

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096566.D
 Acq On : 7 Jul 2017 18:32
 Operator : SJ/MA
 Sample : I4064-12
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF009-01

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-BF070117.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	4.881	470	475	485	rVB	356988	435381	20.18%	2.104%
2	5.310	543	548	551	rBV	2133820	2074170	96.12%	10.024%
3	6.334	717	722	725	rBV	2186963	2105125	97.56%	10.174%
4	6.463	740	744	748	rBV	2245659	2038262	94.46%	9.851%
5	6.692	780	783	787	rVB	738043	636473	29.50%	3.076%
6	6.851	806	810	813	rBV	1835252	1570740	72.79%	7.591%
7	7.251	874	878	881	rBV	1369875	1325220	61.41%	6.405%
8	7.357	890	896	901	rVB	31842	38544	1.79%	0.186%
9	7.975	997	1001	1005	rBV	997831	878375	40.71%	4.245%
10	9.051	1179	1184	1188	rBV	2256822	2157856	100.00%	10.429%
11	9.445	1247	1251	1254	rBV	410641	321413	14.90%	1.553%
12	9.727	1294	1299	1303	rVB	1098734	933754	43.27%	4.513%
13	10.139	1365	1369	1373	rBV2	131099	164597	7.63%	0.795%
14	10.174	1373	1375	1377	rVB	33471	23739	1.10%	0.115%
15	10.510	1427	1432	1436	rBV	1232547	1141754	52.91%	5.518%
16	10.645	1448	1455	1462	rBV	52449	68684	3.18%	0.332%
17	11.092	1527	1531	1534	rBV2	40277	36649	1.70%	0.177%
18	11.204	1546	1550	1554	rVB	1001188	878610	40.72%	4.246%
19	11.745	1637	1642	1645	rBV	106509	103849	4.81%	0.502%
20	11.774	1645	1647	1652	rVB	19759	22344	1.04%	0.108%
21	12.527	1770	1775	1781	rBV2	30721	36661	1.70%	0.177%
22	12.621	1787	1791	1796	rBV2	42427	43865	2.03%	0.212%
23	12.792	1815	1820	1823	rBV	1893806	1771553	82.10%	8.562%
24	13.327	1908	1911	1913	rBV	30653	27742	1.29%	0.134%
25	13.692	1970	1973	1980	rBV	227479	226907	10.52%	1.097%
26	13.833	1993	1997	2002	rVB	772286	678783	31.46%	3.280%
27	14.327	2077	2081	2086	rBV3	25877	34617	1.60%	0.167%
28	14.592	2122	2126	2129	rBV	158376	160732	7.45%	0.777%
29	14.686	2139	2142	2145	rBV	76024	66280	3.07%	0.320%
30	14.933	2181	2184	2189	rBV5	17970	22610	1.05%	0.109%
31	15.233	2230	2235	2241	rBV	496772	579553	26.86%	2.801%
32	15.686	2308	2312	2316	rBV	19682	31285	1.45%	0.151%
33	15.721	2316	2318	2325	rVB8	19257	33667	1.56%	0.163%
34	16.151	2387	2391	2395	rVB5	14379	22065	1.02%	0.107%

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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

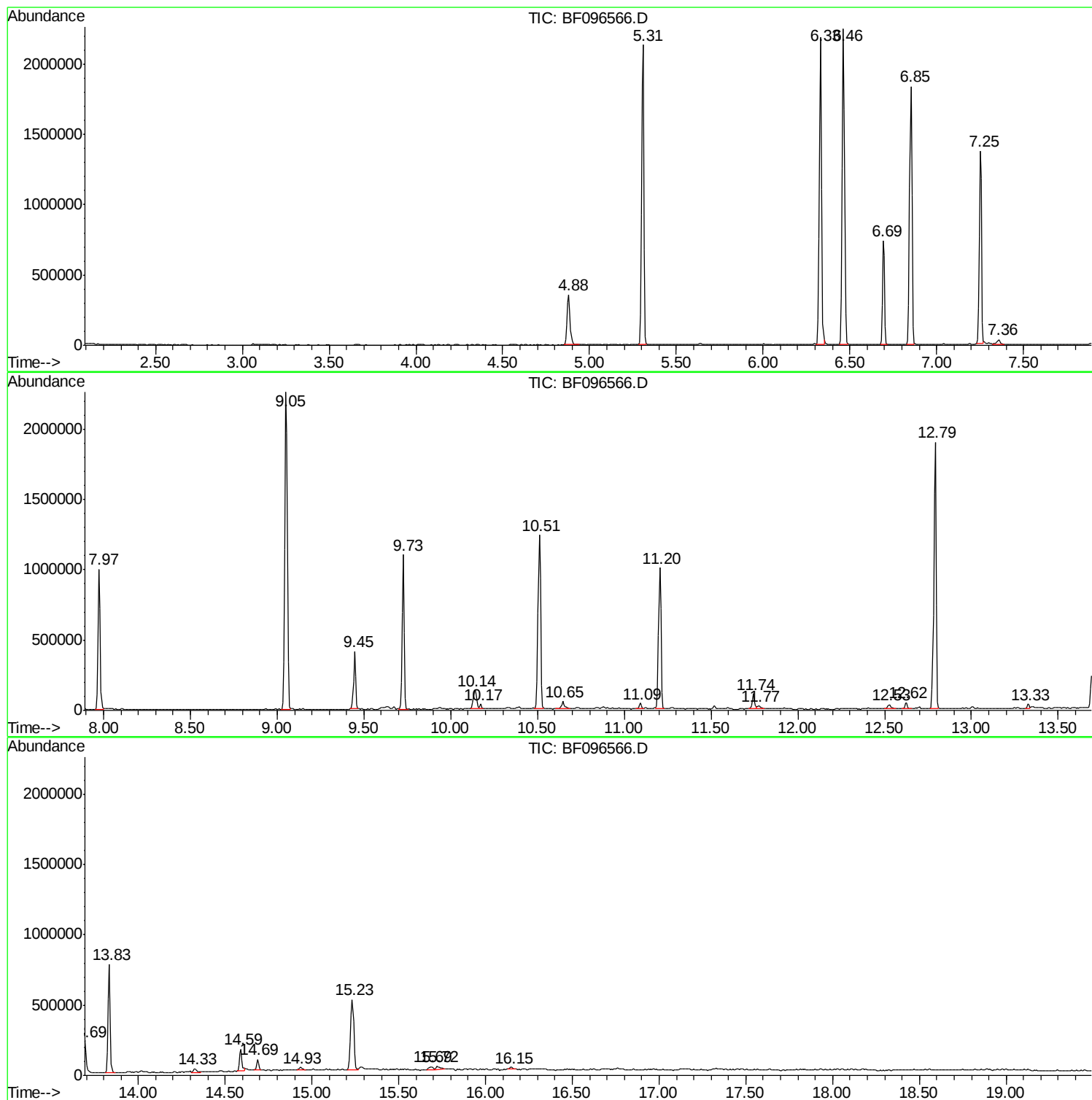
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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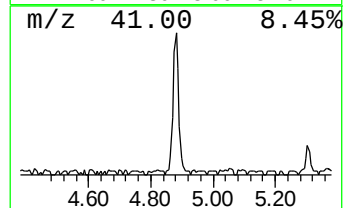
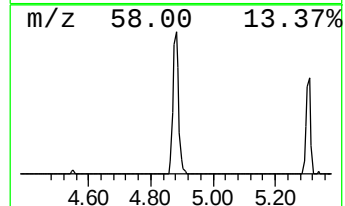
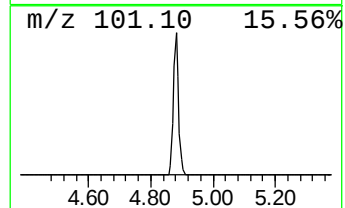
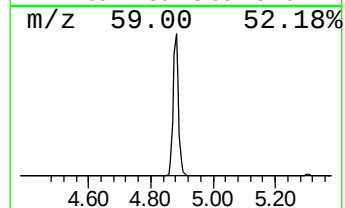
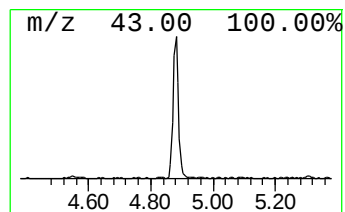
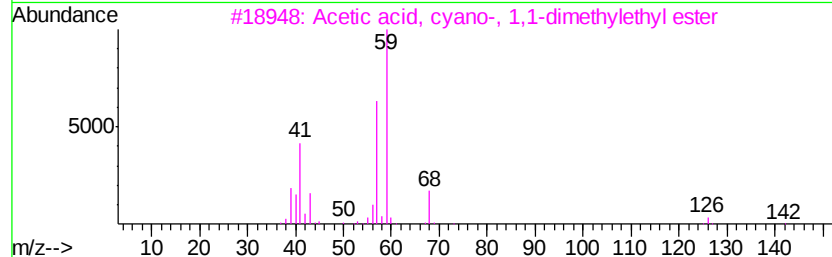
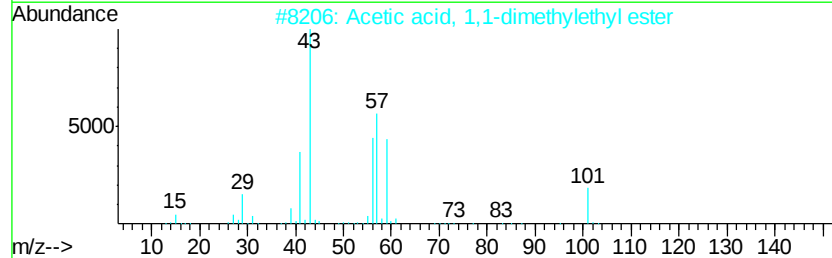
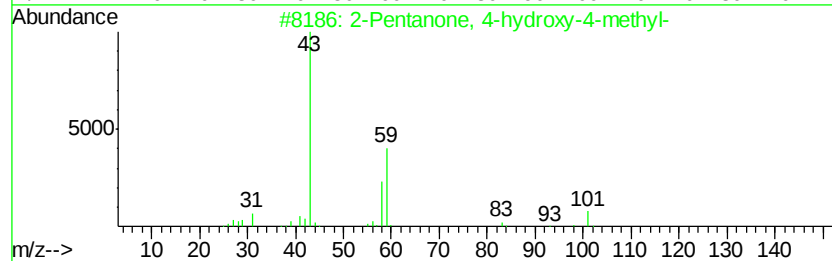
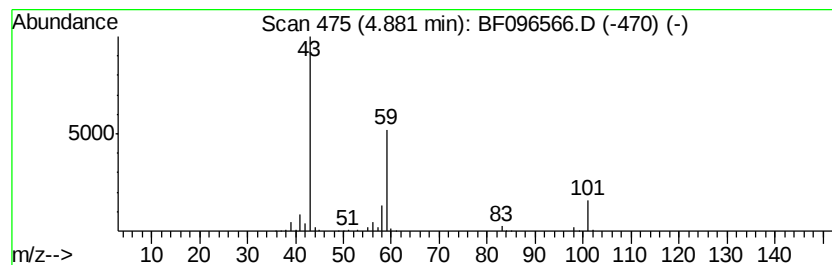
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.88 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	13.68 ng	435381	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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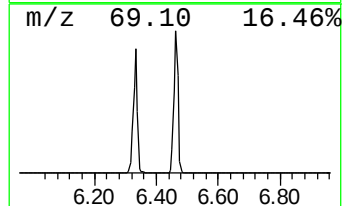
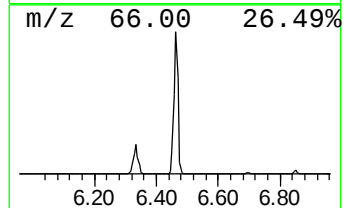
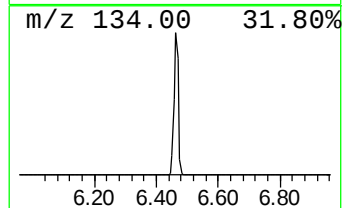
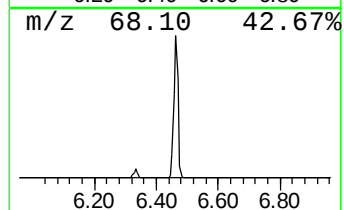
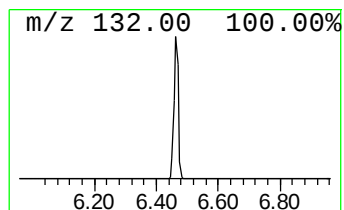
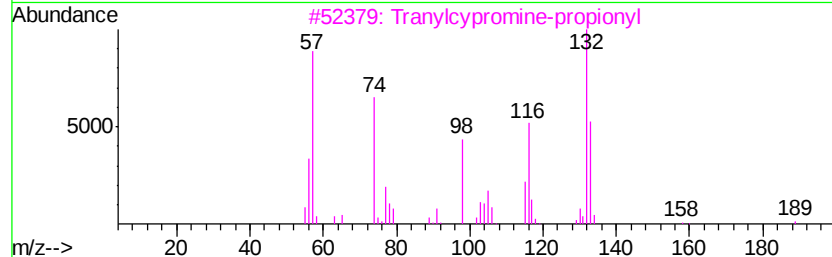
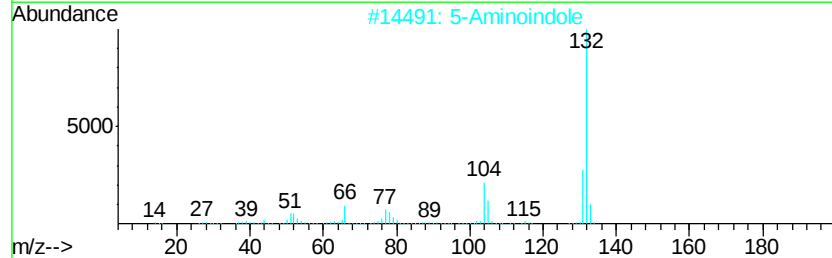
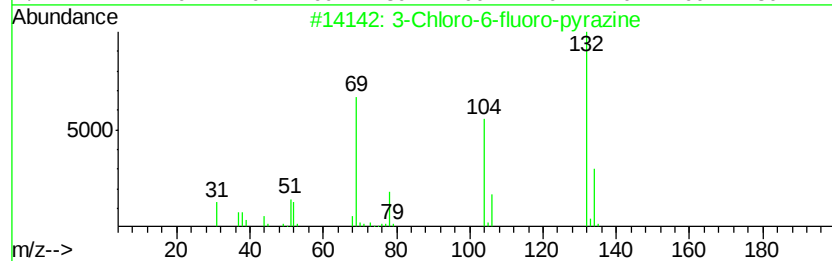
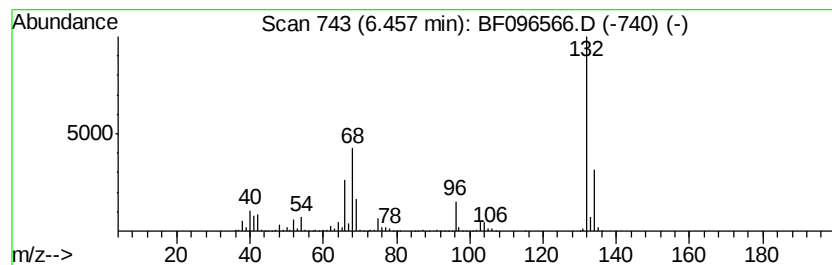
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	64.05 ng	2038260	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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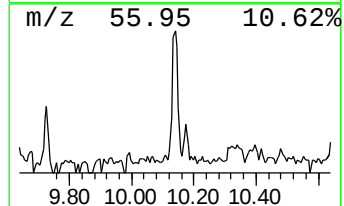
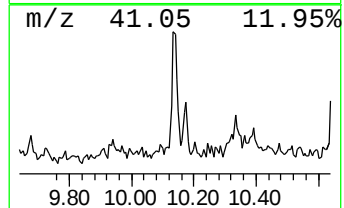
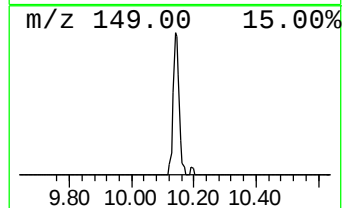
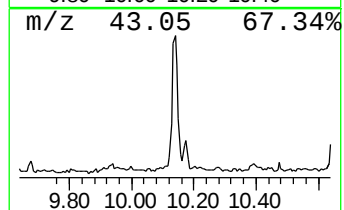
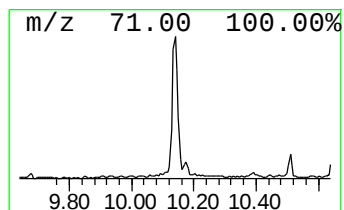
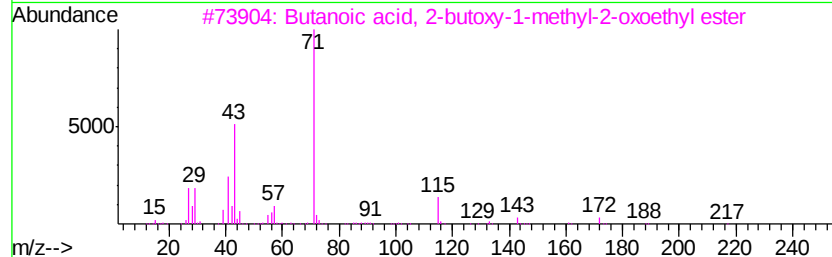
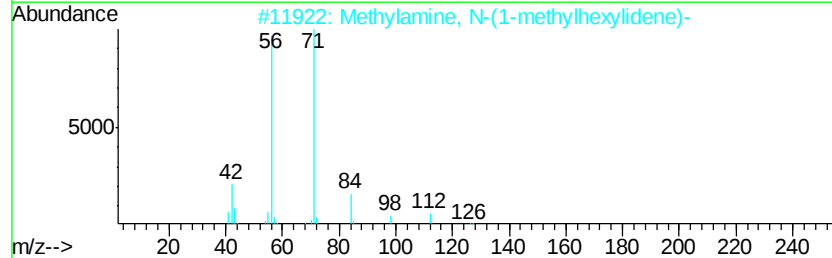
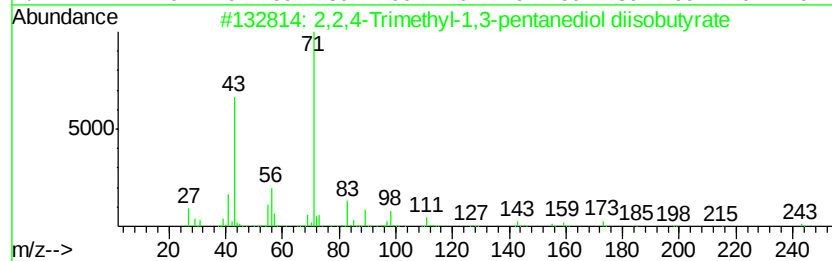
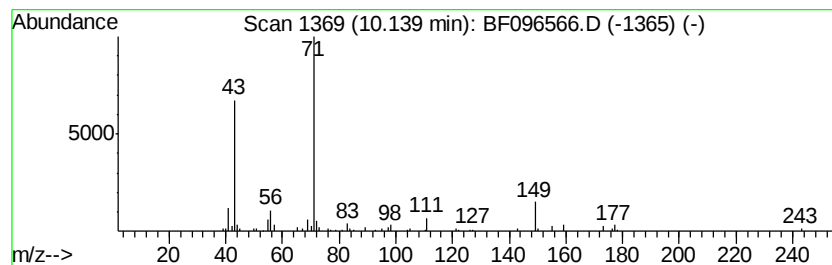
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	3.53 ng	164597	Acenaphthene-d10	9.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
2			Methylamine, N-(1-methylhexylidene)...	127	C8H17N	022058-71-5	50
3			Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	45
4			Oxalic acid, neopentyl nonyl ester	286	C16H30O4	1000309-73-3	45
5			3-Methyl-hepta-1,6-dien-3-ol	126	C8H14O	034780-69-3	42



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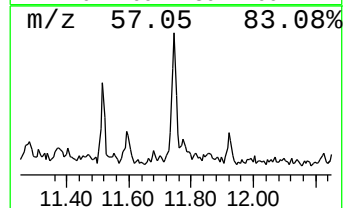
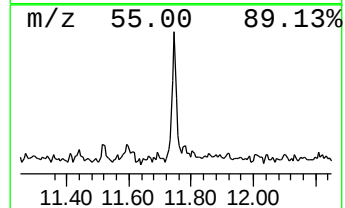
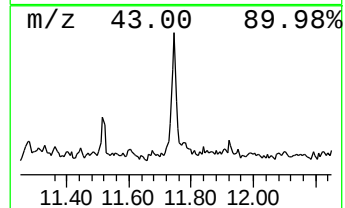
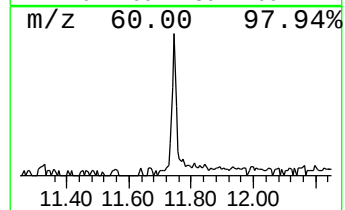
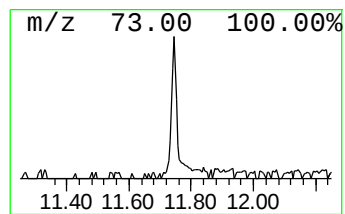
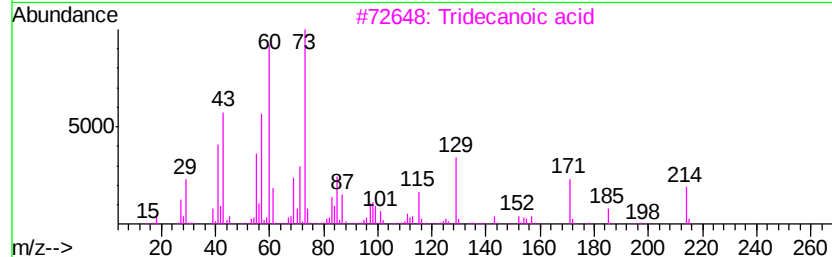
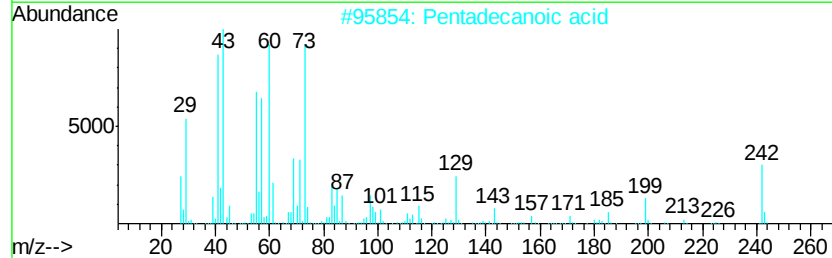
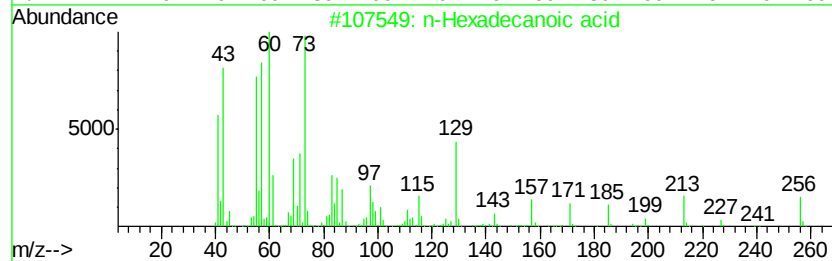
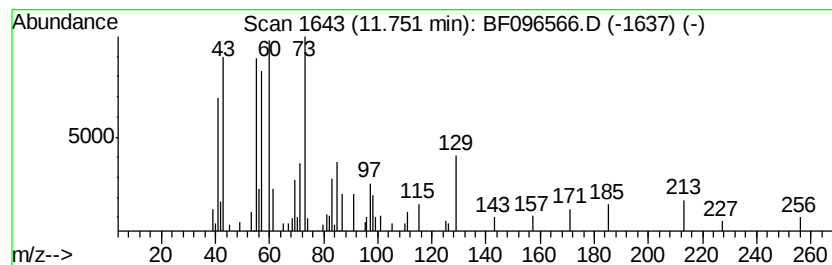
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.75	2.36 ng	103849	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	18



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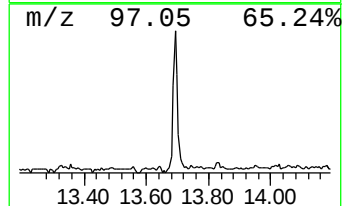
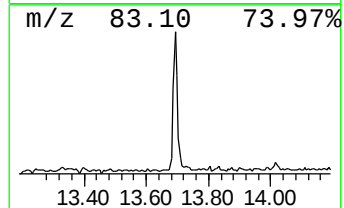
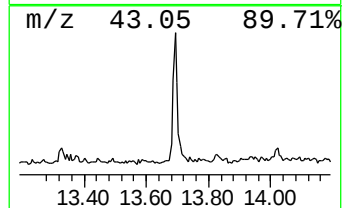
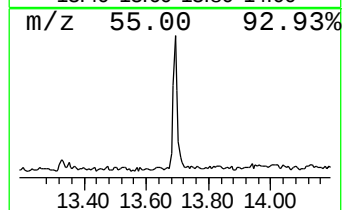
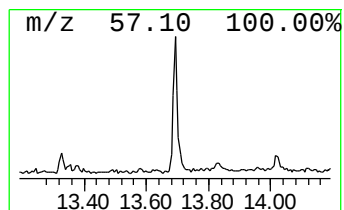
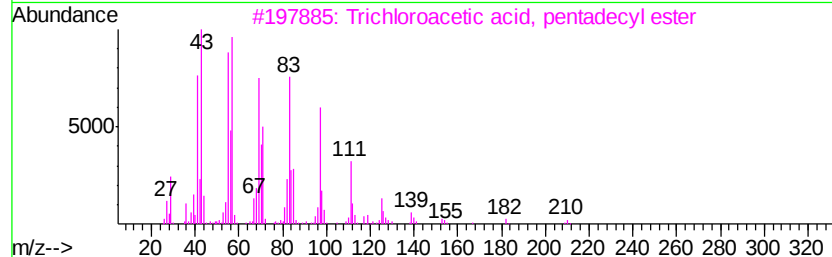
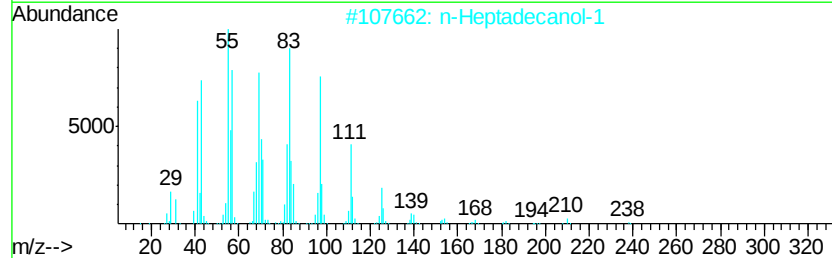
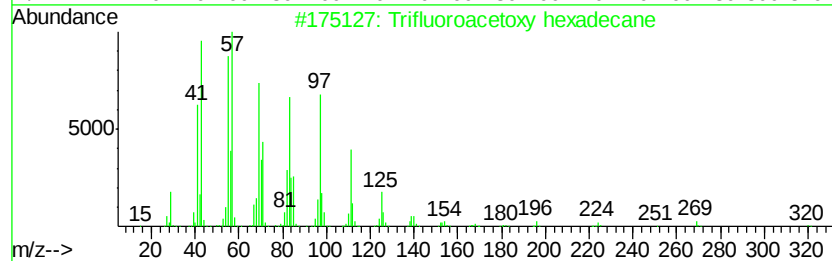
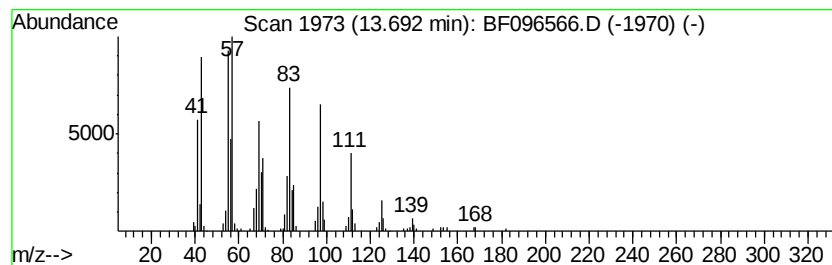
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	6.69 ng	226907	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90



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ClientSampleId :
PET-BF009-01

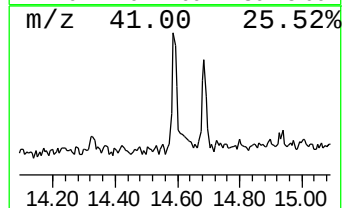
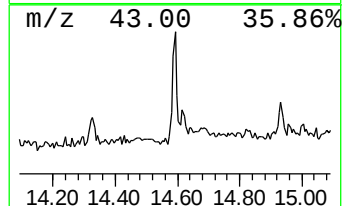
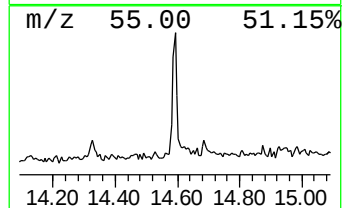
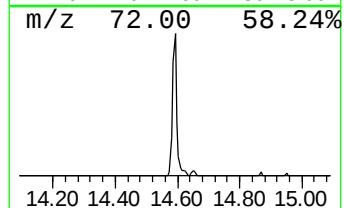
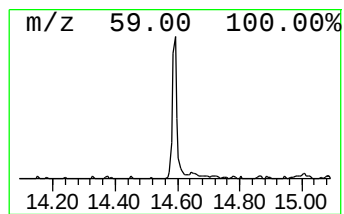
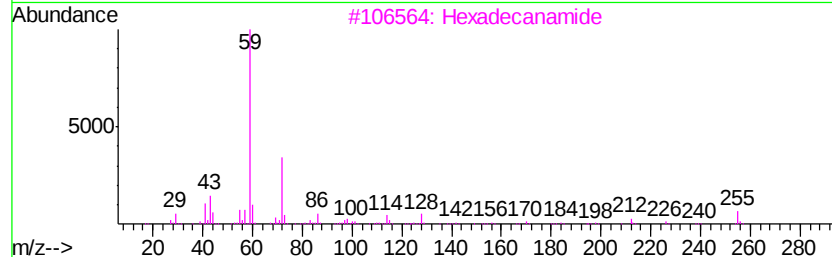
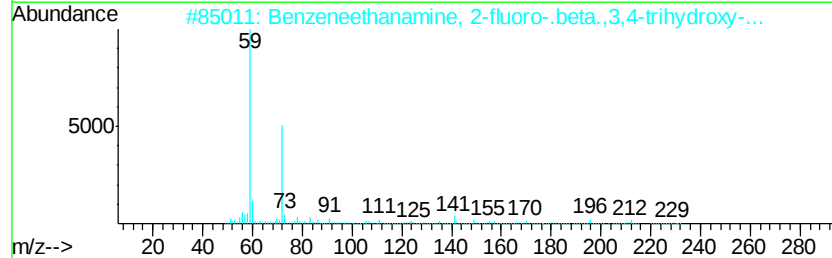
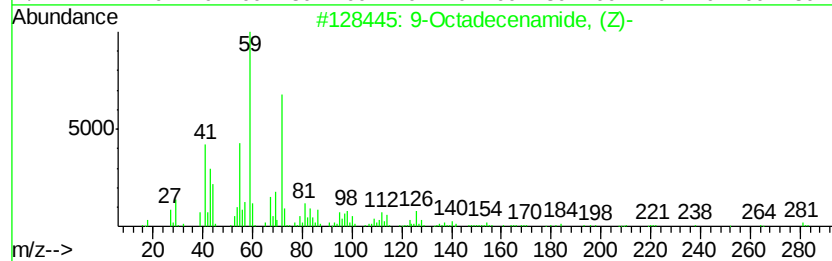
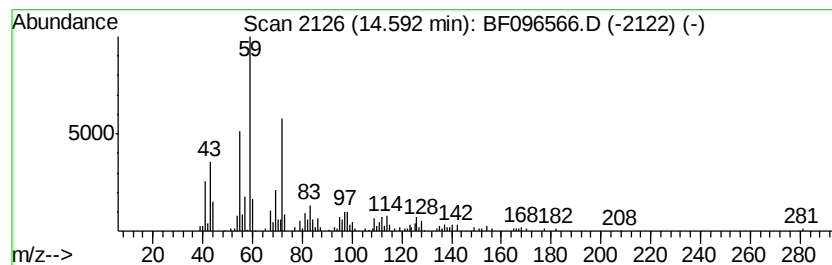
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	5.55 ng	160732	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
5		Decanamide-	171	C10H21NO	002319-29-1	50



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096566.D
Acq On : 7 Jul 2017 18:32
Operator : SJ/MA
Sample : I4064-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF009-01

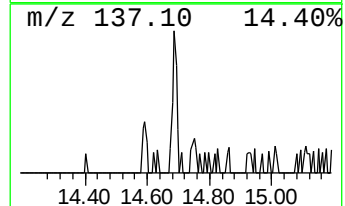
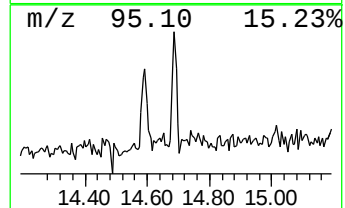
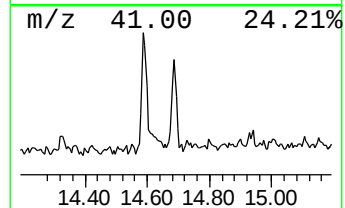
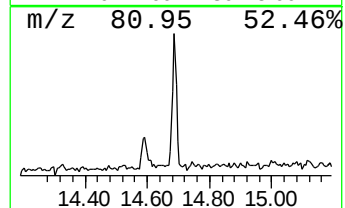
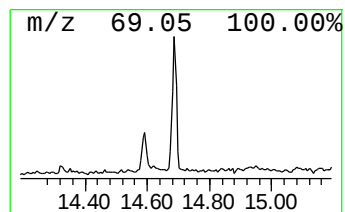
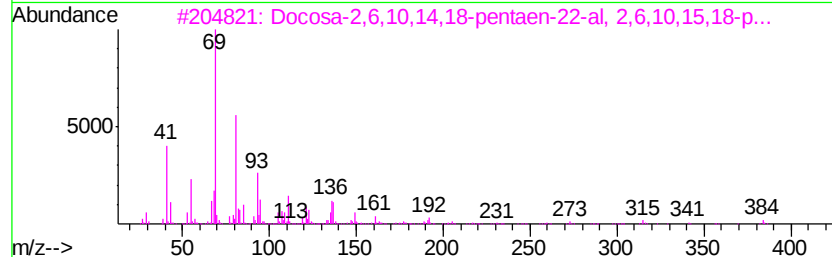
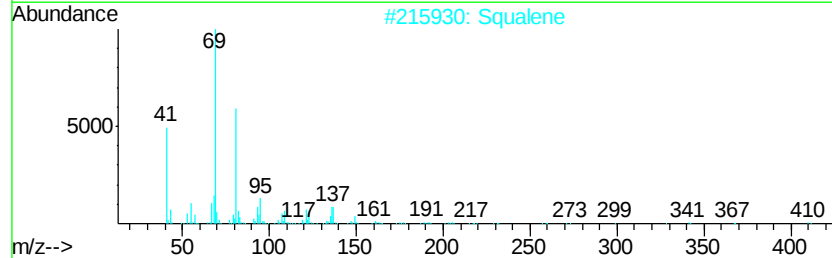
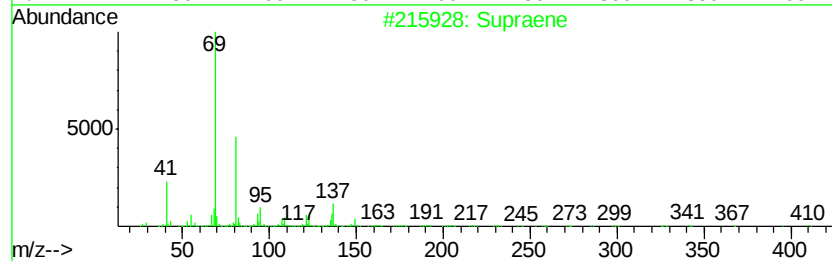
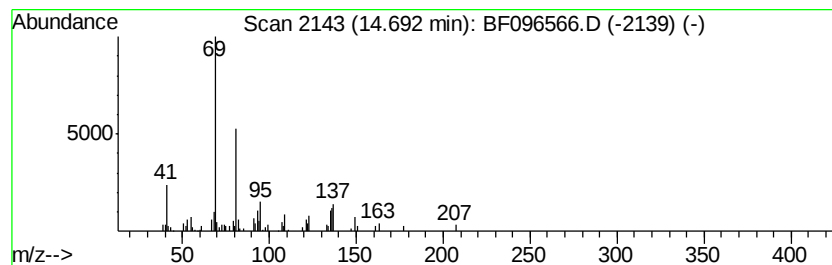
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.29 ng	66280	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
5		6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	59



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096566.D
Acq On : 7 Jul 2017 18:32
Operator : SJ/MA
Sample : I4064-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF009-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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
unknown4.88	4.88	13.7	ng	435381	1	6.69	636473	20.0
unknown6.46	6.46	64.0	ng	2038260	1	6.69	636473	20.0
2,2,4-Trimethyl-1...	10.14	3.5	ng	164597	3	9.73	933754	20.0
n-Hexadecanoic acid	11.75	2.4	ng	103849	4	11.20	878610	20.0
Trifluoroacetoxy ...	13.69	6.7	ng	226907	5	13.83	678783	20.0
9-Octadecenamide,...	14.59	5.5	ng	160732	6	15.23	579553	20.0
Supraene	14.69	2.3	ng	66280	6	15.23	579553	20.0