LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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	4.869	470	473	482	rBV	25849	35416	3.95%	0.305%
2	5.322	545	550	557	rBV4	7889	22053	2.46%	0.190%
3	6.357	721	726	741	rBV3	48546	173710	19.38%	1.494%
4	6.469	741	745	755	rVV	99161	160611	17.92%	1.382%
5	6.692	780	783	794	rBV	269813	406747	45.38%	3.499%
6	6.845	806	809	831	rVB	418533	505137	56.35%	4.346%
7	7.257	876	879	895	rBV	189079	379663	42.35%	3.266%
8	7.475	913	916	918	rVB2	12771	10195	1.14%	0.088%
9	7.716	953	957	962	rVB2	16716	18177	2.03%	0.156%
10	7.816	970	974	978	rVB2	11737	14642	1.63%	0.126%
11	7.975	998	1001	1016	rBV	489308	608111	67.84%	5.232%
12	8.551	1095	1099	1102	rBV	10439	15581	1.74%	0.134%
13	8.633	1110	1113	1117	rVB	28564	22727	2.54%	0.196%
14	8.798	1134	1141	1143	rBV2	12620	16361	1.83%	0.141%
15	8.922	1159	1162	1163	rBV2	8966	10147	1.13%	0.087%
16	9.045	1180	1183	1195	rBV	689976	815088	90.93%	7.012%
17	9.204	1207	1210	1216	rVB4	31486	42444	4.73%	0.365%
18	9.445	1247	1251	1256	rBV	319553	338751	37.79%	2.914%
19	9.633	1280	1283	1286	rBV3	16413	13505	1.51%	0.116%
20	9.722	1292	1298	1311	rBV	759997	775011	86.46%	6.667%
21	9.986	1340	1343	1347	rBV5	11380	11613	1.30%	0.100%
22	10.039	1349	1352	1354	rVV3	13791	15727	1.75%	0.135%
23	10.092	1358	1361	1364	rBV5	8747	10889	1.21%	0.094%
24	10.127	1364	1367	1370	rBV2	29099	32776	3.66%	0.282%
25	10.163	1370	1373	1375	rVB4	9177	11229	1.25%	0.097%
26	10.327	1398	1401	1404	rBV4	9884	14712	1.64%	0.127%
27	10.380	1408	1410	1416	rVB4	16055	20644	2.30%	0.178%
28	10.510	1427	1432	1444	rBV3	113196	254277	28.37%	2.188%
29	10.645	1450	1455	1461	rBV3	42789	67909	7.58%	0.584%
30	10.863	1490	1492	1495	rVB3	21248	16385	1.83%	0.141%
31	11.080	1527	1529	1532	rBV3	20714	24901	2.78%	0.214%
32	11.157	1539	1542	1546	rBV	44609	42347	4.72%	0.364%
33	11.204	1546	1550	1555	rBV	575414	753847	84.10%	6.485%
34	11.245	1555	1557	1563	rVV2	77729	99960	11.15%	0.860%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
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Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.310	1565	1568	1573	rVB	44295	51718	5.77%	0.445%
36	11.422	1584	1587	1589	rBV	80333	74343	8.29%	0.640%
37	11.592	1613	1616	1619	rBV	268063	223364	24.92%	1.922%
38	11.621	1619	1621	1622	rVV	25138	18227	2.03%	0.157%
39	11.669	1626	1629	1631	rBV2	39258	38864	4.34%	0.334%
40	11.845	1656	1659	1661	rVB	45390	39539	4.41%	0.340%
41	12.010	1684	1687	1691	rBV	144500	133554	14.90%	1.149%
42	12.780	1814	1818	1826	rBV	686881	767230	85.59%	6.601%
43	13.833	1993	1997	2003	rBV	422892	551979	61.58%	4.749%
44	14.345	2082	2084	2089	rVB2	172615	214887	23.97%	1.849%
45	14.668	2136	2139	2144	rVB	284432	279266	31.15%	2.403%
46	15.098	2209	2212	2216	rVB	168937	181905	20.29%	1.565%
47	15.186	2224	2227	2231	rVB	223413	251434	28.05%	2.163%
48	15.233	2231	2235	2245	rVB	387306	653298	72.88%	5.620%
49	15.357	2253	2256	2261	rVB3	215329	307685	34.32%	2.647%
50	15.868	2339	2343	2355	rVB	386277	896390	100.00%	7.712%
51	16.268	2406	2411	2417	rVB	483258	801440	89.41%	6.895%
52	16.786	2496	2499	2505	rVB	118522	185878	20.74%	1.599%
53	16.856	2507	2511	2517	rVB4	92389	191436	21.36%	1.647%

Sum of corrected areas: 11623730

LSC Report - Integrated Chromatogram

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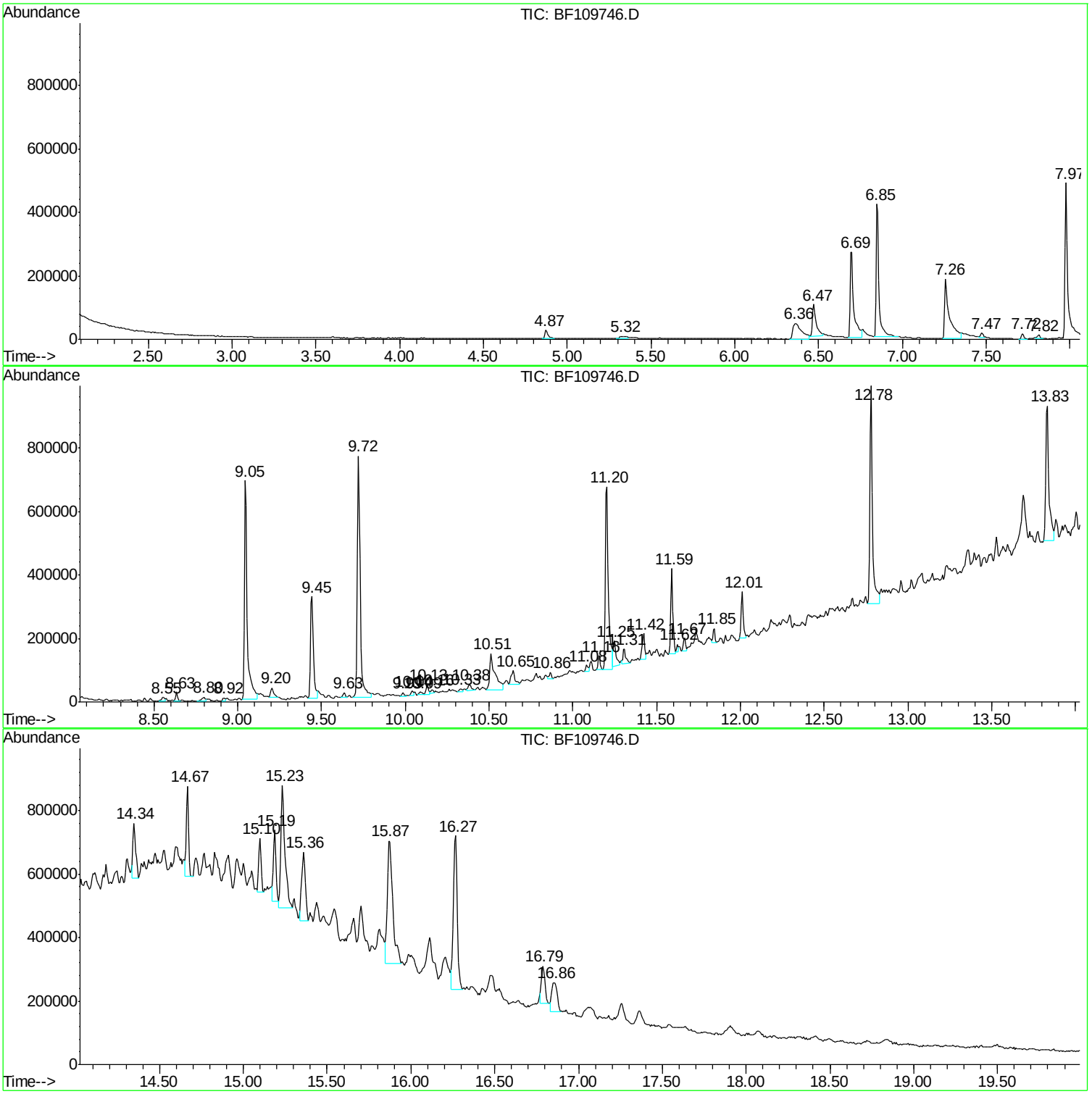
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

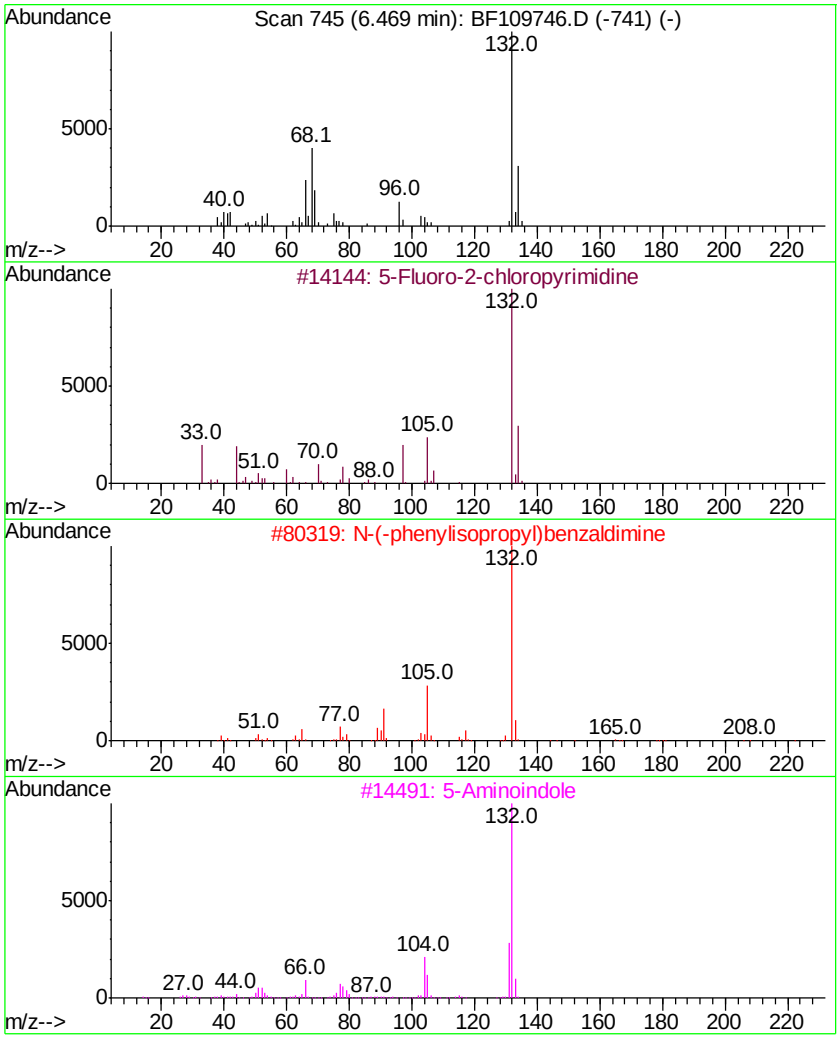
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

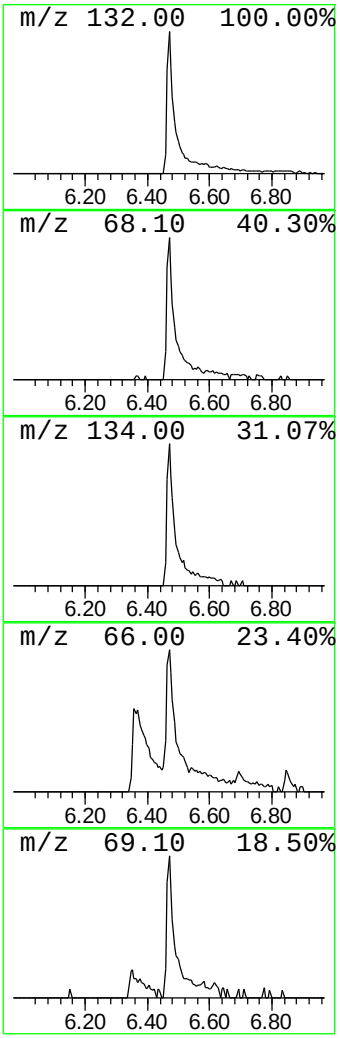
****

Peak Number 1 unknown6.47 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	7.90 ng	160611	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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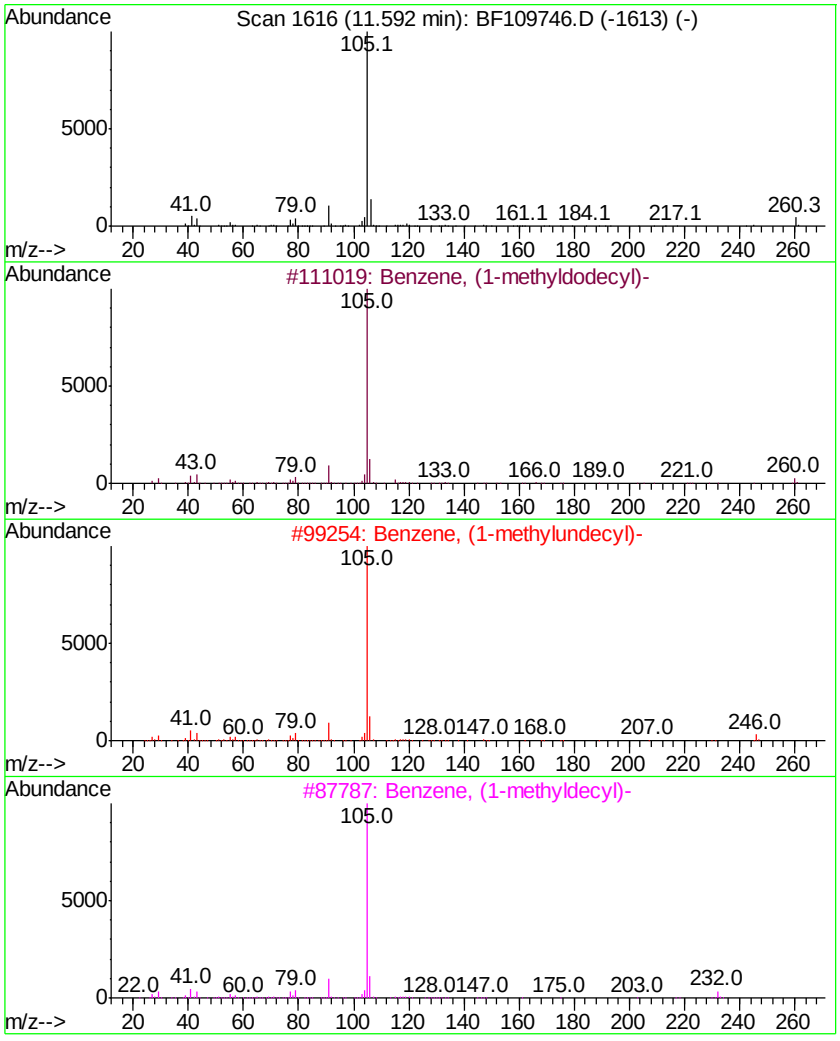
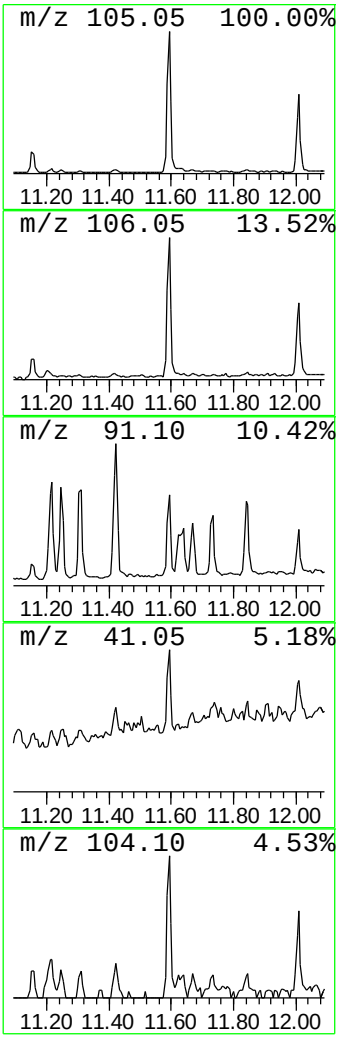
Peak Number 3 Benzene, (1-methyldodecyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	5.93 ng	223364	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	87
2	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
3	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64
4	1-Hexene, 3-methyl-6-phenyl-4-(1...	294	C21H26O	1000194-52-4	50
5	Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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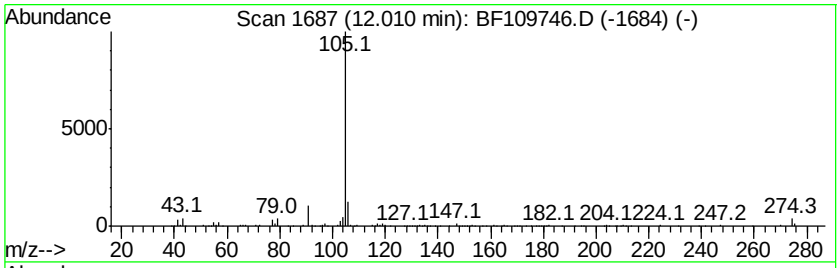
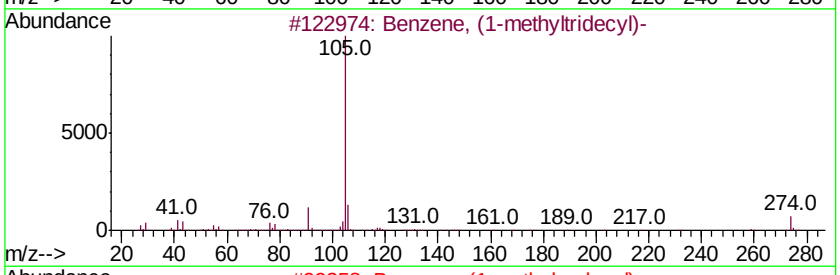
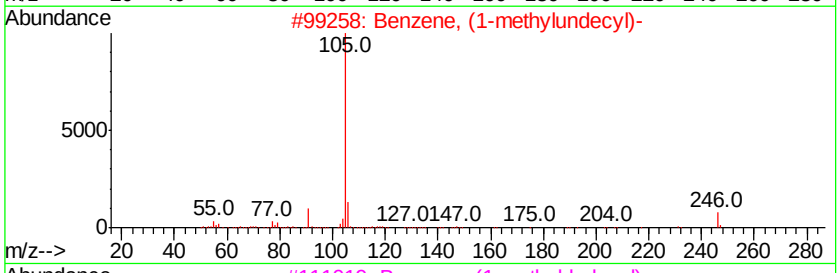
Peak Number 4 Benzene, (1-methyltridecyl)- Concentration Rank 12

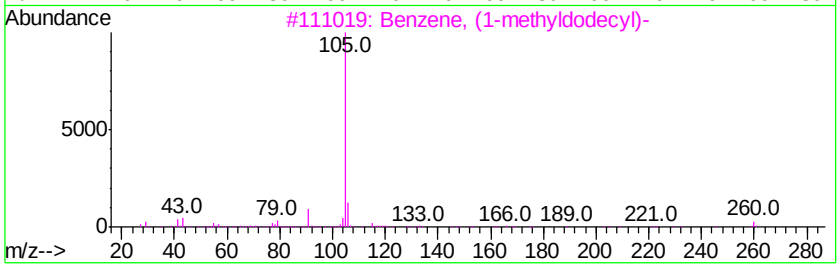
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.54 ng	133554	Phenanthrene-d10	11.20

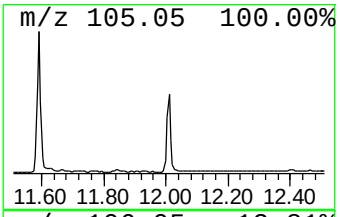
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	64
2	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	53
3	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	53
4	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	53
5	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	53

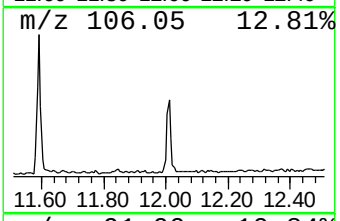


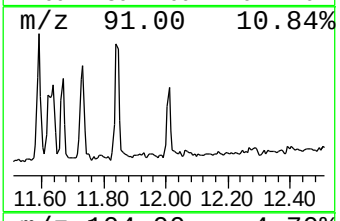


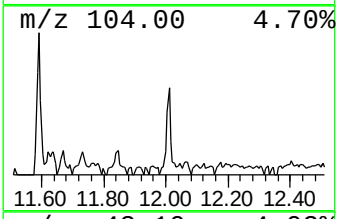


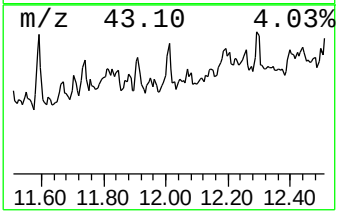












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Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

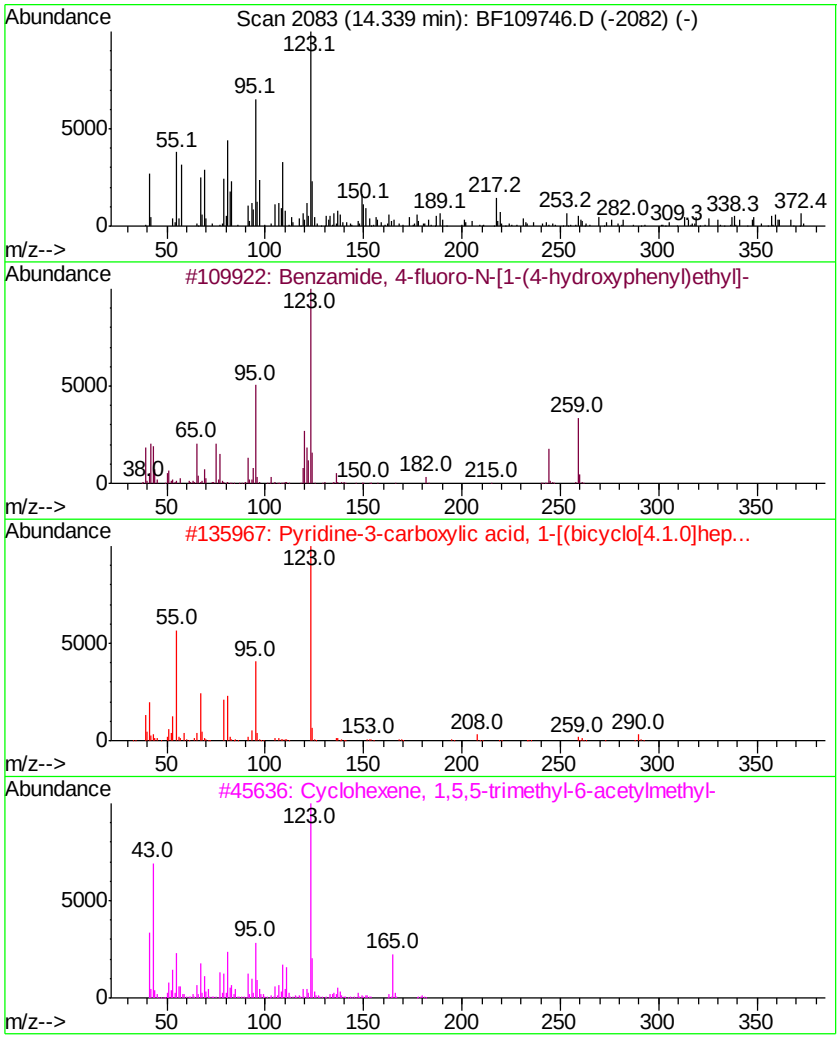
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

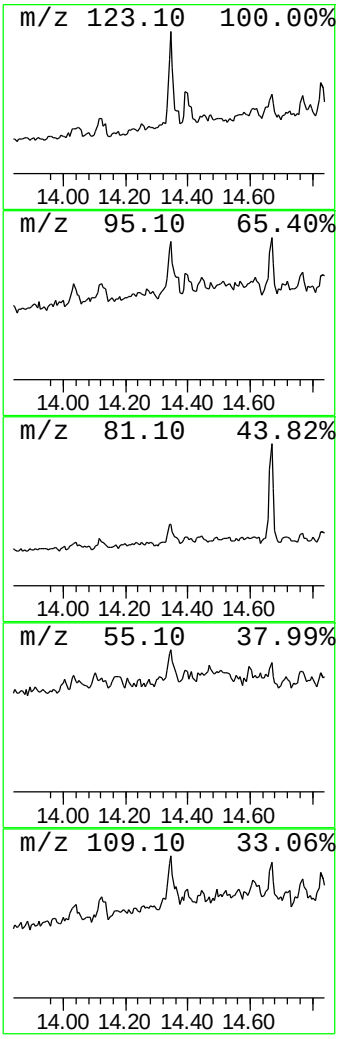
****

Peak Number 5 Benzamide, 4-fluoro-N-[1-(4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	7.79 ng	214887	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 4-fluoro-N-[1-(4-hydr...	259	C15H14FNO2	1000311-09-5	50
2	Pyridine-3-carboxylic acid, 1-[(...	290	C15H18N2O4	1000310-27-9	49
3	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	49
4	trans-2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	115754-87-5	47
5	Octopamine	153	C8H11NO2	000104-14-3	43





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Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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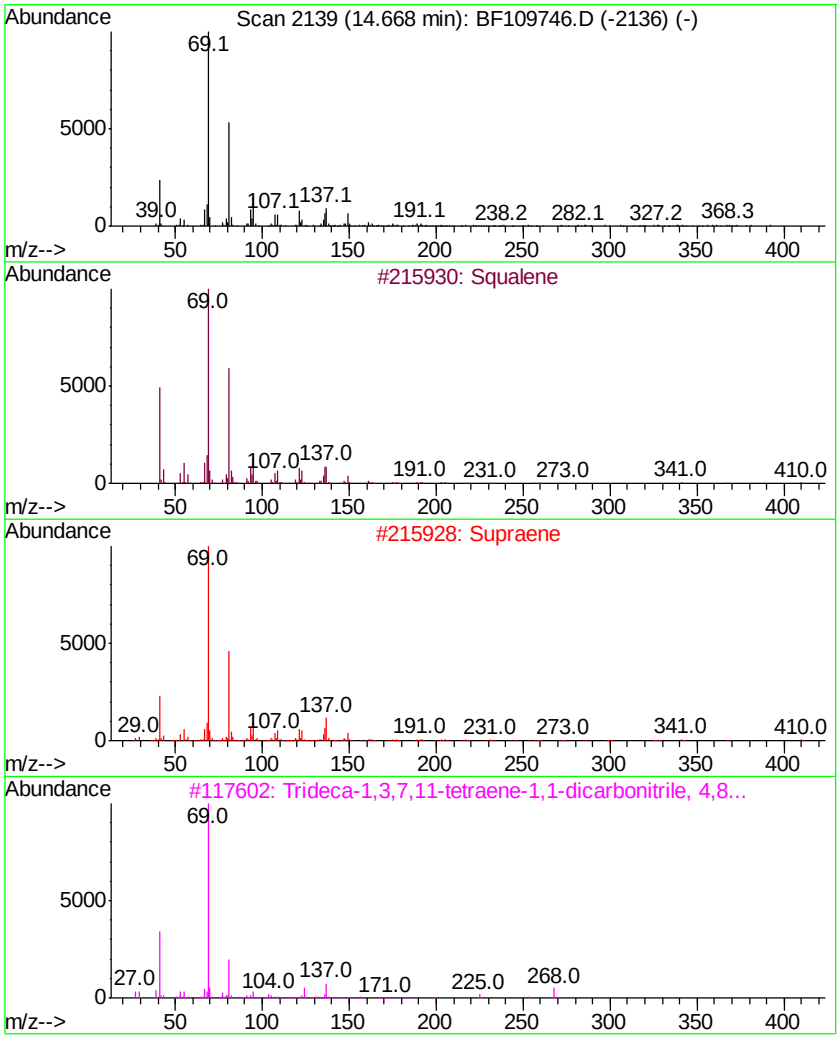
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

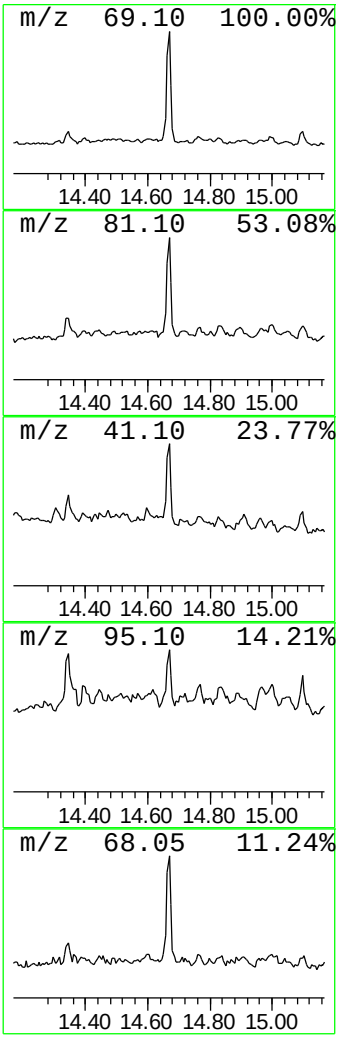
****

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	8.55 ng	279266	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	86
3	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	47





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Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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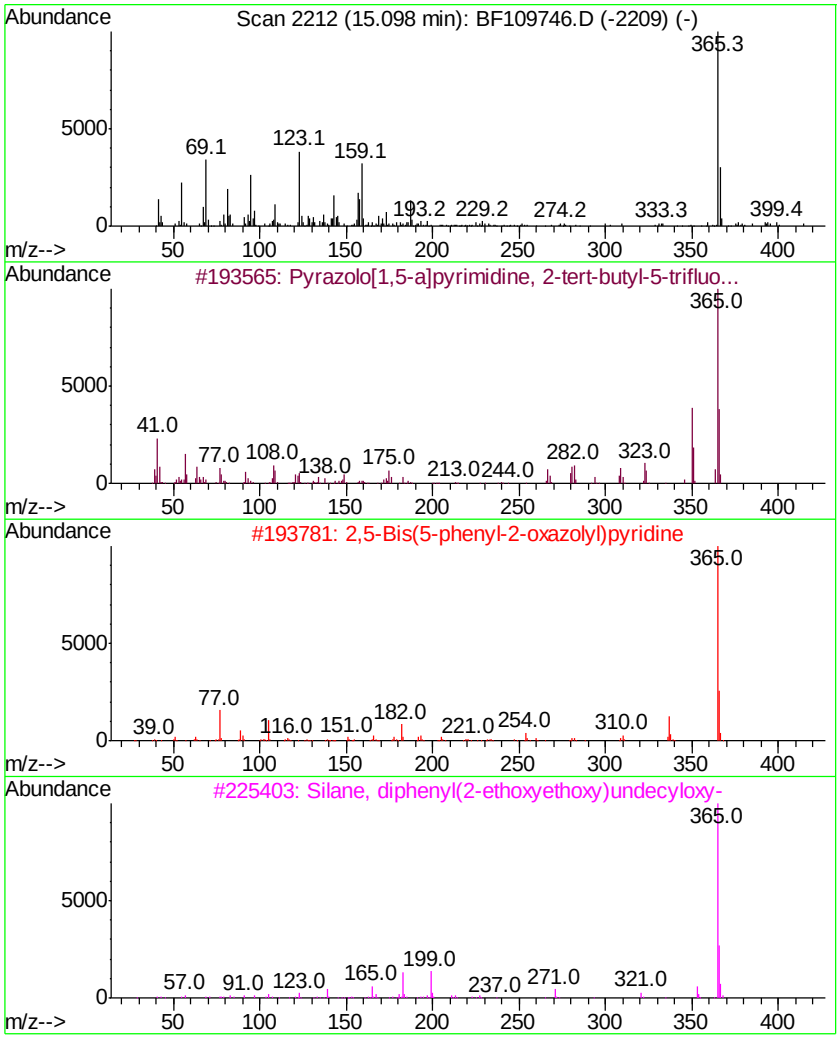
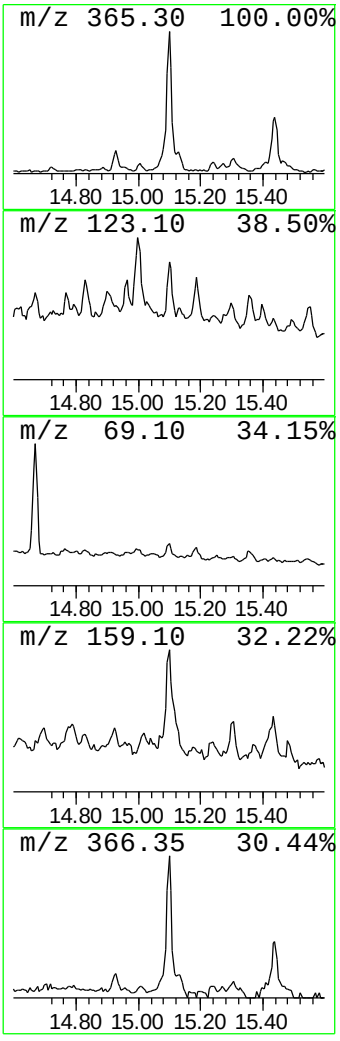
Peak Number 7 unknown15.10 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	5.57 ng	181905	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo[1,5-a]pyrimidine, 2-ter...	365	C18H18F3N3O2	1000268-76-7	38
2	2,5-Bis(5-phenyl-2-oxazolyl)pyri...	365	C23H15N3O2	040875-87-4	32
3	Silane, diphenyl(2-ethoxyethoxy)...	442	C27H42O3Si	1000367-66-8	23
4	Imidazo[5,1-a]isoquinoline-1,3-d...	456	C28H28N2O4	115684-13-4	23
5	Isonipecotic acid, N-methacryloy...	365	C22H39NO3	1000360-96-3	23





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ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

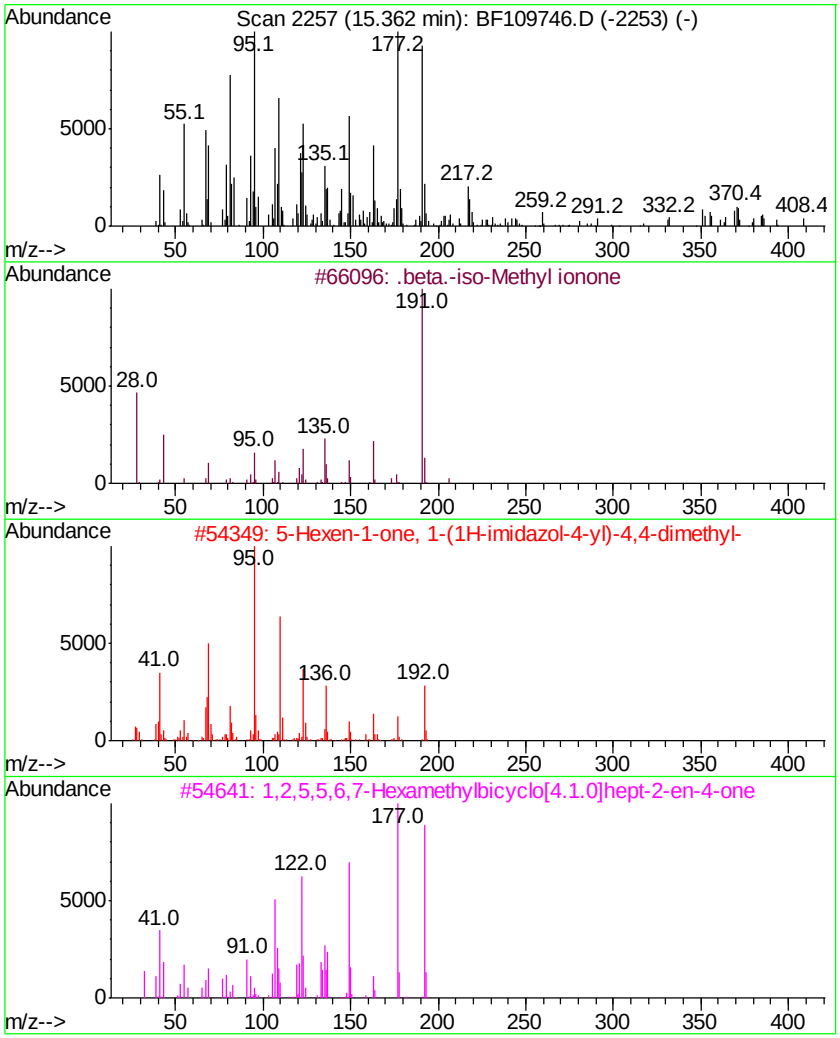
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

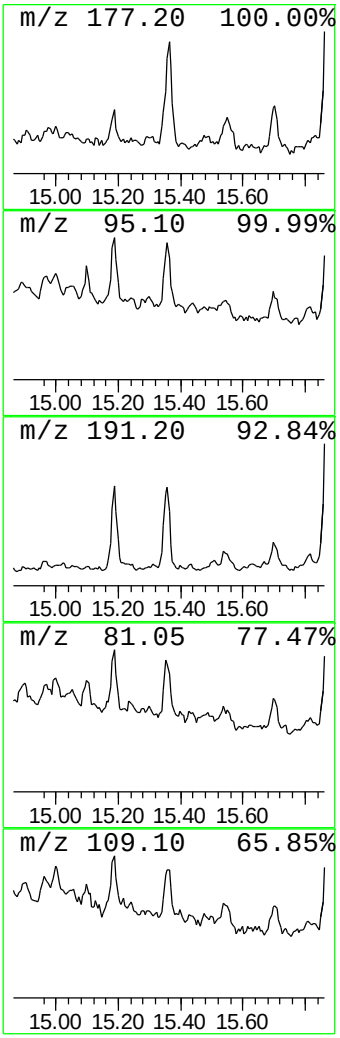
****

Peak Number 8 unknown15.36 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	9.42 ng	307685	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
2	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	42
3	1,2,5,5,6,7-Hexamethylbicyclo[4....	192	C13H20O	1000110-52-5	38
4	Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	35
5	23,28-Bisnor-17.alpha.(H)-hopane	384	C28H48	1000101-35-1	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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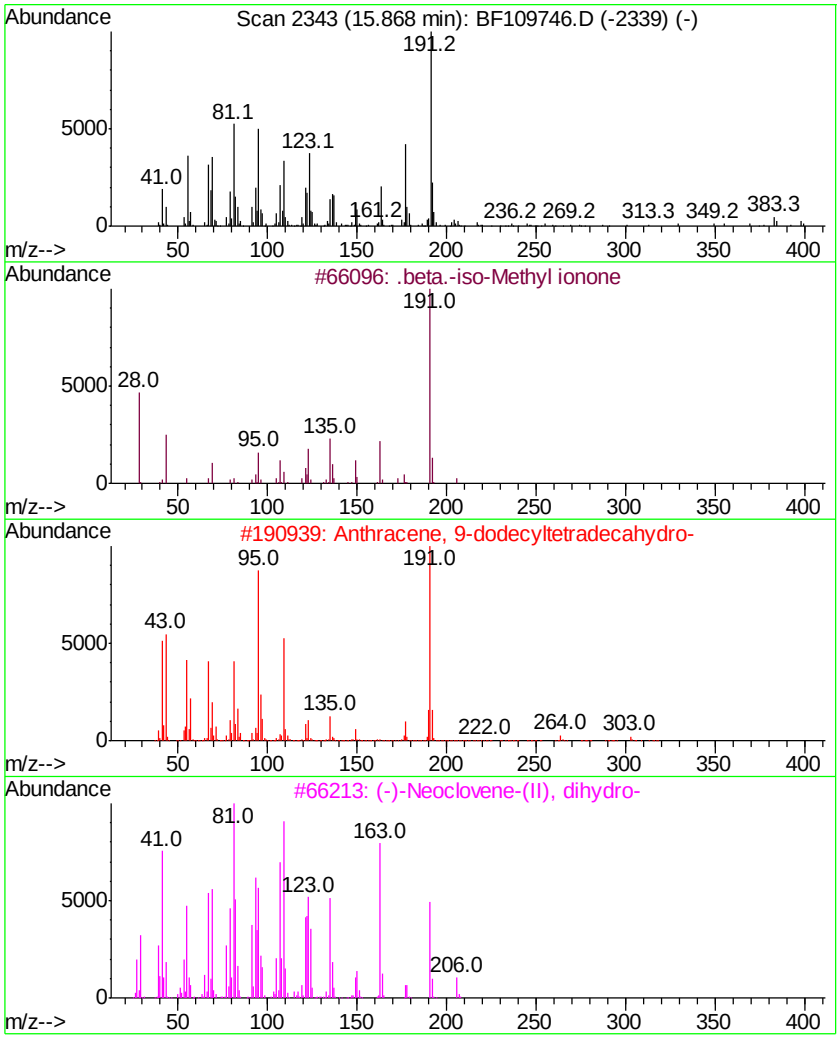
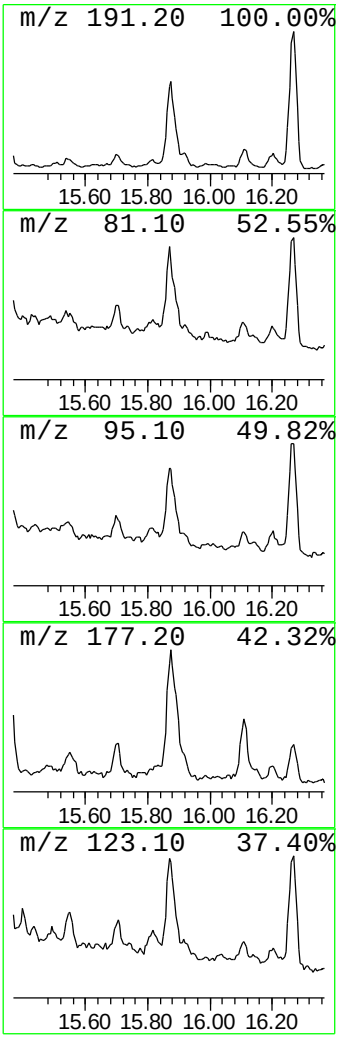
Peak Number 9 unknown15.87 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	27.44 ng	896390	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38
3	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	38
4	Azuleno[4,5-b]furan-2(3H)-one, d...	266	C15H22O4	005090-67-5	37
5	7-Hydroxy-2,5,8-quinoline trione	191	C9H5NO4	015544-54-4	32





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Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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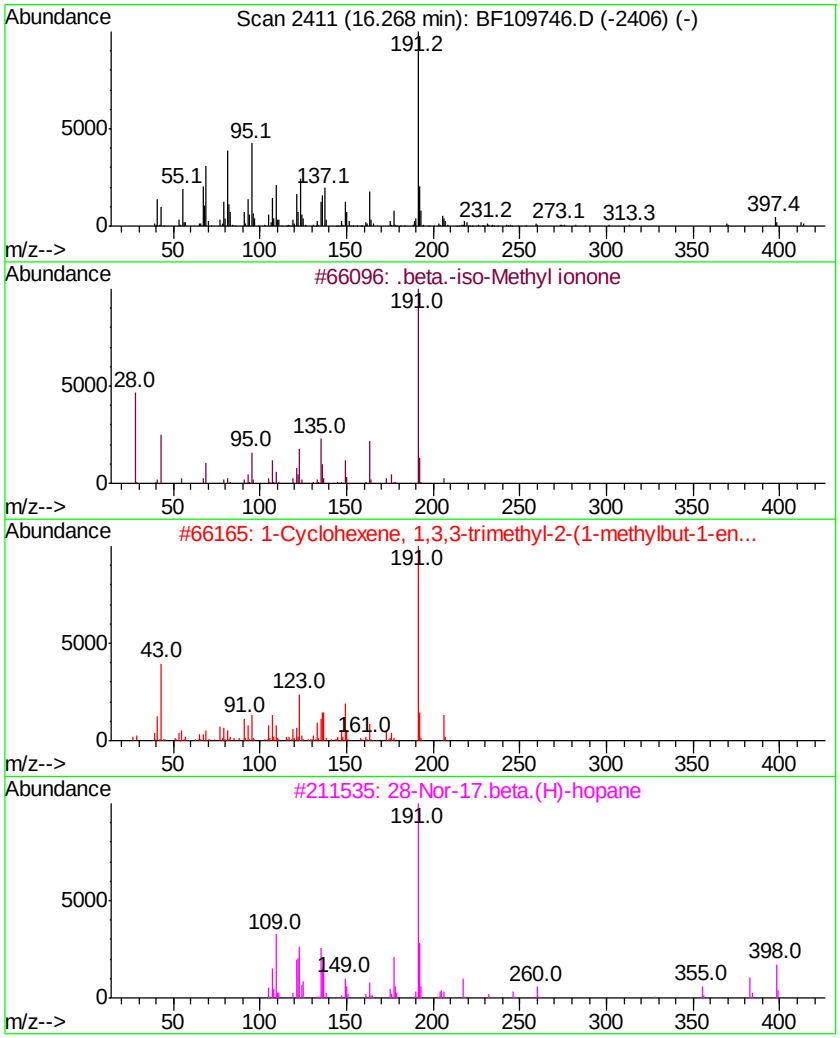
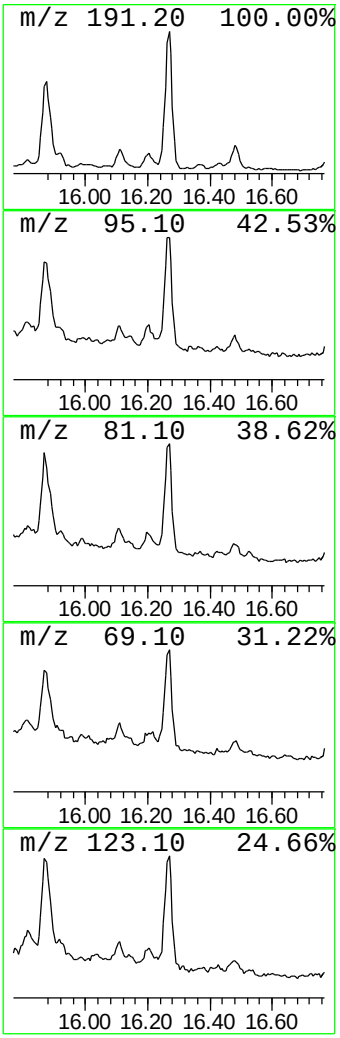
Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	24.54 ng	801440	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	53
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	50
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	45
5	2,5,5,8a-Tetramethyl-4-methylene...	206	C14H22O	093175-76-9	37





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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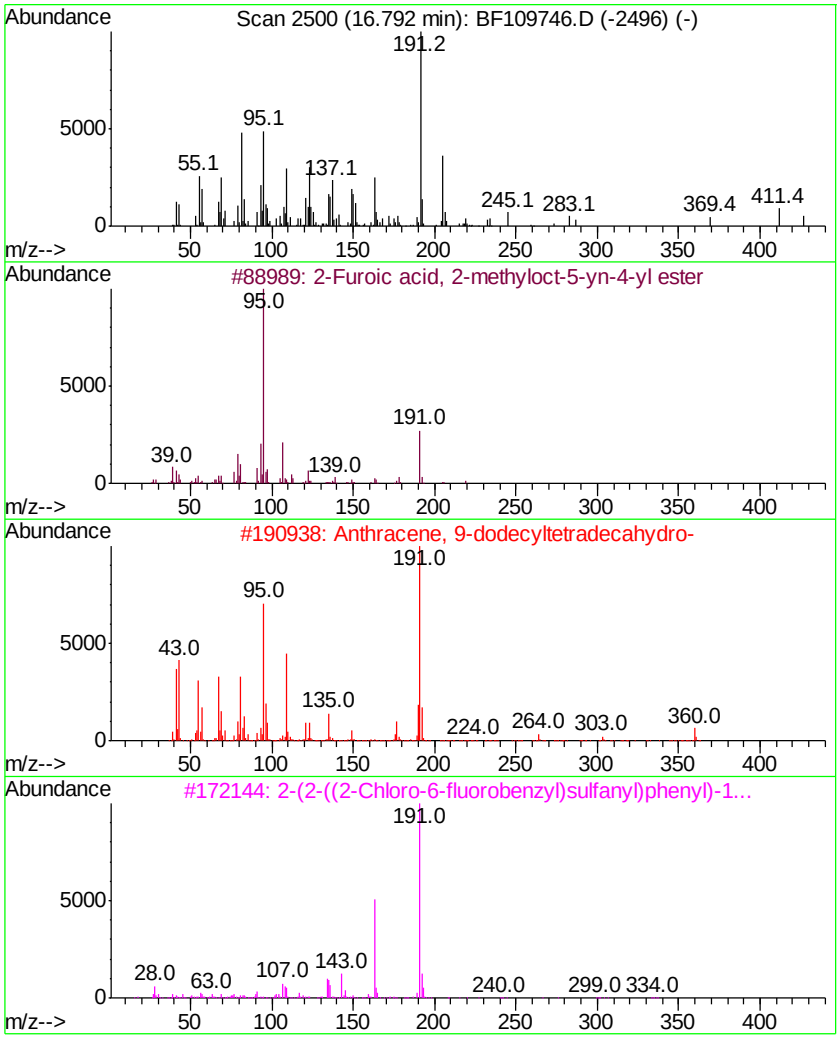
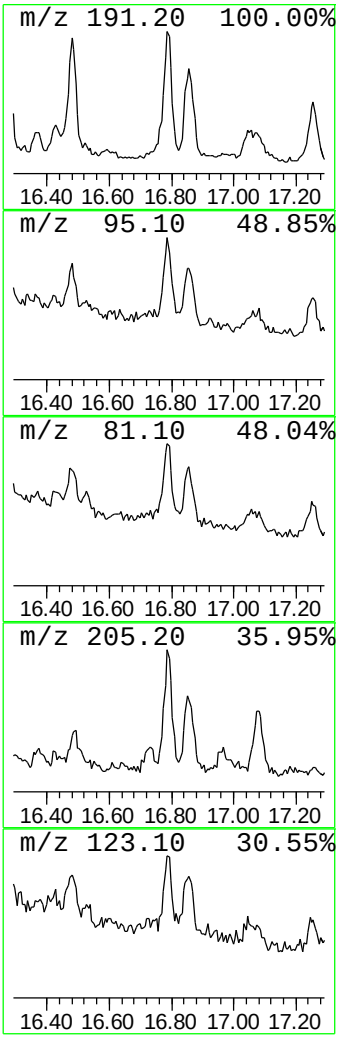
Peak Number 11 unknown16.79 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	5.69 ng	185878	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furoic acid, 2-methyloct-5-yn-...	234	C14H18O3	1000299-23-7	43
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	35
3	2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	35
4	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	35
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	30





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Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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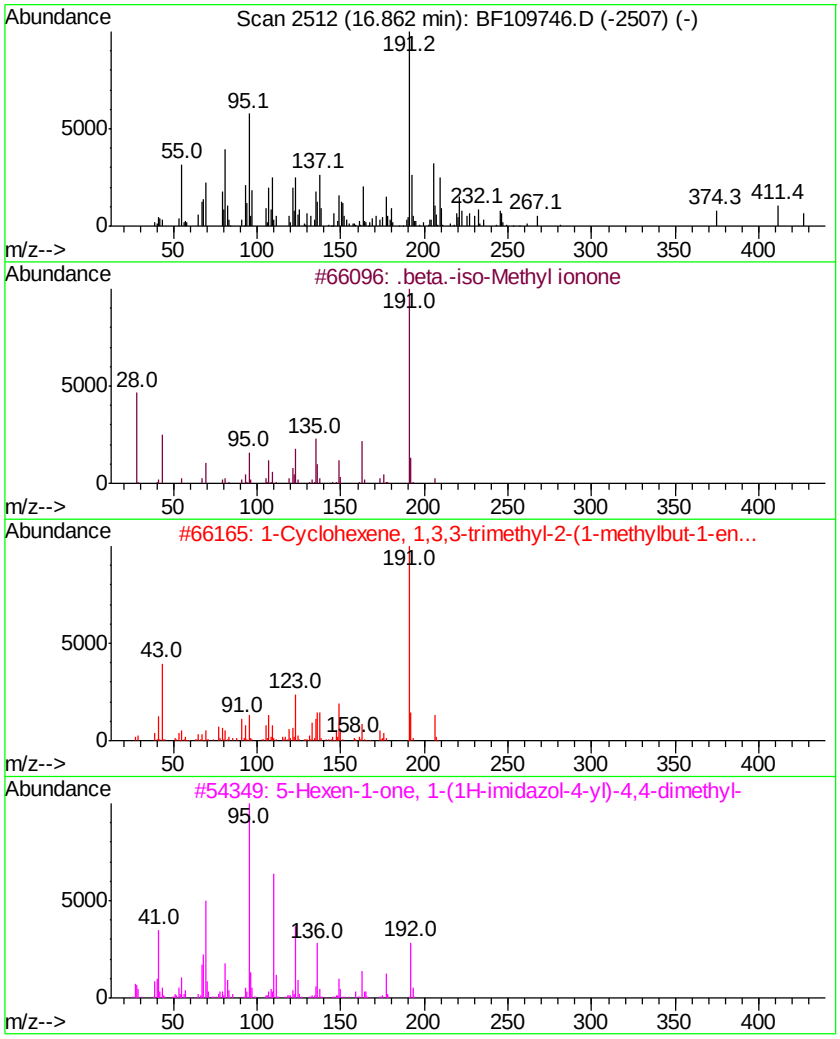
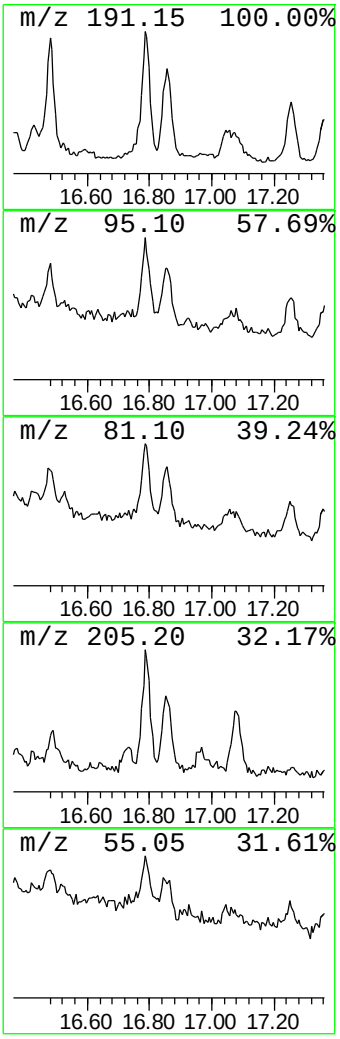
Peak Number 12 unknown16.86 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	5.86 ng	191436	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	49
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	43
3	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	38
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5	Propenamide, 3-(3,4-dimethoxyphe...	313	C18H19NO4	339165-72-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
Data File : BF109746.D
Acq On : 10 Oct 2018 17:00
Operator : JU/SJ
Sample : J5367-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DS-VB-16202

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.47	6.47	7.9	ng	160611	1	6.70	406747	20.0
Benzene, (1-methy...	11.59	5.9	ng	223364	4	11.20	753847	20.0
Benzene, (1-methy...	12.01	3.5	ng	133554	4	11.20	753847	20.0
Benzamide, 4-fluo...	14.34	7.8	ng	214887	5	13.83	551979	20.0
Squalene	14.67	8.6	ng	279266	6	15.23	653298	20.0
unknown15.10	15.10	5.6	ng	181905	6	15.23	653298	20.0
unknown15.36	15.36	9.4	ng	307685	6	15.23	653298	20.0
unknown15.87	15.87	27.4	ng	896390	6	15.23	653298	20.0
.beta.-iso-Methyl...	16.27	24.5	ng	801440	6	15.23	653298	20.0
unknown16.79	16.79	5.7	ng	185878	6	15.23	653298	20.0
unknown16.86	16.86	5.9	ng	191436	6	15.23	653298	20.0