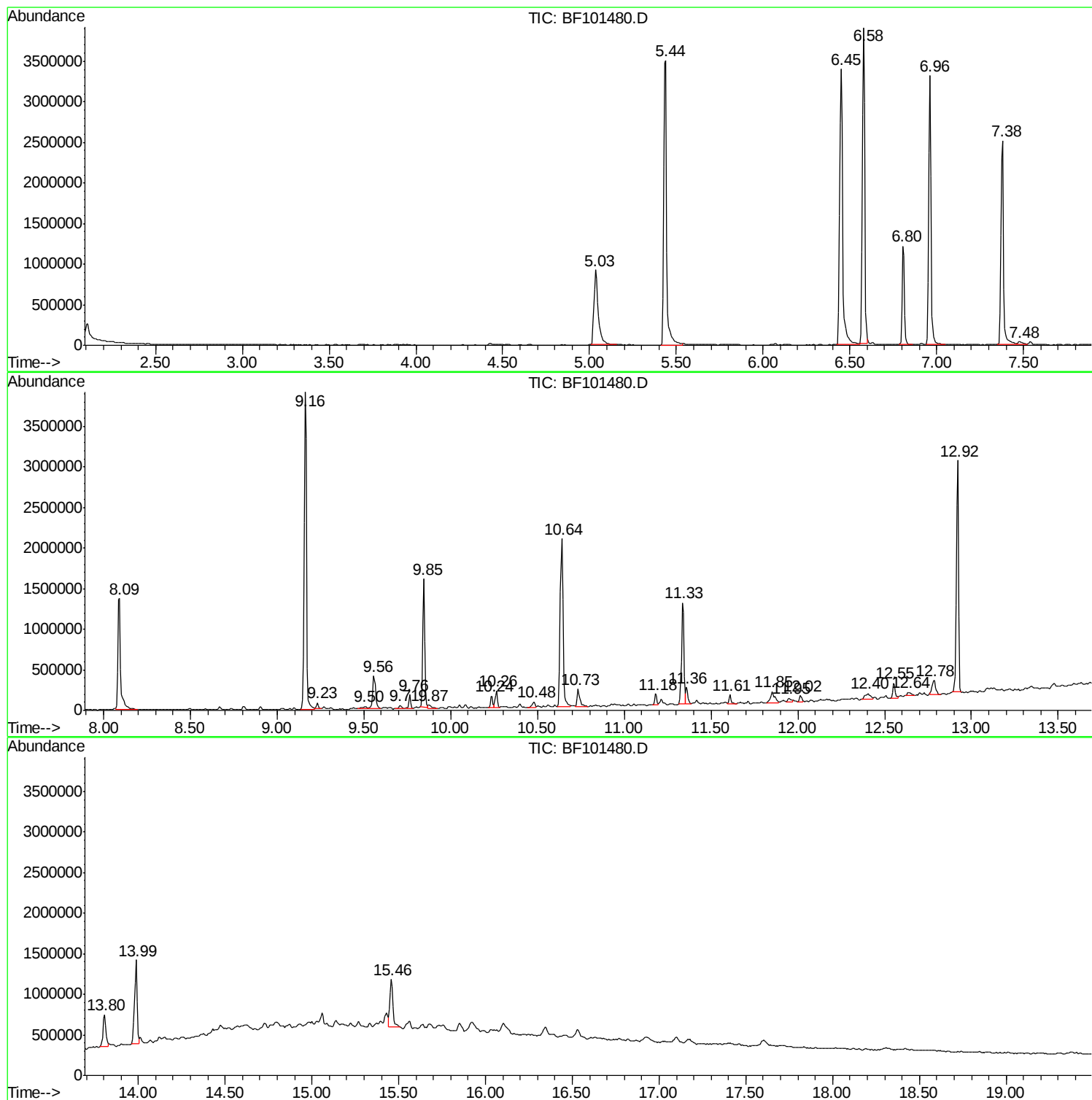
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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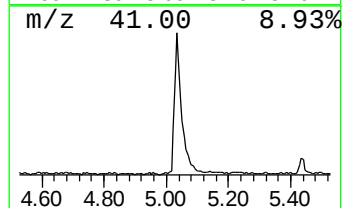
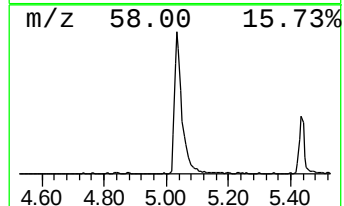
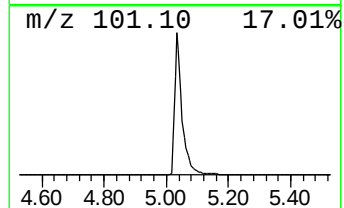
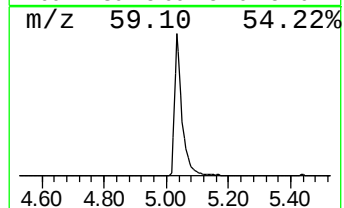
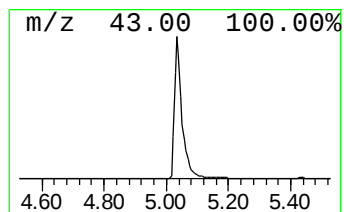
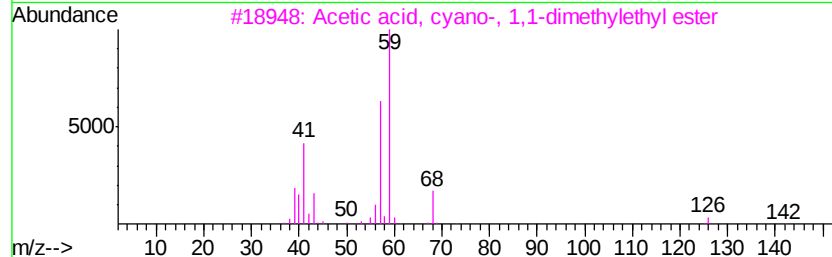
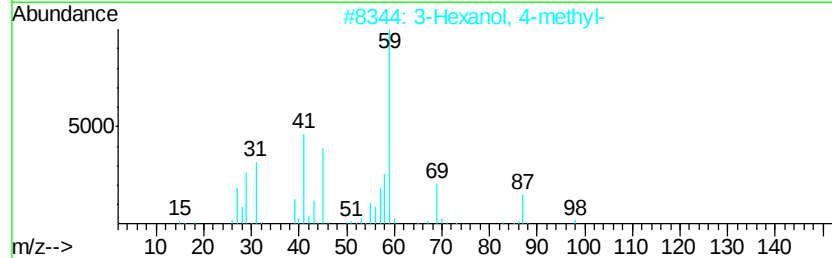
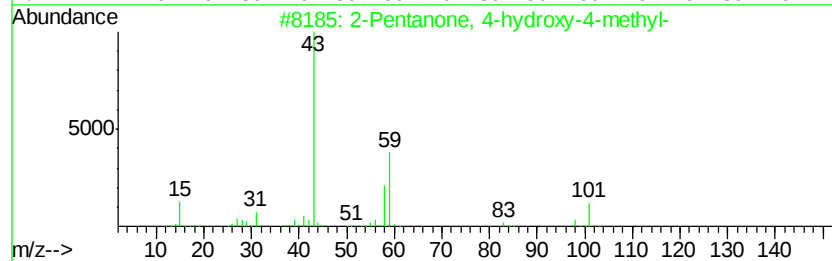
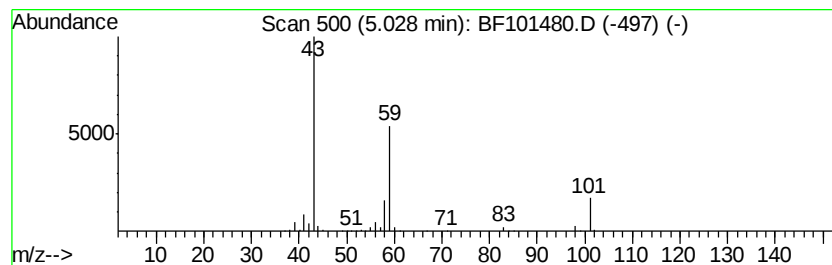
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.03 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	26.54 ng	1540600	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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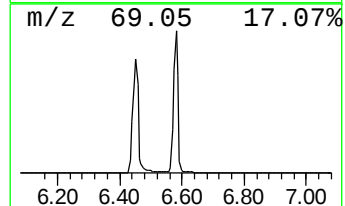
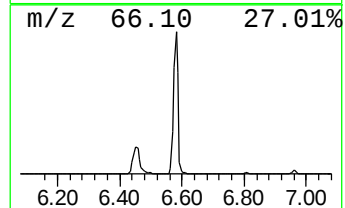
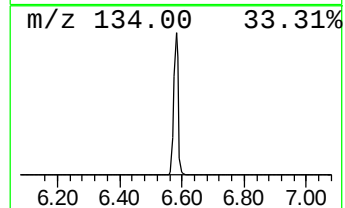
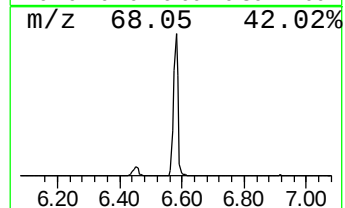
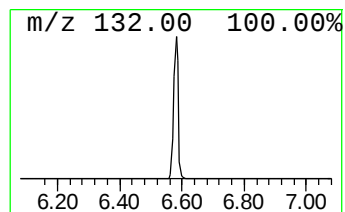
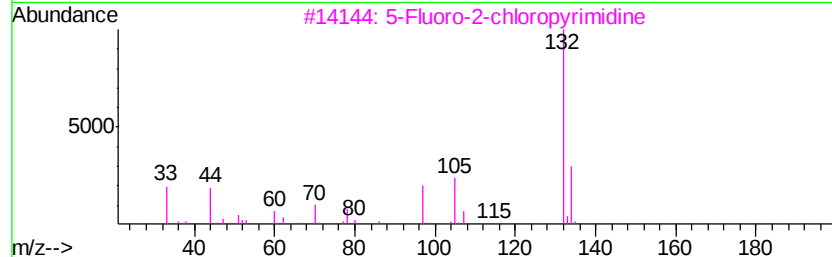
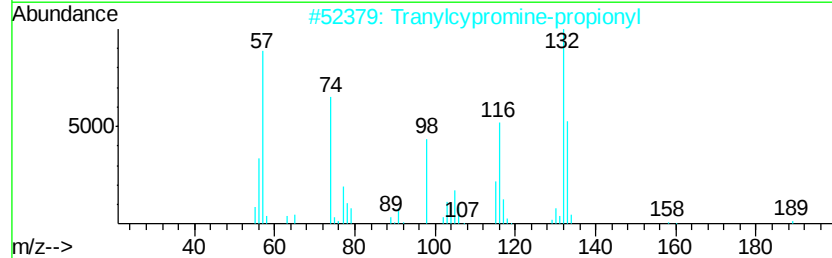
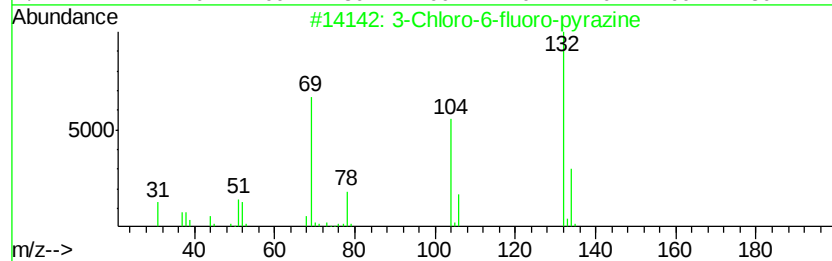
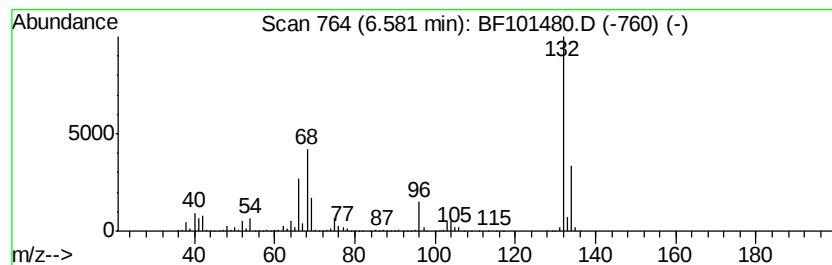
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	69.05 ng	4008060	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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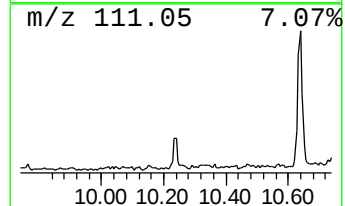
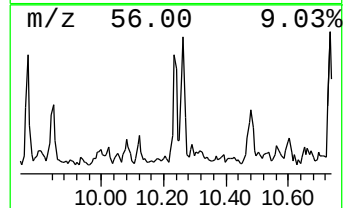
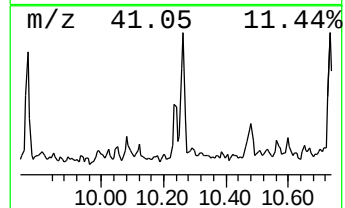
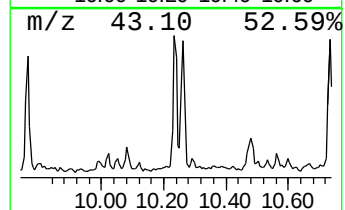
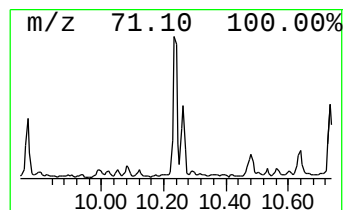
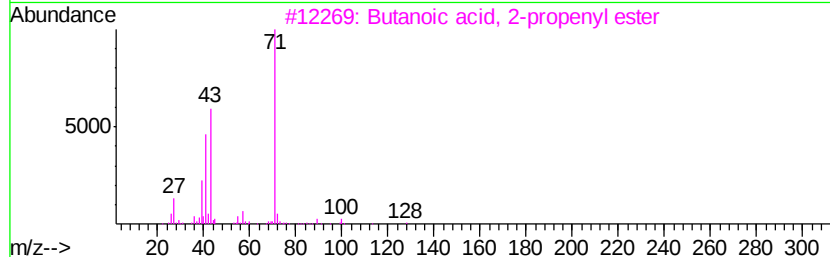
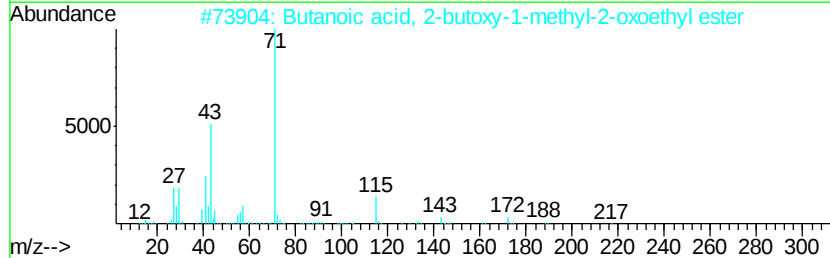
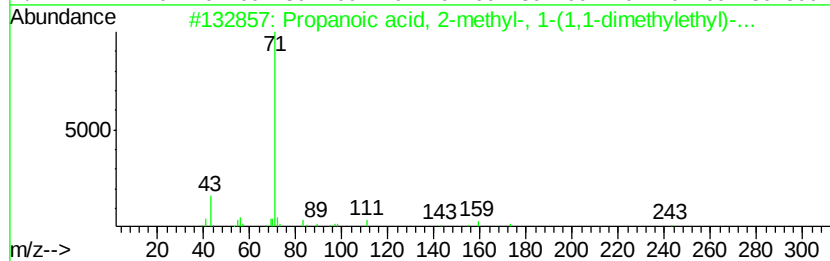
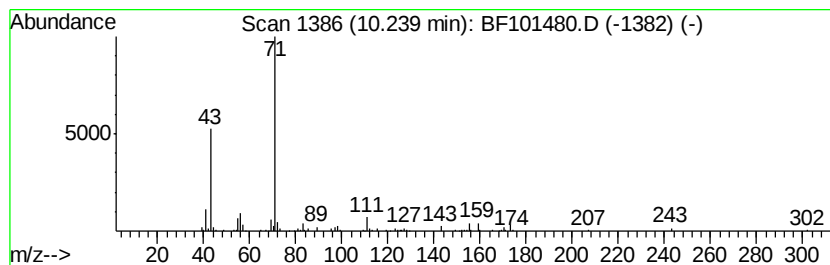
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.24	2.02 ng	140958	Acenaphthene-d10	9.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	78	
2	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	64	
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	53	
4	Methylamine, N-(1-methylhexylid...	127	C8H17N	022058-71-5	53	
5	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	53	



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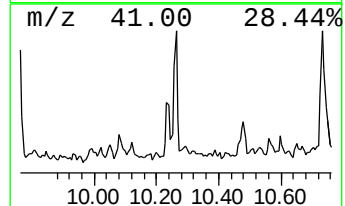
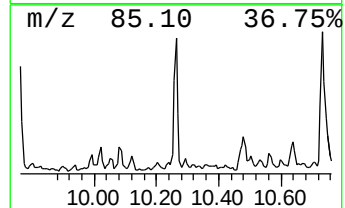
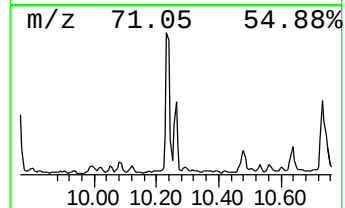
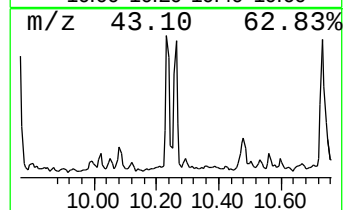
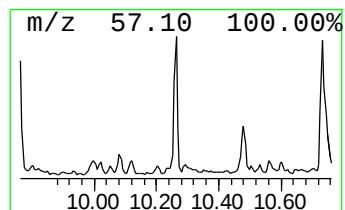
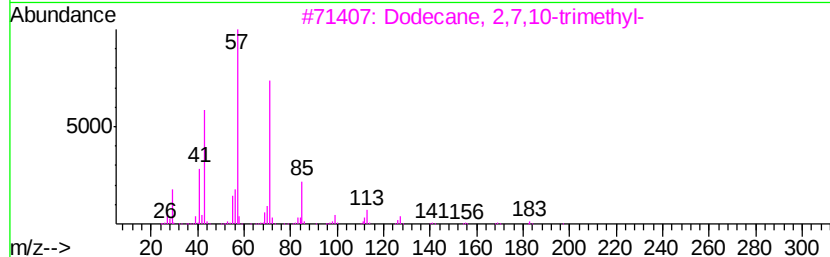
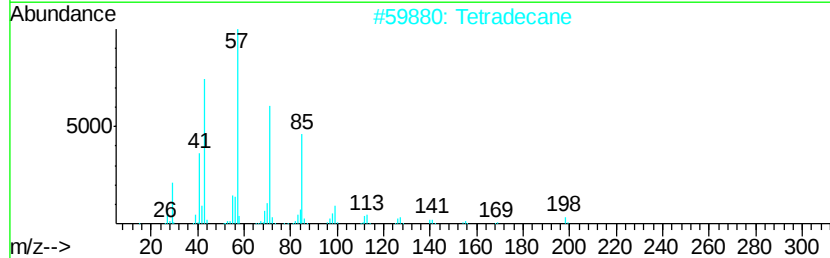
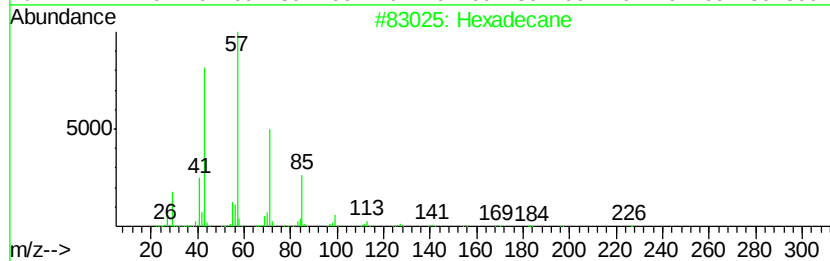
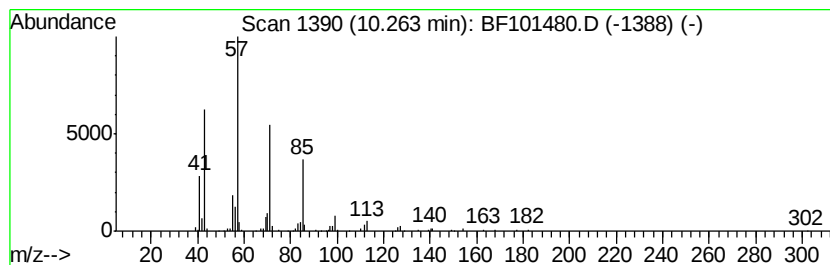
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Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.26 ng	157353	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	86
2	Tetradecane	198 C14H30	000629-59-4	78
3	Dodecane, 2,7,10-trimethyl-	212 C15H32	074645-98-0	64
4	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	64
5	Heptacosane	380 C27H56	000593-49-7	59



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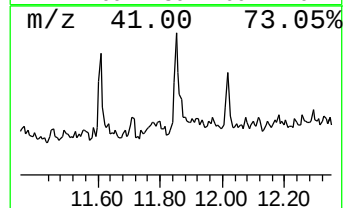
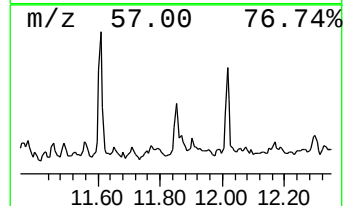
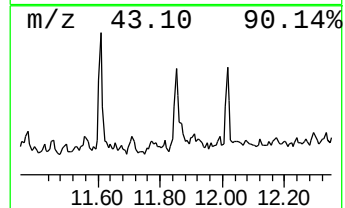
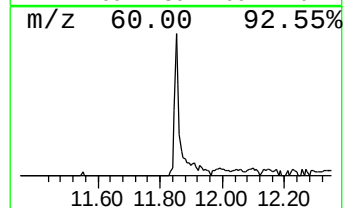
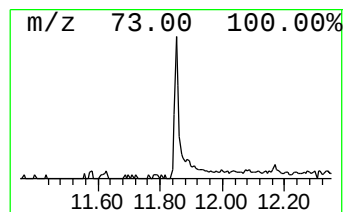
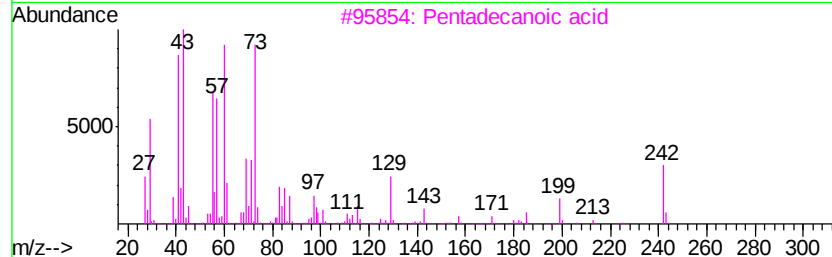
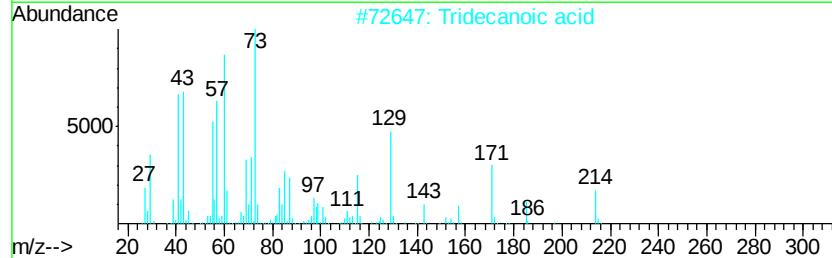
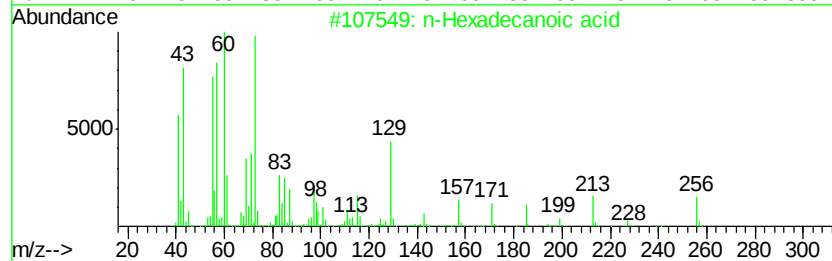
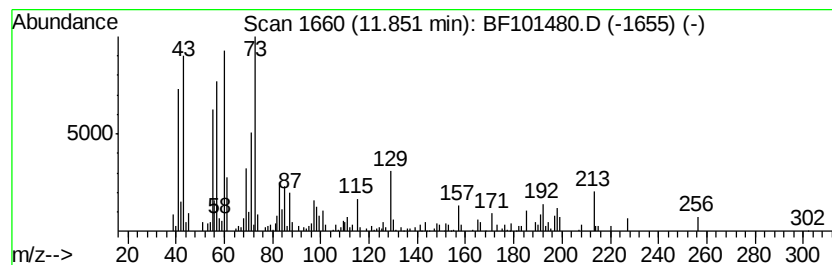
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	4.01 ng	243268	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101480.D
Acq On : 18 Dec 2017 15:04
Operator : SJ/JU
Sample : I6680-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-121417-A

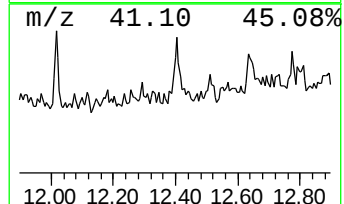
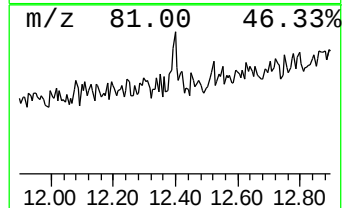
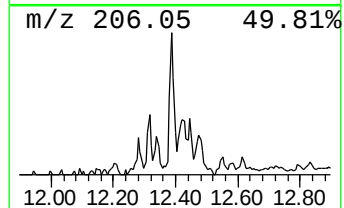
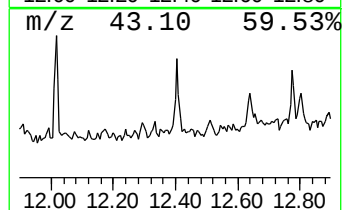
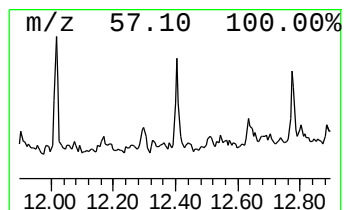
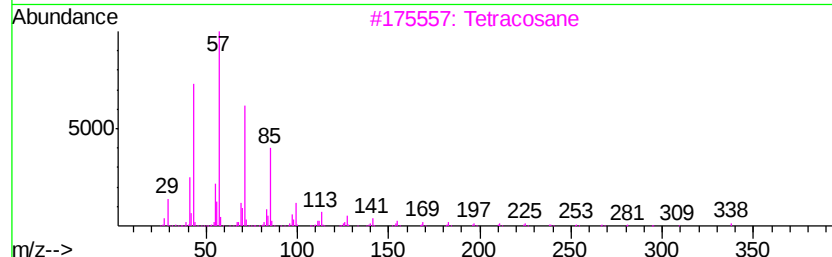
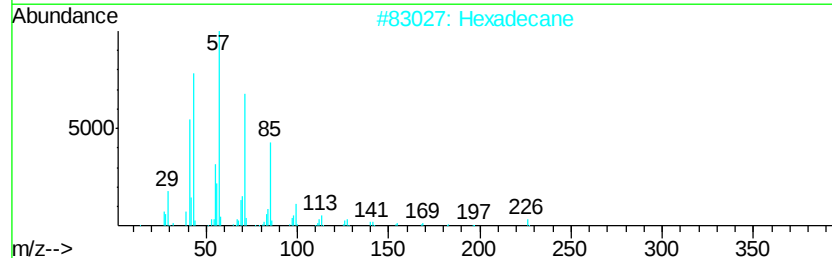
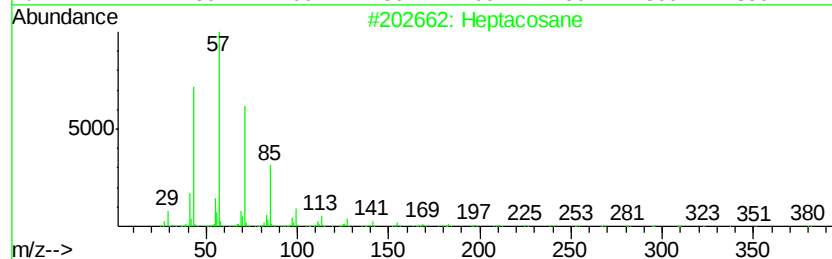
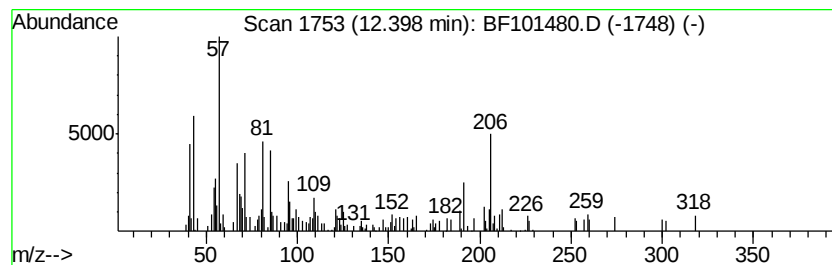
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	2.55 ng	154436	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	74
2	Hexadecane		226	C16H34	000544-76-3	74
3	Tetracosane		338	C24H50	000646-31-1	72
4	Hexacosane		366	C26H54	000630-01-3	72
5	Pentadecane		212	C15H32	000629-62-9	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101480.D
Acq On : 18 Dec 2017 15:04
Operator : SJ/JU
Sample : I6680-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

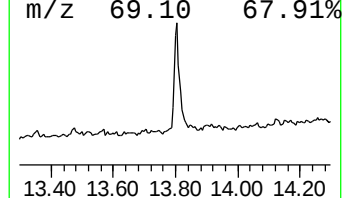
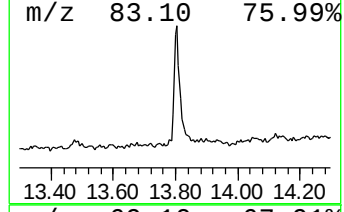
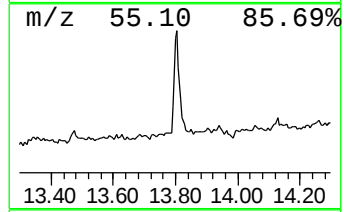
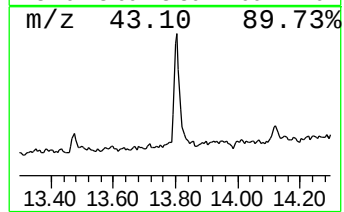
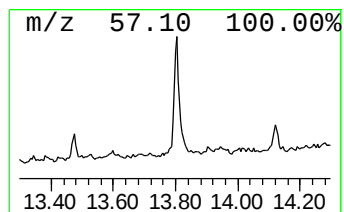
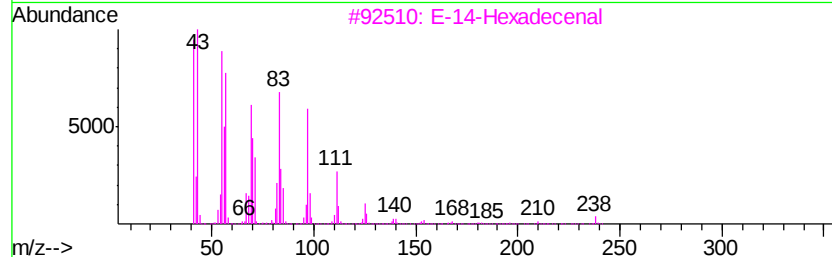
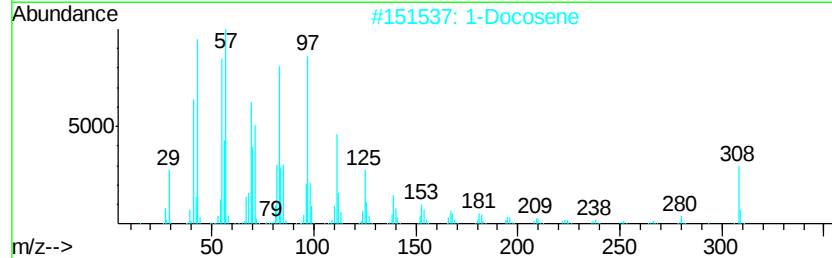
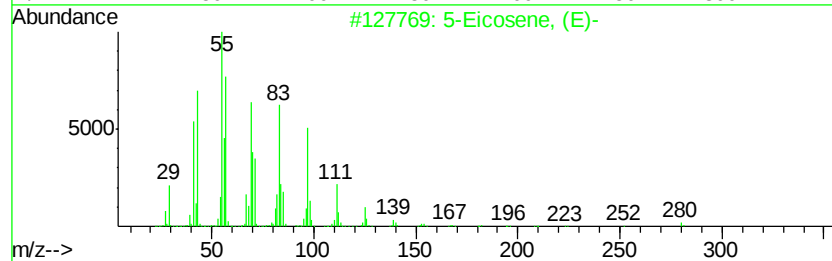
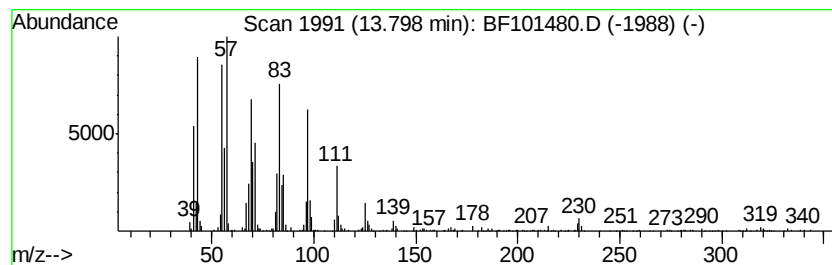
Instrument :
BNA_F
ClientSampleId :
CL-02-121417-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.80	9.62 ng	474796	Chrysene-d12		13.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	E-14-Hexadecenal	238	C16H30O	330207-53-9	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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Sample : I6680-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-121417-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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
unknown5.03	5.03	26.5	ng	1540600	1	6.80	1160980	20.0
unknown6.58	6.58	69.0	ng	4008060	1	6.80	1160980	20.0
Propanoic acid, 2...	10.24	2.0	ng	140958	3	9.85	1392610	20.0
Hexadecane	10.26	2.3	ng	157353	3	9.85	1392610	20.0
n-Hexadecanoic acid	11.85	4.0	ng	243268	4	11.33	1213390	20.0
Heptacosane	12.40	2.5	ng	154436	4	11.33	1213390	20.0
5-Eicosene, (E)-	13.80	9.6	ng	474796	5	13.99	987075	20.0