LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

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-BF022218.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	5.104	509	513	528	rBV	45750	102720	2.83%	0.337%
2	5.492	576	579	619	rBV	1688783	3624078	100.00%	11.878%
3	6.504	748	751	769	rBV	2016945	3492948	96.38%	11.448%
4	6.634	769	773	799	rVB	2800394	3576766	98.69%	11.723%
5	6.857	808	811	831	rVV	679597	926682	25.57%	3.037%
6	7.010	833	837	869	rVB	2200419	2636493	72.75%	8.641%
7	7.428	904	908	925	rBV	1641391	2262400	62.43%	7.415%
8	8.139	1026	1029	1050	rBV	935638	1297997	35.82%	4.254%
9	9.216	1208	1212	1221	rBV	3099864	3288956	90.75%	10.780%
10	9.280	1221	1223	1228	rVB	67800	63876	1.76%	0.209%
11	9.610	1273	1279	1285	rBV	252492	290826	8.02%	0.953%
12	9.810	1309	1313	1317	rBV	138518	109477	3.02%	0.359%
13	9.898	1324	1328	1333	rBV2	1193832	1210639	33.41%	3.968%
14	10.127	1364	1367	1372	rVB3	33788	38315	1.06%	0.126%
15	10.310	1395	1398	1401	rVB	159694	124385	3.43%	0.408%
16	10.457	1421	1423	1428	rVB	34028	40259	1.11%	0.132%
17	10.527	1431	1435	1438	rBV	44581	52546	1.45%	0.172%
18	10.698	1460	1464	1476	rBV	1451545	1748048	48.23%	5.729%
19	10.780	1476	1478	1487	rVB	137639	172634	4.76%	0.566%
20	11.233	1551	1555	1557	rBV	76362	64553	1.78%	0.212%
21	11.398	1579	1583	1586	rBV	895206	972889	26.85%	3.189%
22	11.422	1586	1587	1594	rVV	210204	184605	5.09%	0.605%
23	11.480	1594	1597	1605	rVB	34020	51057	1.41%	0.167%
24	11.657	1622	1627	1630	rBV2	35995	38016	1.05%	0.125%
25	11.904	1665	1669	1672	rBV2	61110	78481	2.17%	0.257%
26	11.933	1672	1674	1680	rVB2	40930	50459	1.39%	0.165%
27	12.016	1684	1688	1691	rBV2	35367	42553	1.17%	0.139%
28	12.621	1787	1791	1799	rBV	145289	186899	5.16%	0.613%
29	12.851	1827	1830	1836	rVB	145791	151564	4.18%	0.497%
30	12.980	1848	1852	1863	rBV	2090109	2043133	56.38%	6.696%
31	13.180	1879	1886	1891	rBV2	27956	62800	1.73%	0.206%
32	13.857	1998	2001	2006	rBV	117219	141192	3.90%	0.463%
33	14.057	2030	2035	2039	rBV	630652	724790	20.00%	2.375%
34	14.868	2171	2173	2178	rVB	55655	62311	1.72%	0.204%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.568	2287	2292	2303	rVB	404149	595787	16.44%	1.953%

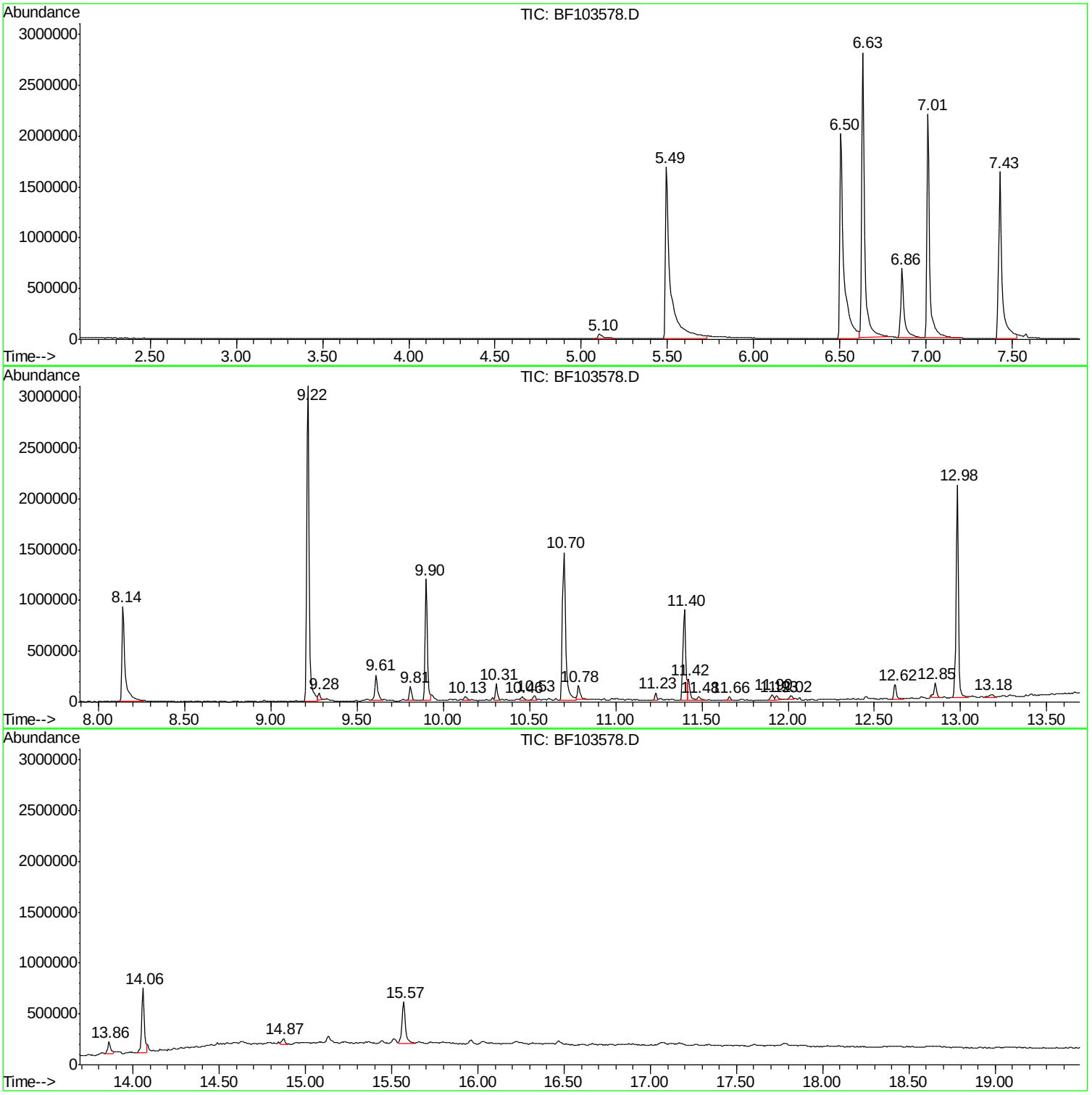
Sum of corrected areas: 30511134

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

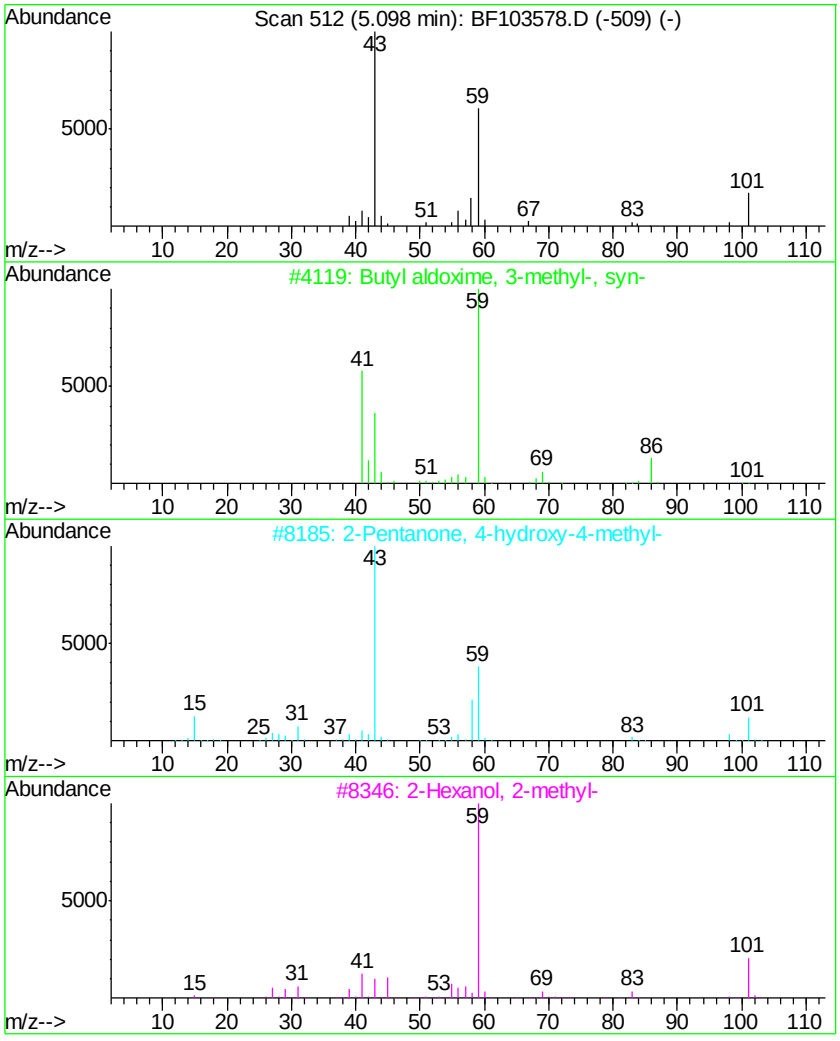
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

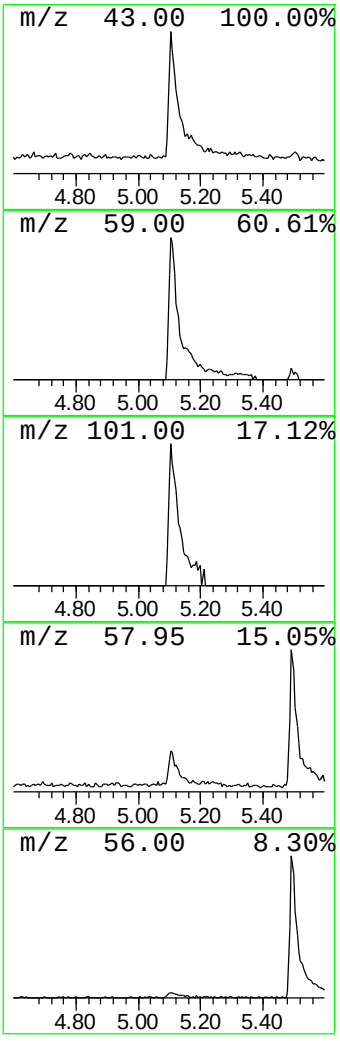
****

Peak Number 1 unknown5.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.22 ng	102720	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	43
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

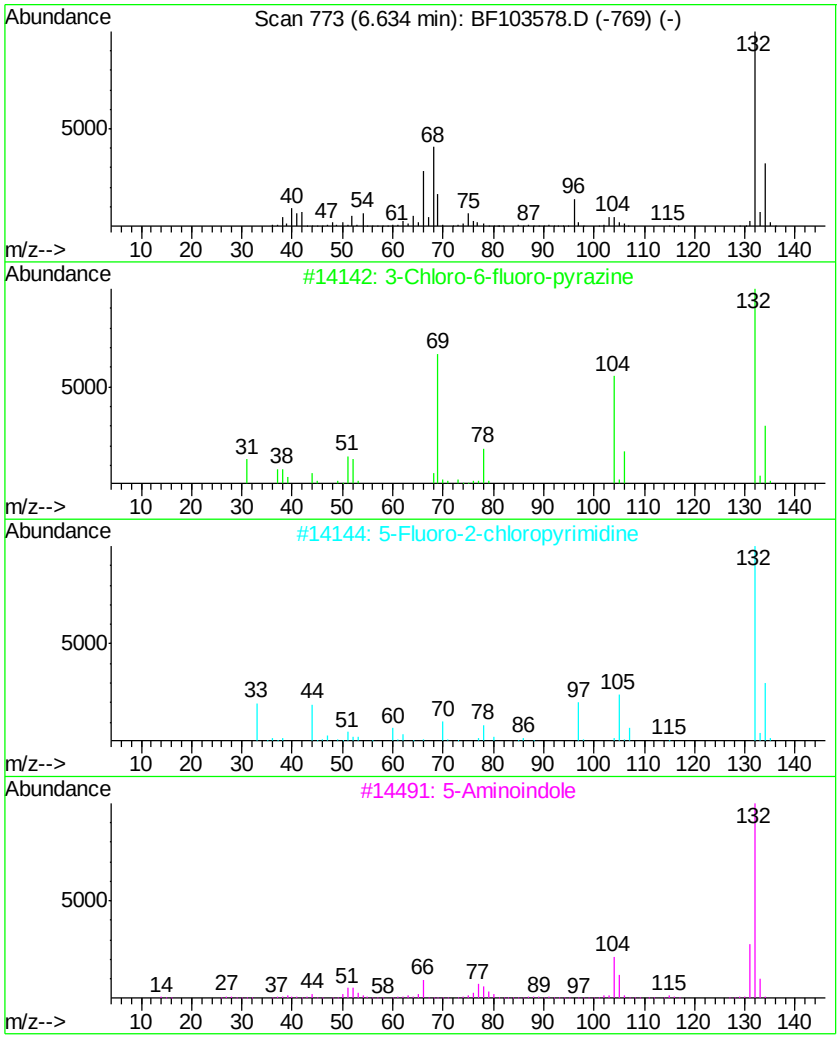
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

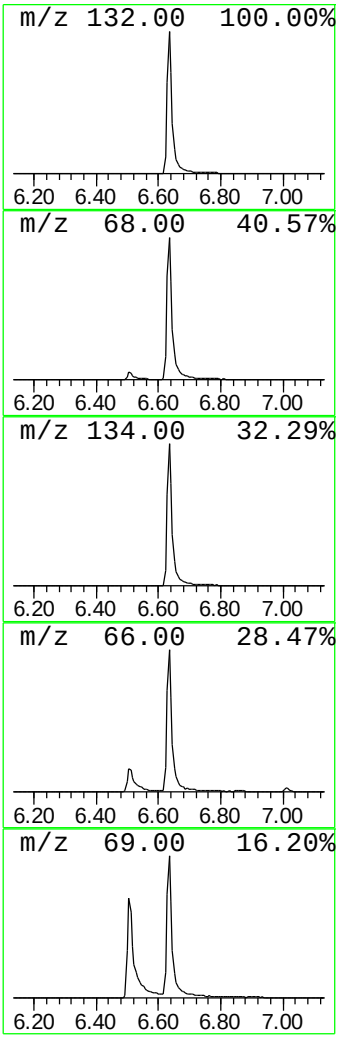
****

Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	77.20 ng	3576770	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

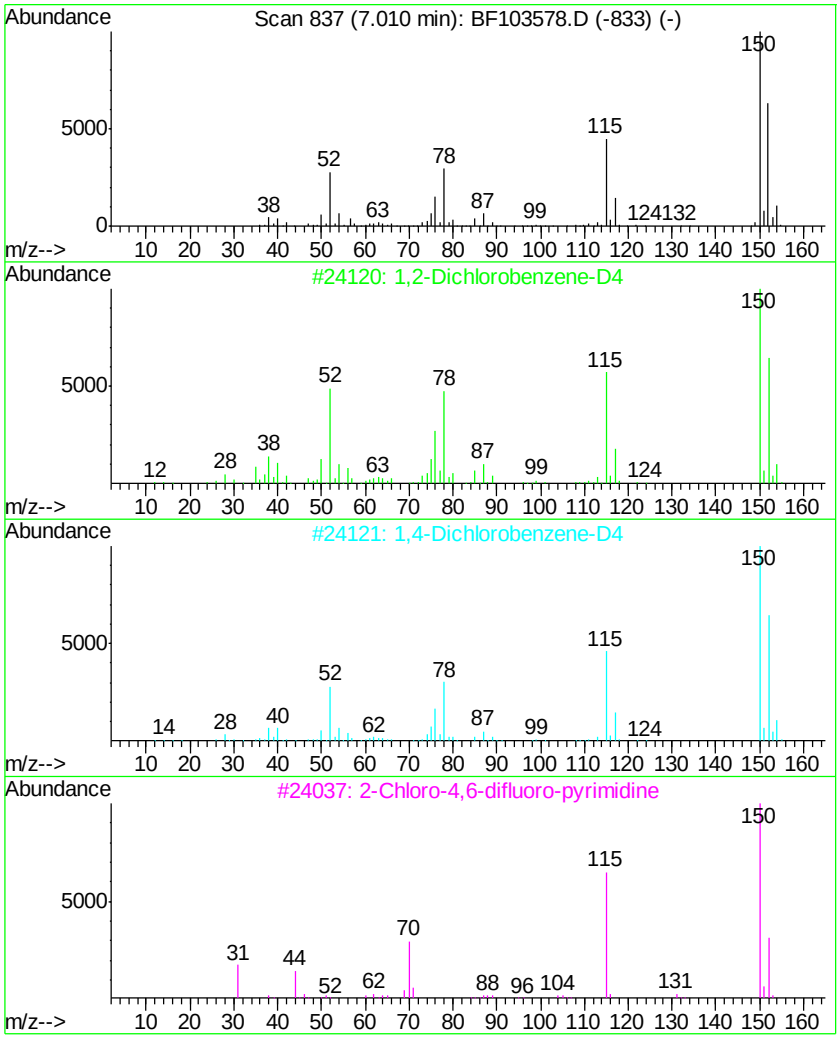
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

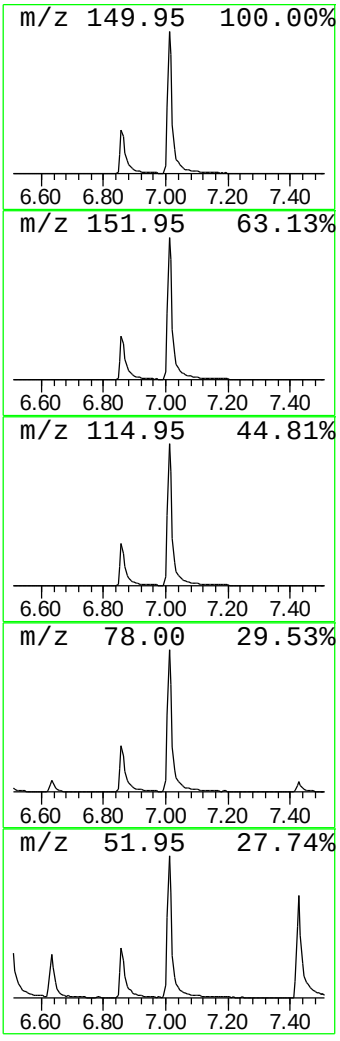
****

Peak Number 3 1,2-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.01	56.90 ng	2636490	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
2	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
3	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	38
4	2-Bromo-2'-nitroacetophenone	243	C8H6BrNO3	006851-99-6	22
5	2-Bromo-3'-nitroacetophenone	243	C8H6BrNO3	002227-64-7	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

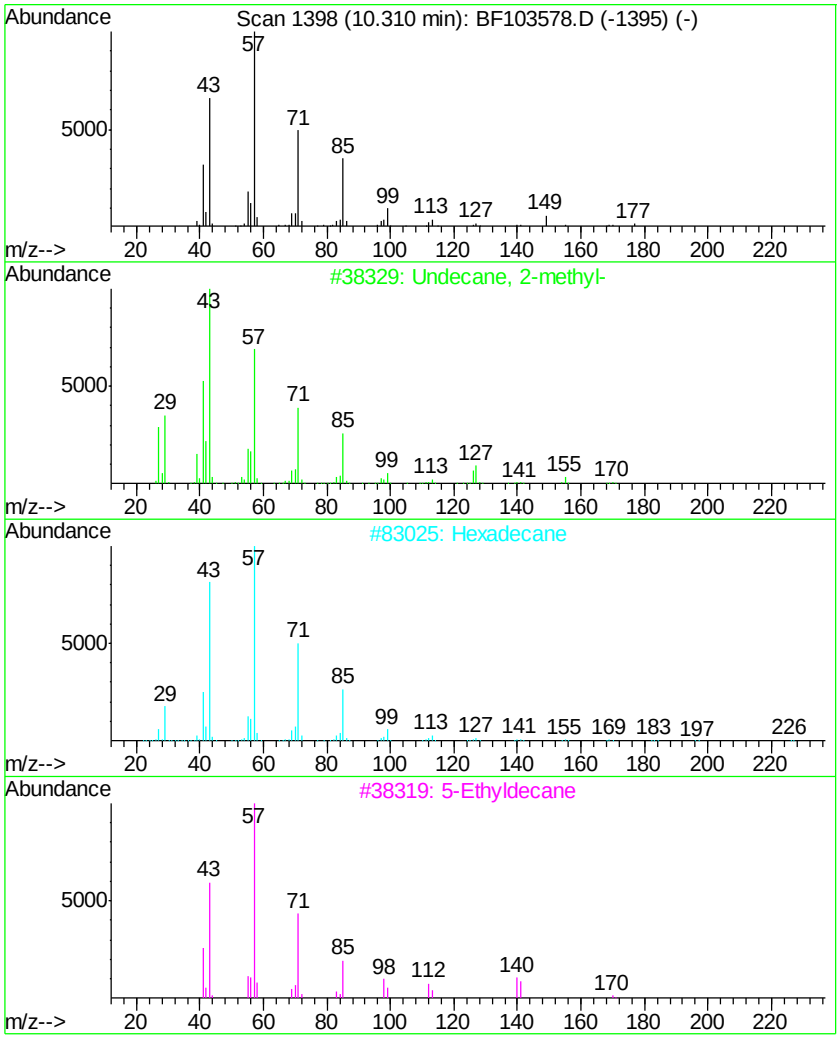
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

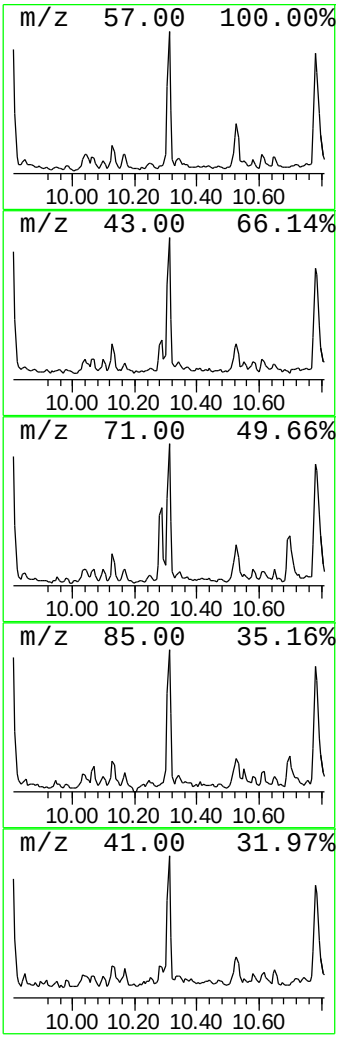
****

Peak Number 4 Undecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.31	2.05 ng	124385	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2-methyl-	170	C12H26	007045-71-8	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	5-Ethyldecane	170	C12H26	017302-36-2	83
4	Heneicosane	296	C21H44	000629-94-7	80
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

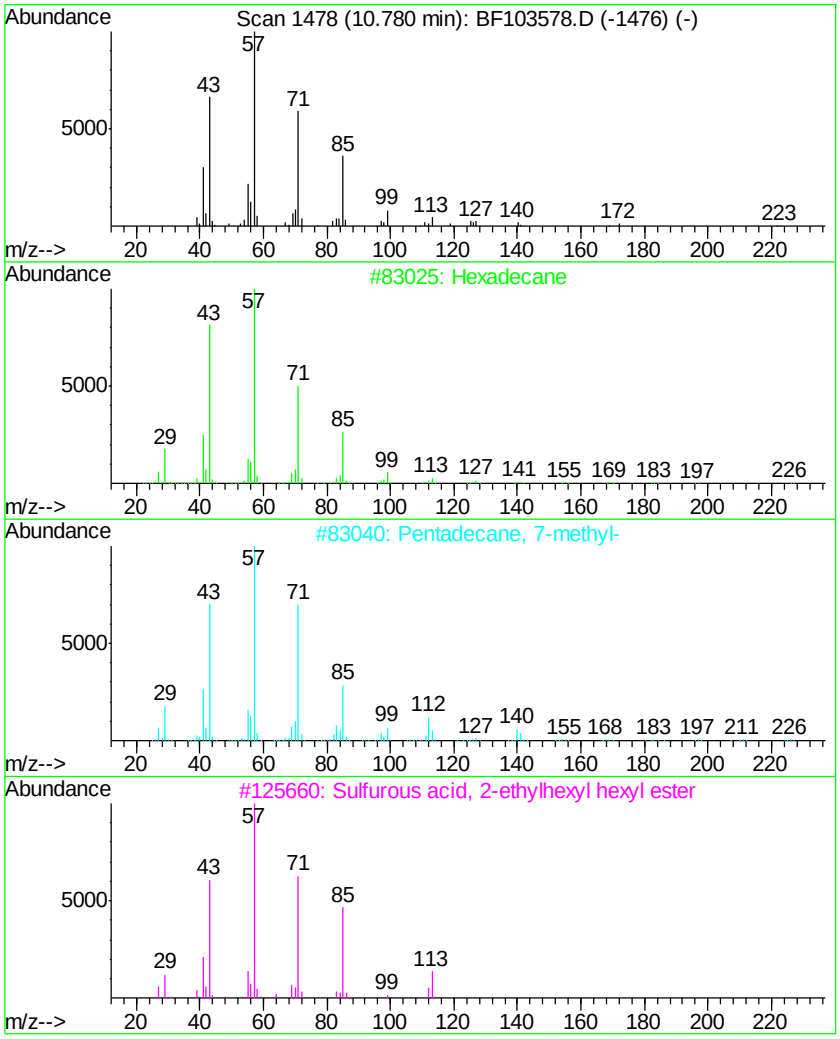
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

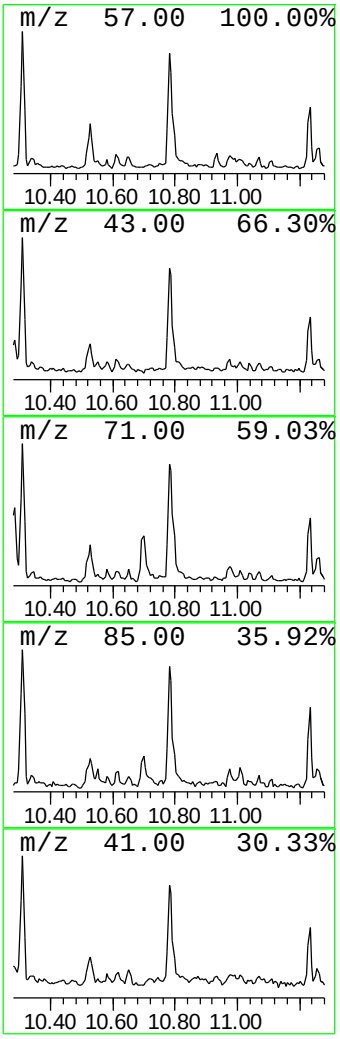
****

Peak Number 5 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.55 ng	172634	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	83
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	78
4	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

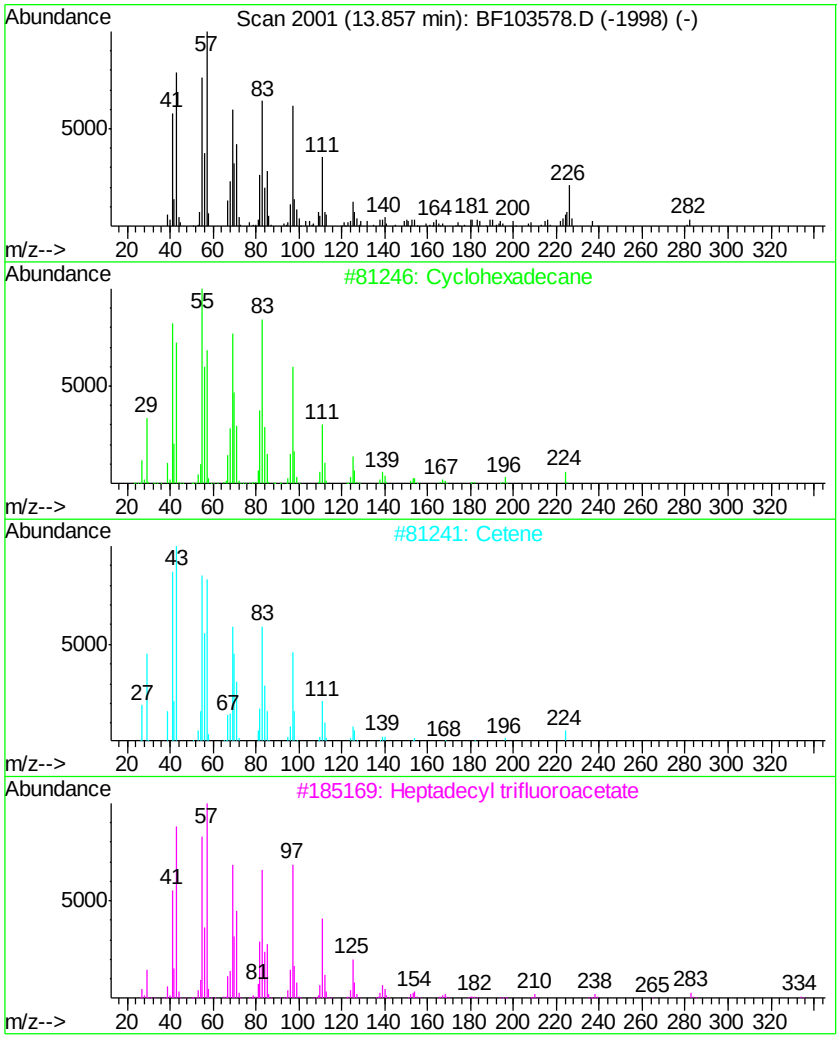
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

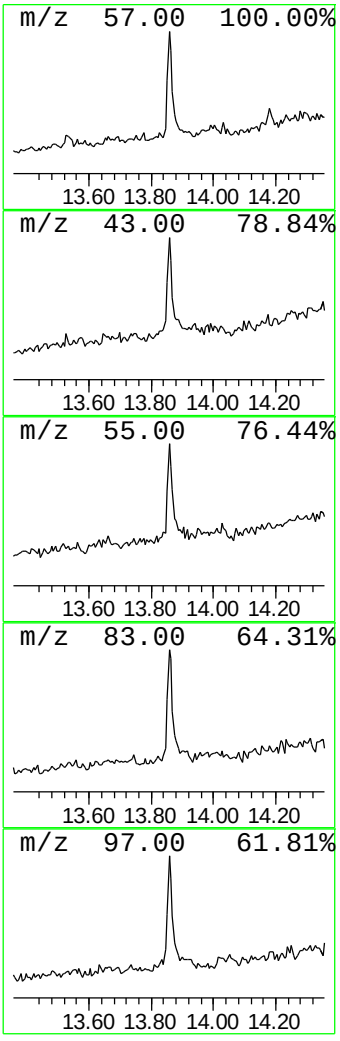
****

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.90 ng	141192	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Cetene	224	C16H32	000629-73-2	87
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

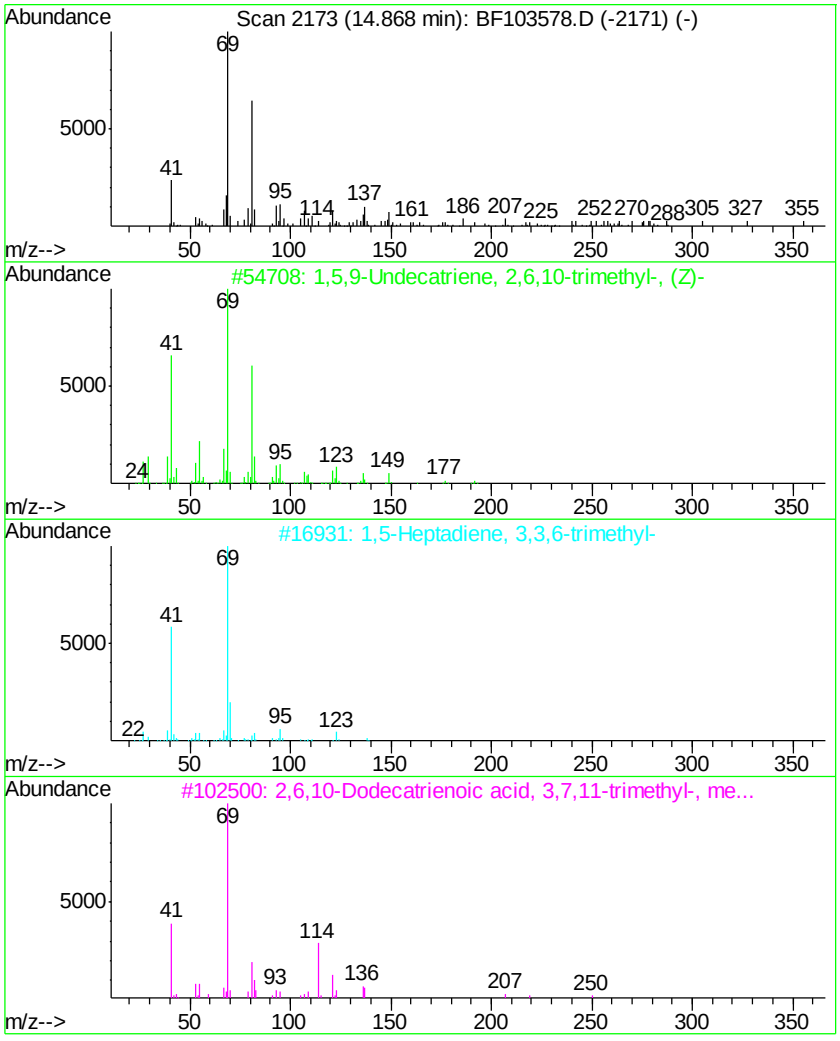
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

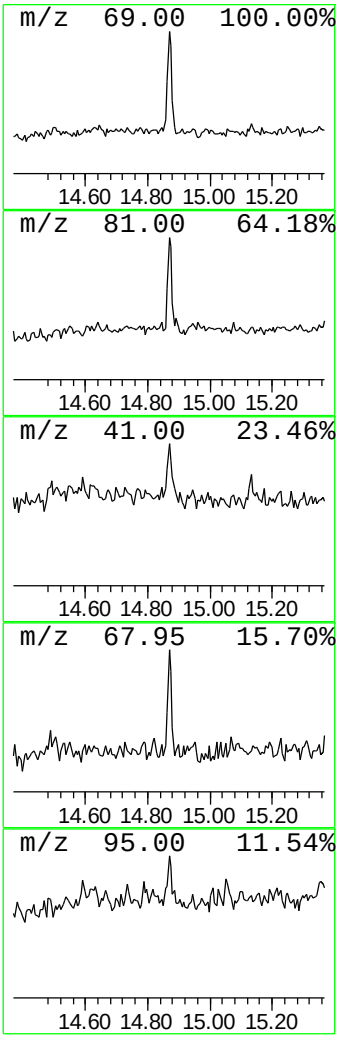
****

Peak Number 7 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.09 ng	62311	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
2	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	59
3	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	59
4	1,6-Octadiene, 2,7-dimethyl-	138	C10H18	040195-09-3	53
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031218\
Data File : BF103578.D
Acq On : 12 Mar 2018 13:33
Operator : SJ/JU
Sample : J1776-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-6FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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
unknown5.10	5.10	2.2	ng	102720	1	6.86	926682	20.0
3-Chloro-6-fluoro...	6.63	77.2	ng	3576770	1	6.86	926682	20.0
1,2-Dichlorobenze...	7.01	56.9	ng	2636490	1	6.86	926682	20.0
Undecane, 2-methyl-	10.31	2.1	ng	124385	3	9.90	1210640	20.0
Hexadecane	10.78	3.5	ng	172634	4	11.40	972889	20.0
Cyclohexadecane	13.86	3.9	ng	141192	5	14.06	724790	20.0
1,5,9-Undecatrien...	14.87	2.1	ng	62311	6	15.57	595787	20.0