LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

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-BF063016.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	1.724	11	12	18	rVV	19922	28790	1.21%	0.127%
2	1.850	21	23	32	rVV	190369	268049	11.28%	1.180%
3	1.975	32	34	43	rVB	46893	72059	3.03%	0.317%
4	2.993	121	123	140	rBB	7483	24016	1.01%	0.106%
5	4.947	291	294	299	rBB	181711	229095	9.64%	1.008%
6	5.382	329	332	334	rVB	2029985	2376820	100.00%	10.462%
7	6.422	420	423	425	rBV	2237655	2351040	98.92%	10.348%
8	6.547	432	434	437	rBV	1943722	2200505	92.58%	9.686%
9	6.787	453	455	457	rBV	648664	623174	26.22%	2.743%
10	6.936	466	468	471	rVB	1323116	1760473	74.07%	7.749%
11	7.347	501	504	506	rBV	1619340	1462452	61.53%	6.437%
12	7.393	506	508	510	rVB	33292	28078	1.18%	0.124%
13	8.068	565	567	569	rBV	1016266	818748	34.45%	3.604%
14	9.142	659	661	664	rBV	2126032	2160186	90.89%	9.508%
15	9.542	694	696	698	rBV	134195	164187	6.91%	0.723%
16	9.759	714	715	718	rBV	30849	31160	1.31%	0.137%
17	9.816	718	720	722	rVV	906129	750643	31.58%	3.304%
18	10.262	757	759	760	rVB	35319	27049	1.14%	0.119%
19	10.605	786	789	791	rBV2	872724	1121199	47.17%	4.935%
20	10.731	798	800	804	rVB	42905	52215	2.20%	0.230%
21	11.176	837	839	841	rBV	73621	67639	2.85%	0.298%
22	11.291	847	849	853	rVV	715118	661297	27.82%	2.911%
23	11.359	853	855	857	rVB2	22927	39437	1.66%	0.174%
24	11.554	871	872	875	rBV	13124	25206	1.06%	0.111%
25	11.599	875	876	879	rVB	29934	34610	1.46%	0.152%
26	11.828	894	896	898	rVB2	39489	45102	1.90%	0.199%
27	11.896	901	902	907	rVB3	21721	42066	1.77%	0.185%
28	12.011	908	912	915	rBV4	13791	43170	1.82%	0.190%
29	12.239	929	932	933	rBV2	13395	28204	1.19%	0.124%
30	12.342	939	941	942	rBV	20598	24873	1.05%	0.109%
31	12.502	953	955	957	rBV	101004	126631	5.33%	0.557%
32	12.548	957	959	961	rBV3	36555	43003	1.81%	0.189%
33	12.719	972	974	977	rBV	114400	159461	6.71%	0.702%
34	12.879	986	988	990	rBV	1657060	1607056	67.61%	7.074%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.119	1007	1009	1011	rBV2	33828	37462	1.58%	0.165%
36	13.154	1011	1012	1017	rVV3	28551	63680	2.68%	0.280%
37	13.245	1018	1020	1022	rBV	29826	38954	1.64%	0.171%
38	13.805	1067	1069	1072	rBV2	74339	118101	4.97%	0.520%
39	13.920	1076	1079	1080	rBV	701897	688516	28.97%	3.031%
40	15.200	1189	1191	1194	rBV	124950	172108	7.24%	0.758%
41	15.314	1199	1201	1203	rVB	370383	411763	17.32%	1.812%
42	15.463	1212	1214	1217	rVB2	125654	187592	7.89%	0.826%
43	15.977	1257	1259	1267	rVB	258807	574850	24.19%	2.530%
44	16.377	1291	1294	1301	rVB	295482	560226	23.57%	2.466%
45	16.903	1338	1340	1343	rVV	96838	163061	6.86%	0.718%
46	16.971	1344	1346	1350	rVB2	105441	205261	8.64%	0.903%

Sum of corrected areas: 22719267

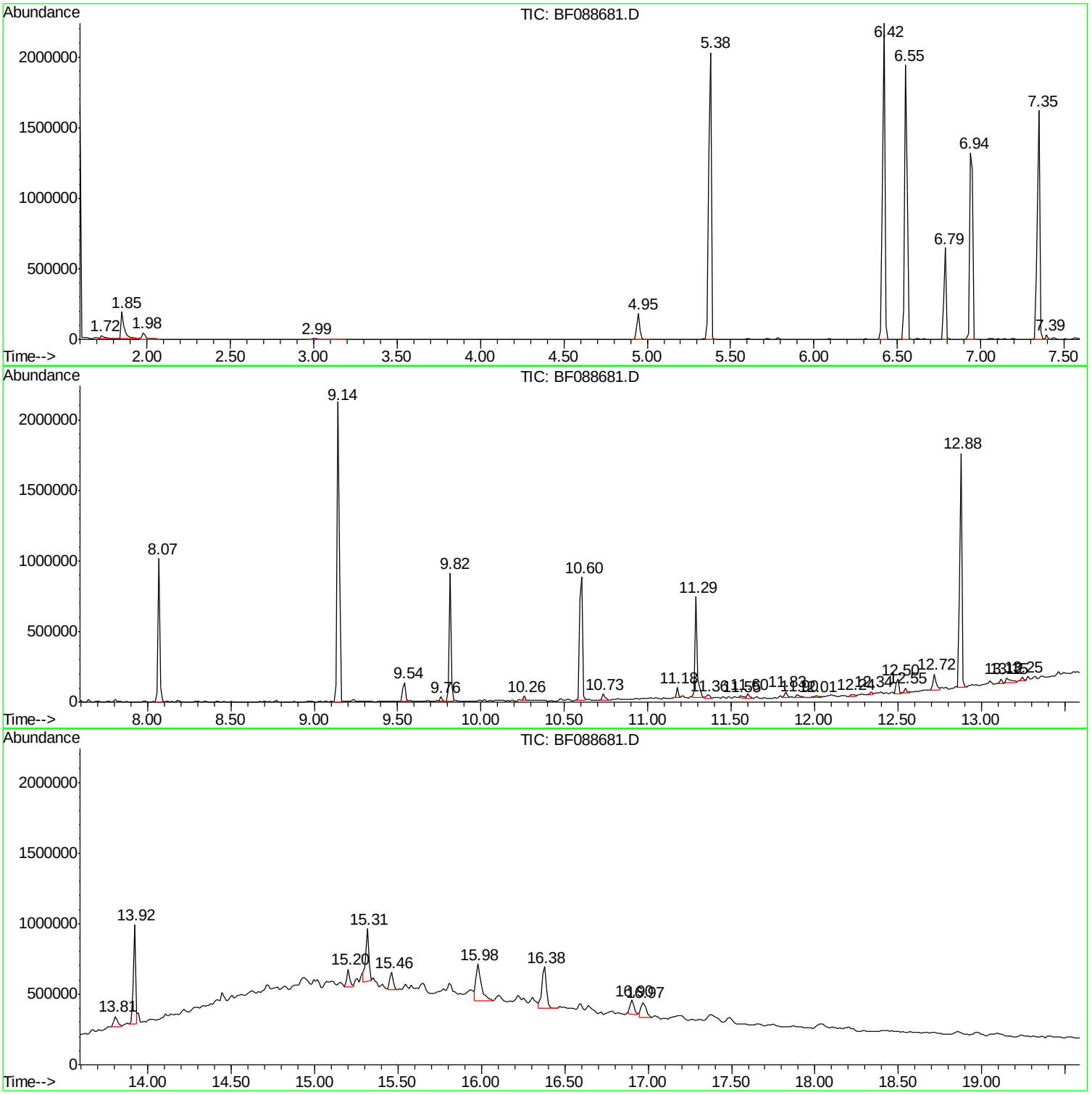
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

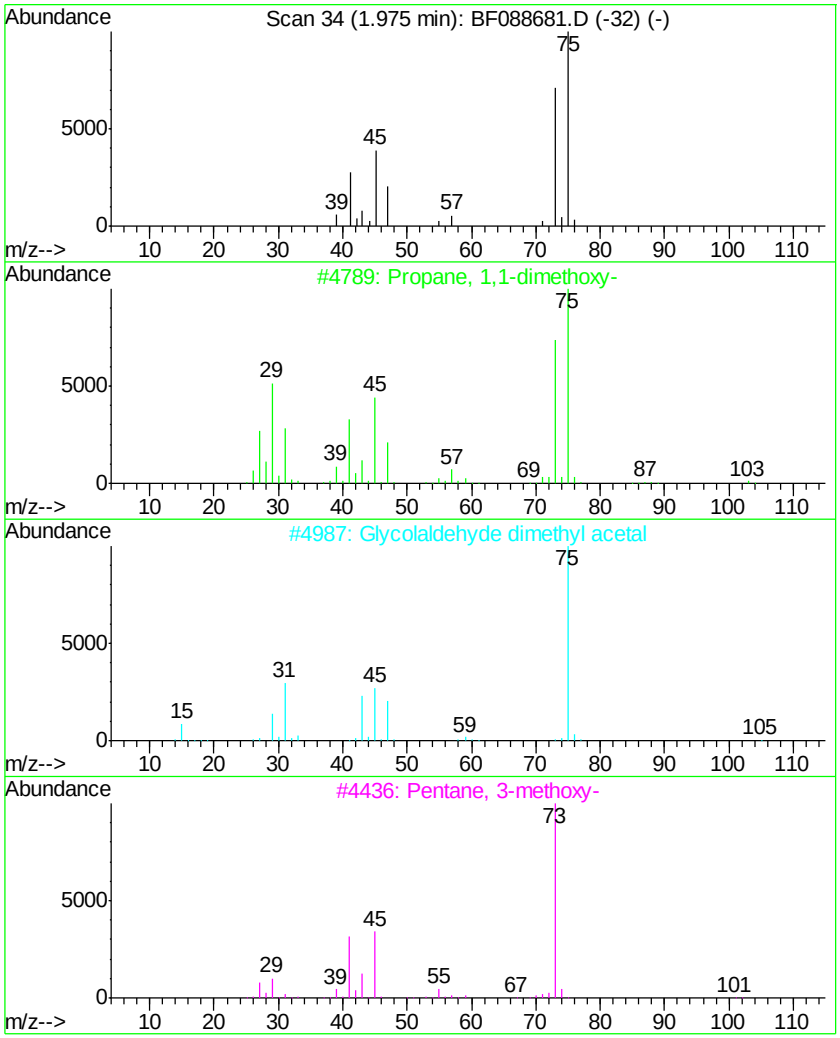
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

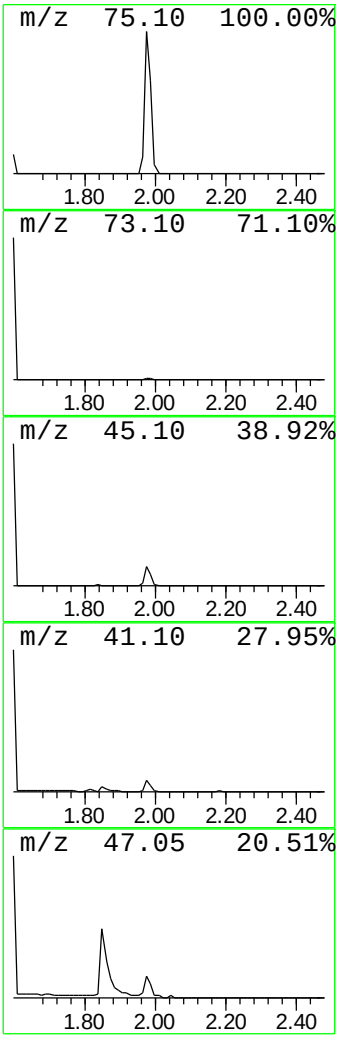
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.98	2.31 ng	72059	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5	Glycine	75	C2H5NO2	000056-40-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

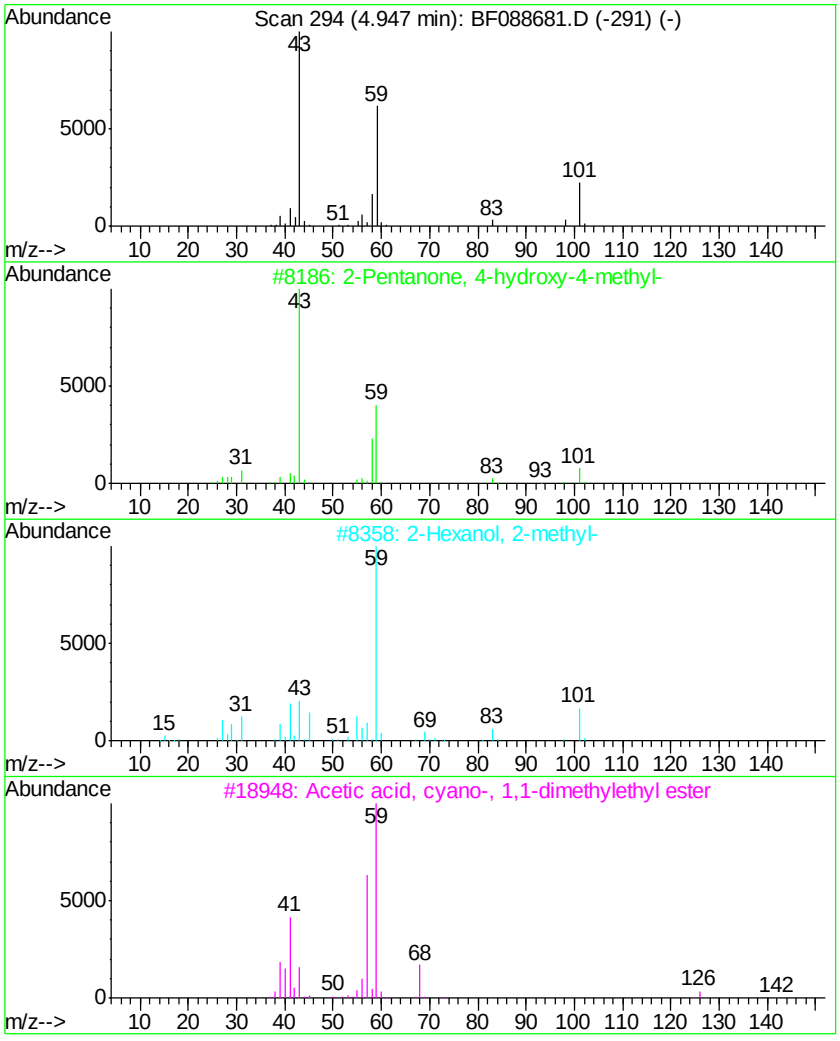
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

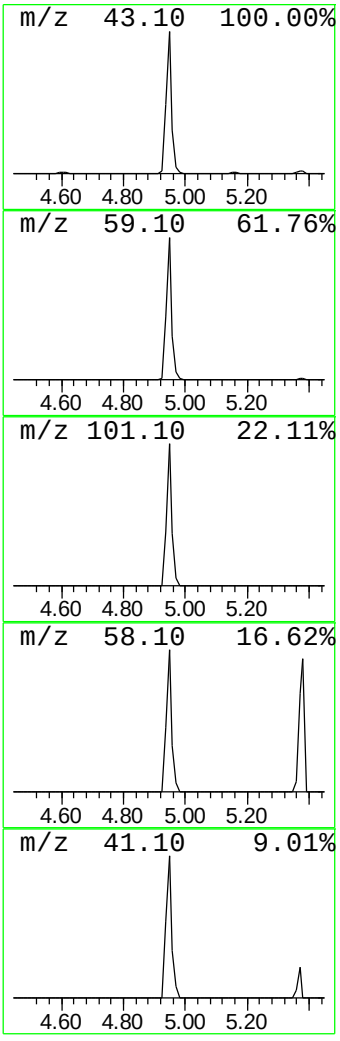
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	7.35 ng	229095	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

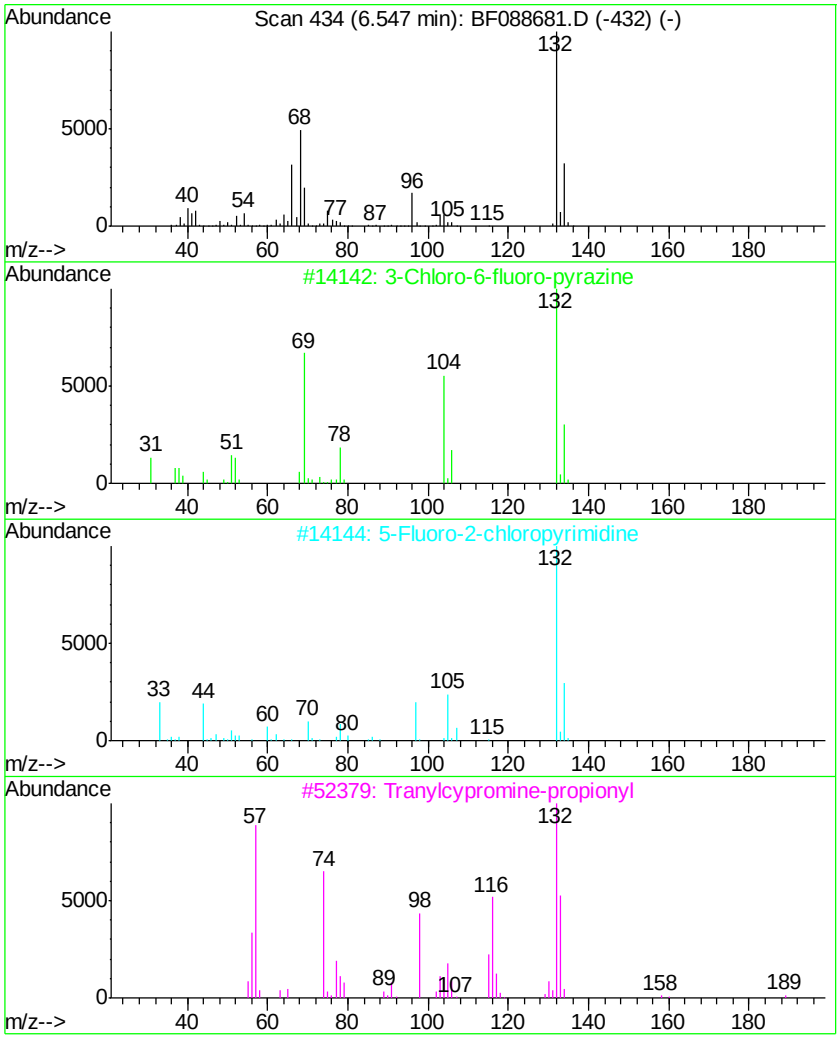
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

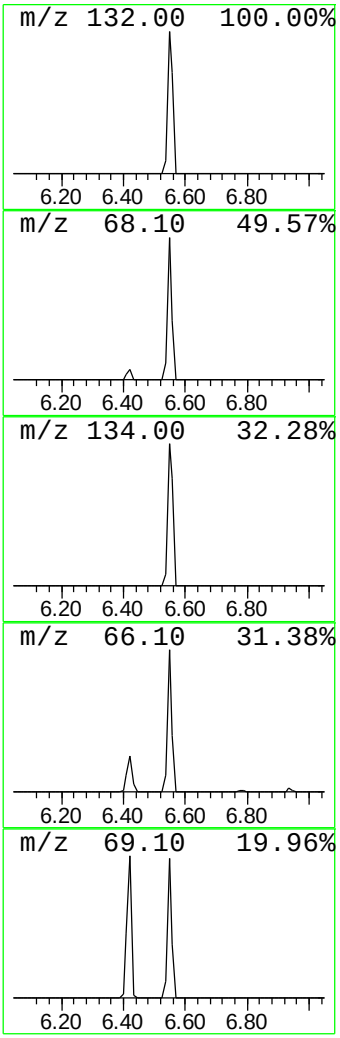
****

Peak Number 4 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	70.62 ng	2200510	1,4-Dichlorobenzene-d4	6.79

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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

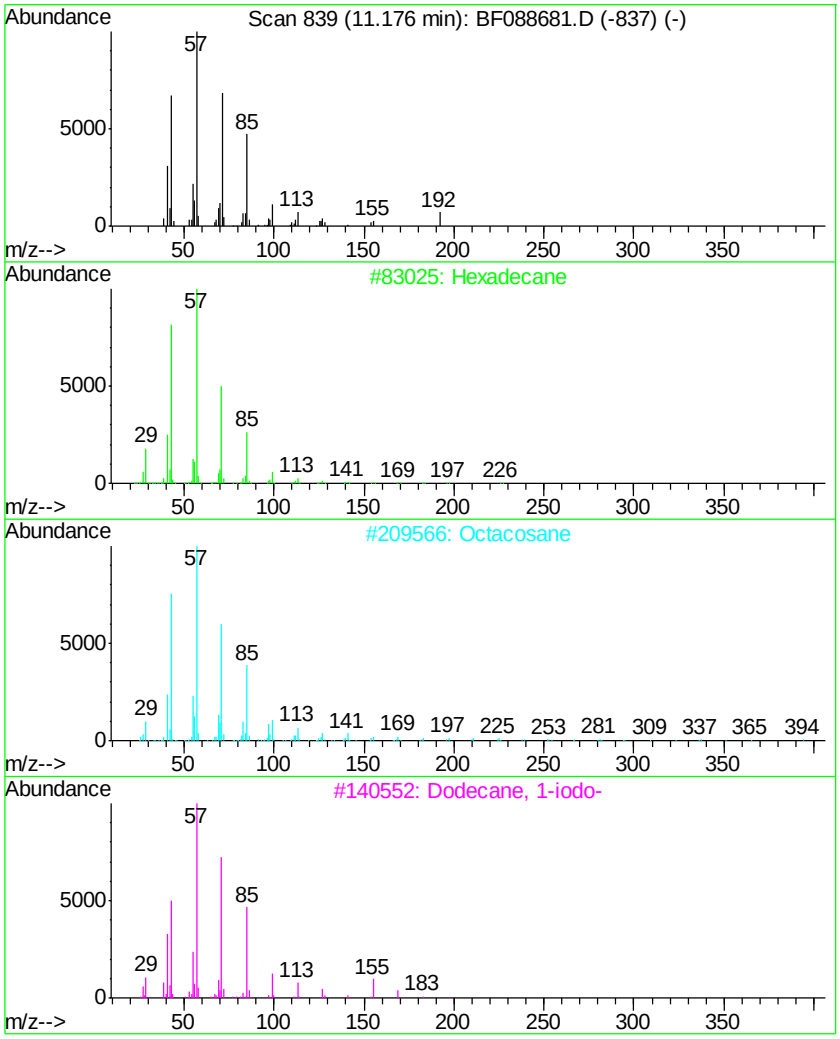
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

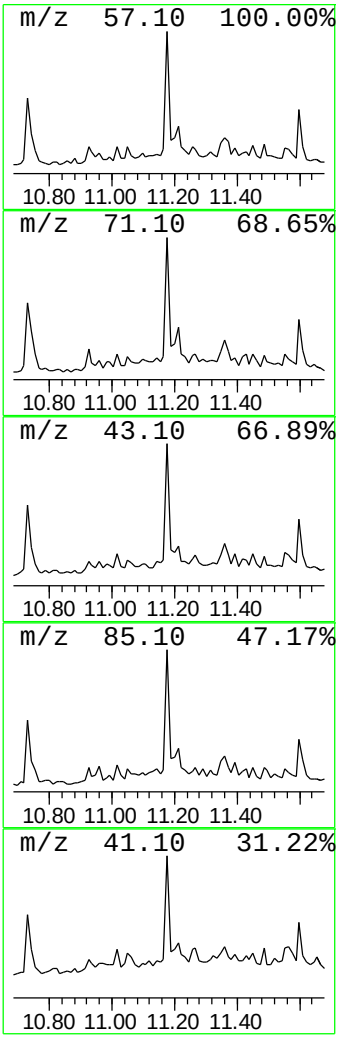
****

Peak Number 6 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	2.05 ng	67639	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Octacosane	394	C28H58	000630-02-4	86
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Tetracosane	338	C24H50	000646-31-1	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

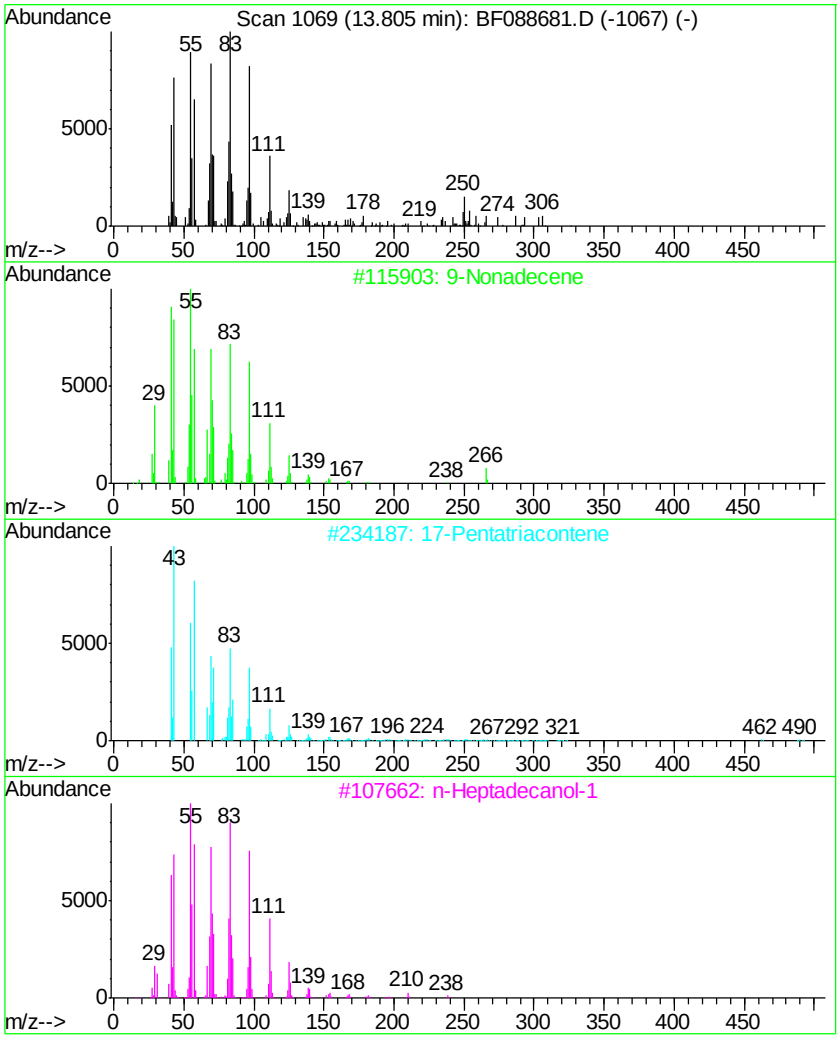
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

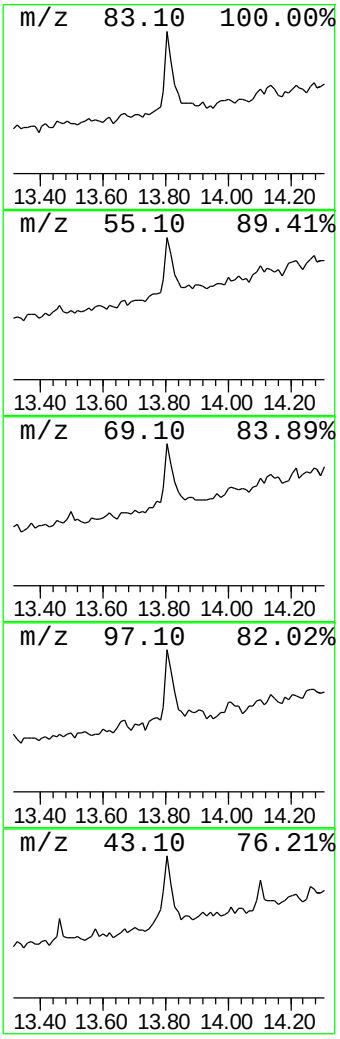
****

Peak Number 7 9-Nonadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.43 ng	118101	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Nonadecene	266	C19H38	031035-07-1	92
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	86
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	80
5	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

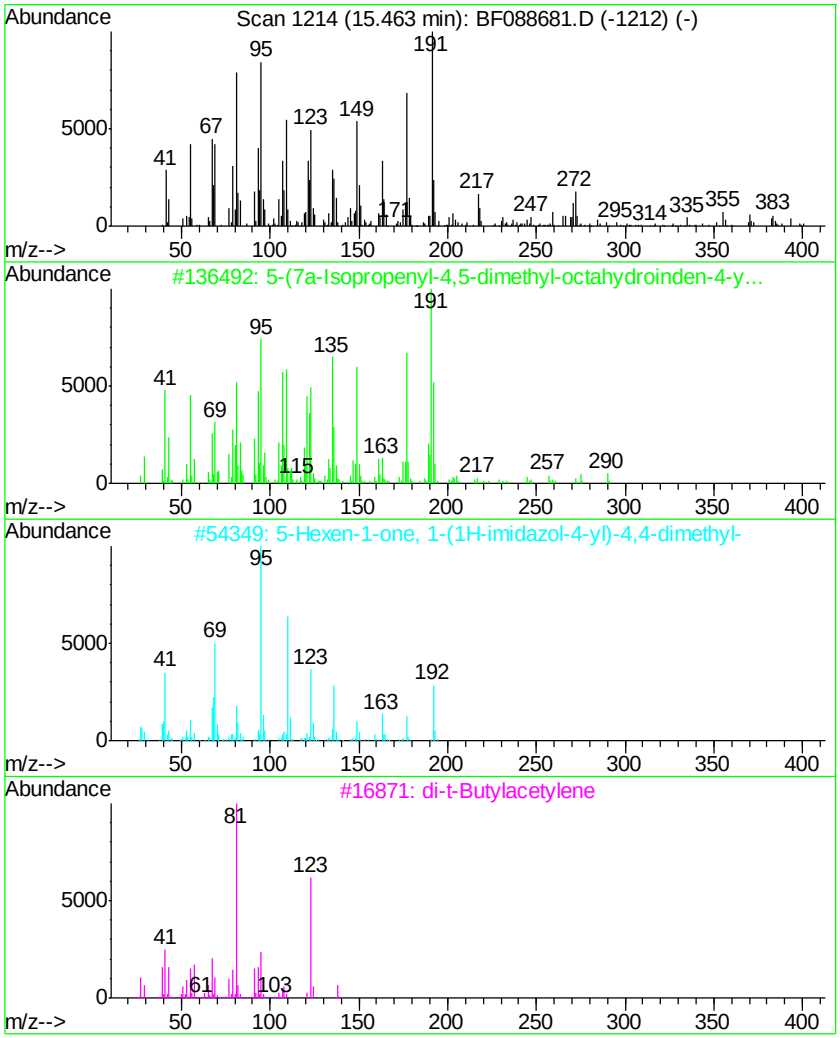
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

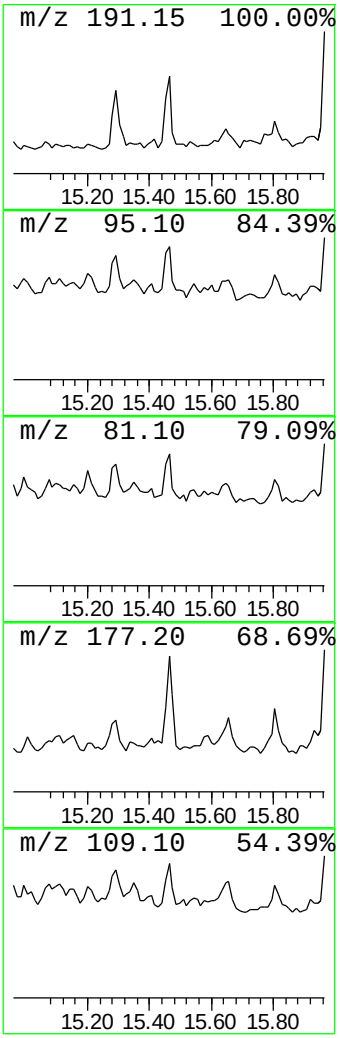
****

Peak Number 9 5-(7a-Isopropenyl-4,5-dimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	9.11 ng	187592	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(7a-Isopropenyl-4,5-dimethyl-o...	290	C20H34O	1000193-54-0	53
2	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	18
3	di-t-Butylacetylene	138	C10H18	017530-24-4	18
4	3,4-Dihydrocoumarin, 6-amino-4,4...	191	C11H13NO2	1000128-49-9	14
5	Divinylbis(cyclopropyl)silane	164	C10H16Si	1000109-95-2	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

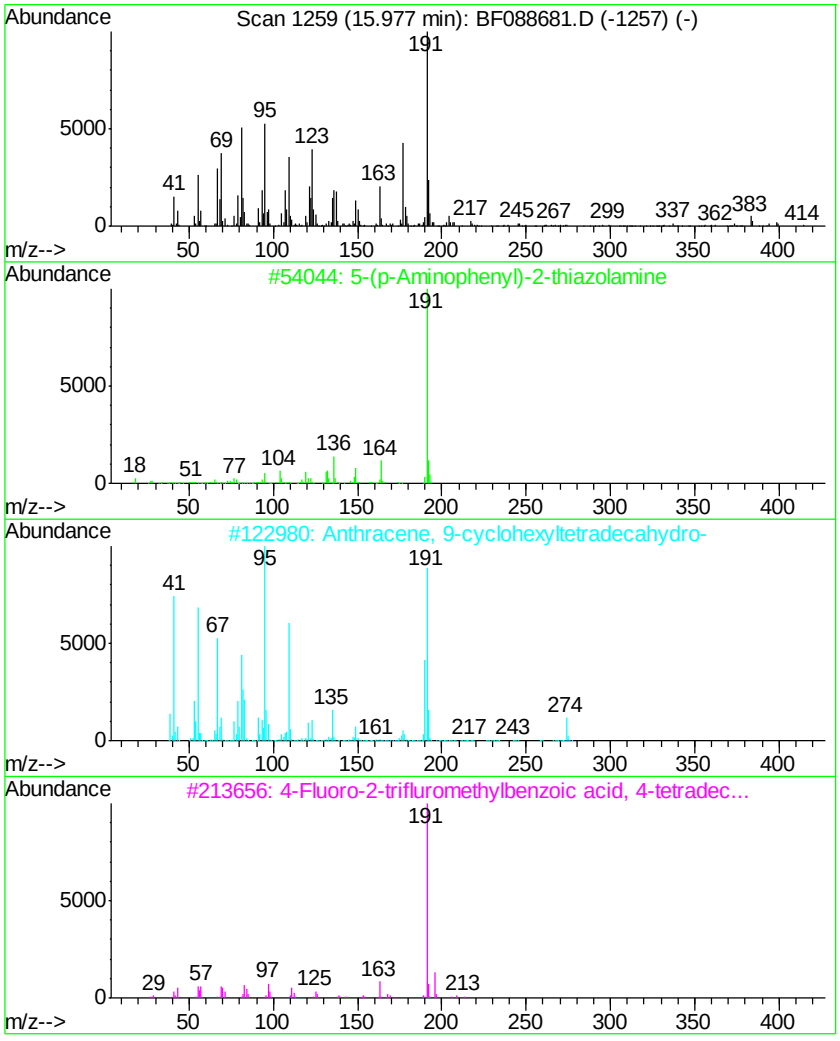
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

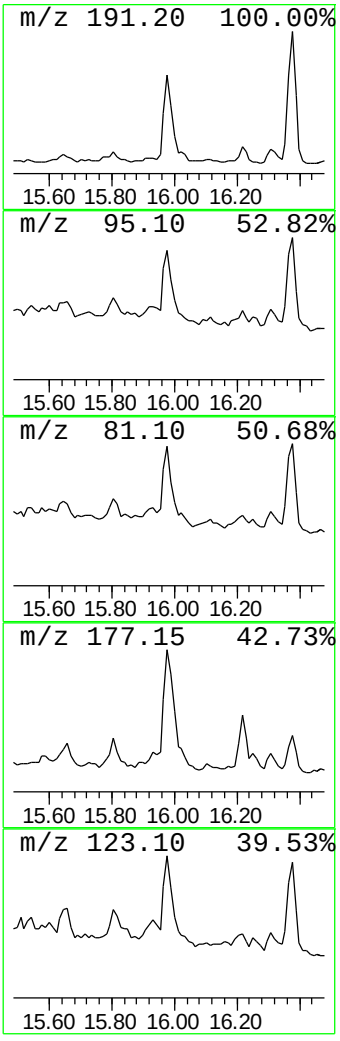
****

Peak Number 10 unknown15.98 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	27.92 ng	574850	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	30
2	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	27
3	4-Fluoro-2-trifluromethylbenzoic...	404	C22H32F4O2	1000338-50-2	22
4	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	22
5	Isophthalic acid, 2,6-dichloroph...	352	C17H14Cl2O4	1000344-61-9	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

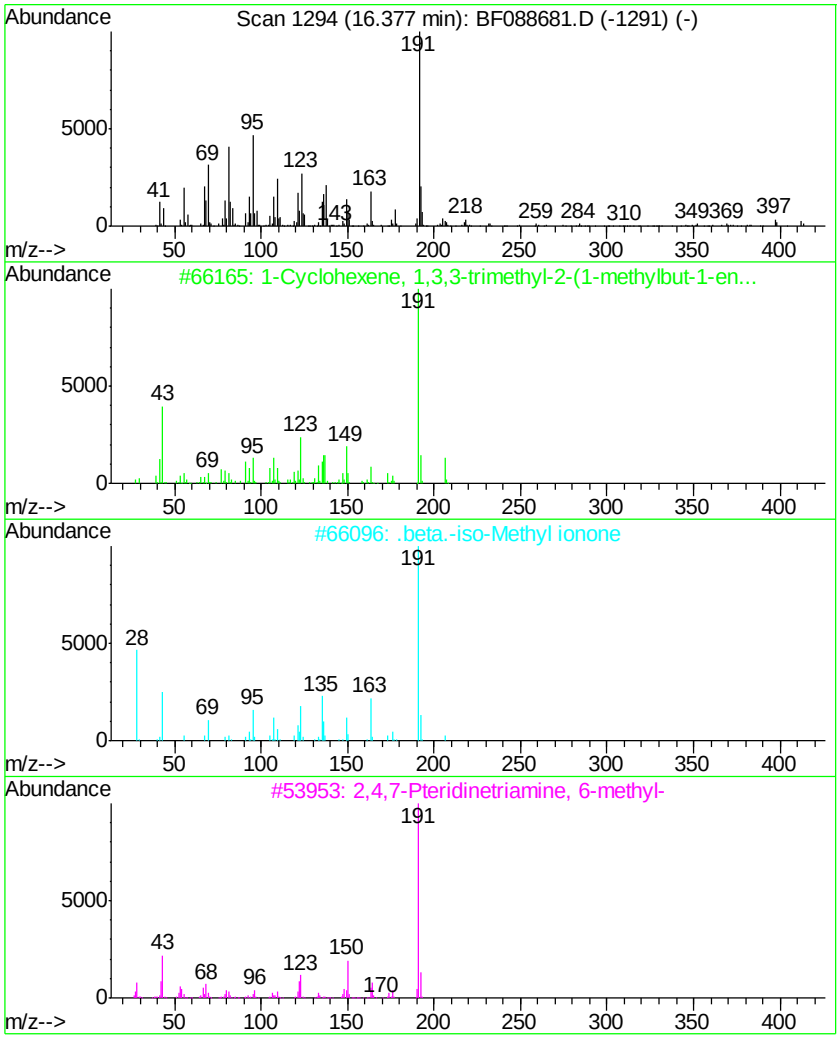
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

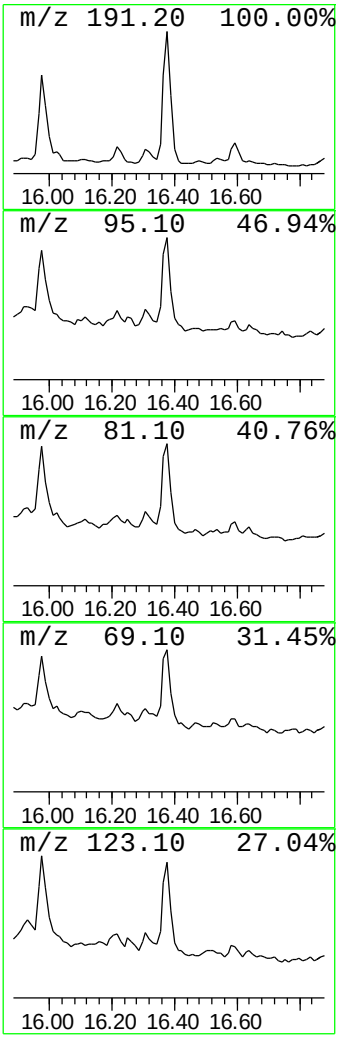
****

Peak Number 11 1-Cyclohexene, 1,3,3-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	27.21 ng	560226	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	53
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	52
3	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	38
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	38
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

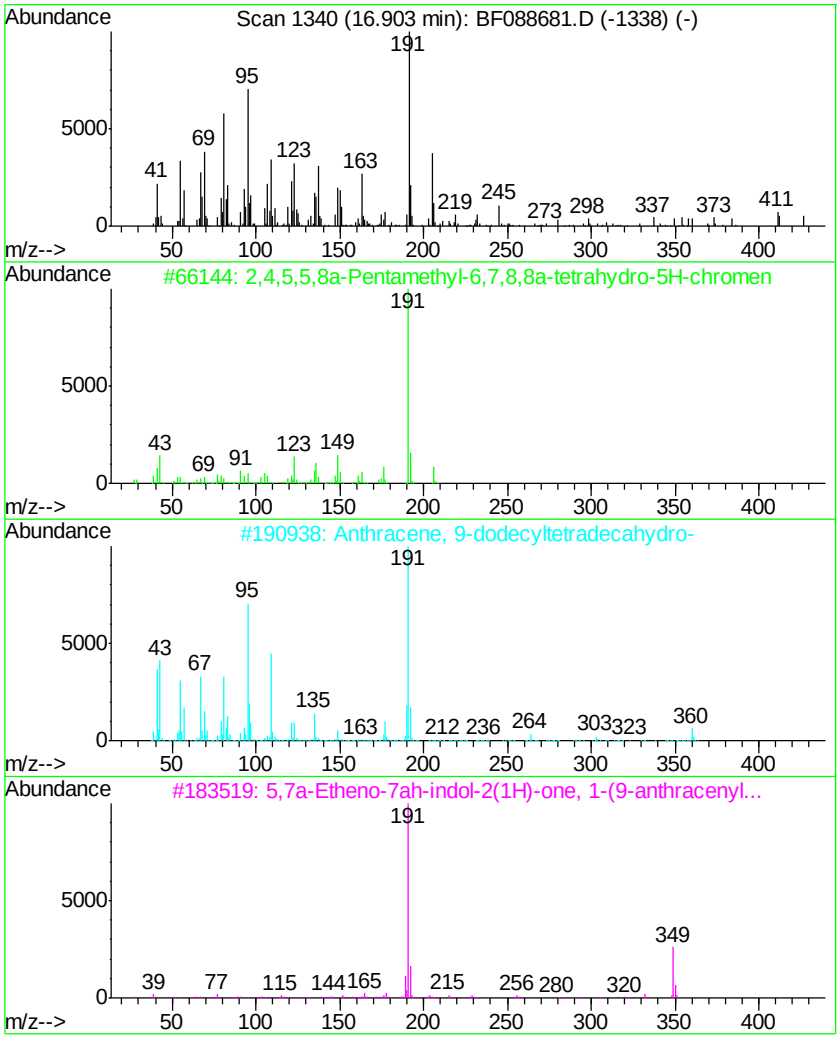
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

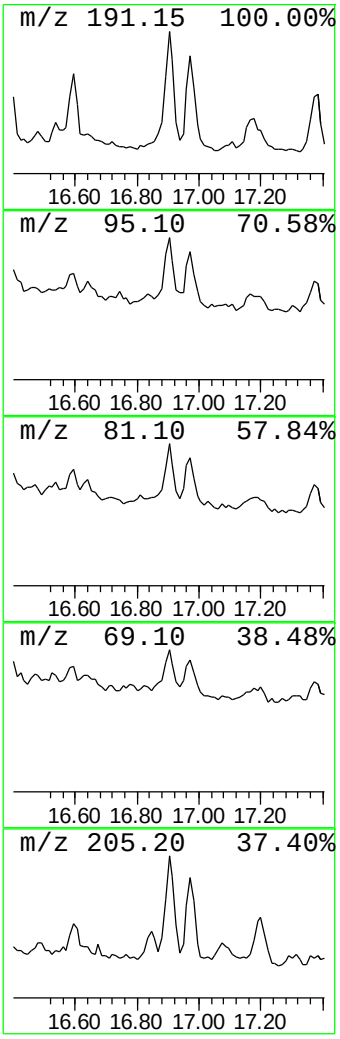
****

Peak Number 12 unknown16.90 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	7.92 ng	163061	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	46
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38
3	5,7a-Etheno-7ah-indol-2(1H)-one,...	349	C25H19NO	117800-57-4	38
4	1H-Inden-1-one, 2,3-dihydro-5,6-...	206	C12H14O3	004082-25-1	38
5	Anthracene, 9-(3-butenyl)-	232	C18H16	097451-55-3	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

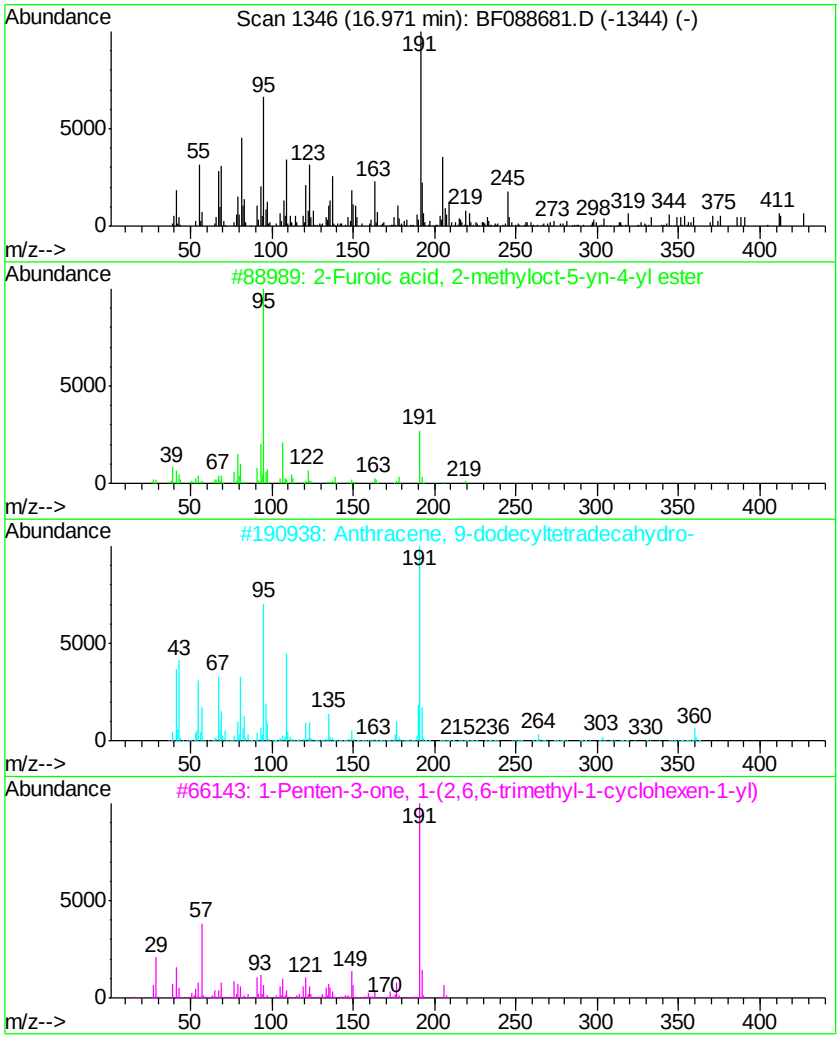
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

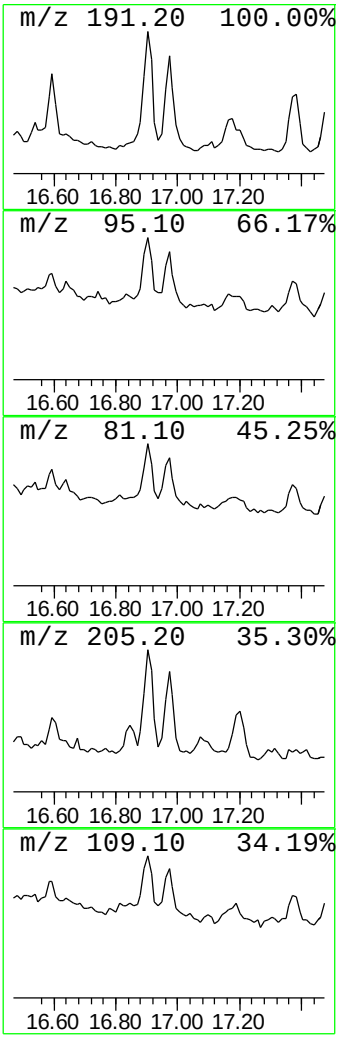
****

Peak Number 13 2-Furoic acid, 2-methyloct-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	9.97 ng	205261	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furoic acid, 2-methyloct-5-yn-...	234	C14H18O3	1000299-23-7	50
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	50
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	50
4	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	45
5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088681.D
Acq On : 4 Jul 2016 8:15
Operator : UM/SJ
Sample : H3849-01
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F11-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 1,1-dime...	1.98	2.3	ng	72059	1	6.79	623174	20.0
2-Pentanone, 4-hy...	4.95	7.3	ng	229095	1	6.79	623174	20.0
unknown6.55	6.55	70.6	ng	2200510	1	6.79	623174	20.0
Hexadecane	11.18	2.0	ng	67639	4	11.29	661297	20.0
9-Nonadecene	13.81	3.4	ng	118101	5	13.92	688516	20.0
5-(7a-Isopropenyl...	15.46	9.1	ng	187592	6	15.31	411763	20.0
unknown15.98	15.98	27.9	ng	574850	6	15.31	411763	20.0
1-Cyclohexene, 1,...	16.38	27.2	ng	560226	6	15.31	411763	20.0
unknown16.90	16.90	7.9	ng	163061	6	15.31	411763	20.0
2-Furoic acid, 2-...	16.97	10.0	ng	205261	6	15.31	411763	20.0