LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

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-BF060716.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	1.747	12	14	23	rVB	187955	371299	5.80%	1.572%
2	1.873	23	25	98	rVB	2713508	6404882	100.00%	27.118%
3	4.970	294	296	300	rBV	71186	77109	1.20%	0.326%
4	5.393	331	333	336	rVB	850240	1177148	18.38%	4.984%
5	6.444	422	425	427	rBV	1290188	1334393	20.83%	5.650%
6	6.570	434	436	439	rBV	1025798	1241718	19.39%	5.257%
7	6.810	455	457	459	rBV	948070	761562	11.89%	3.224%
8	6.970	468	471	473	rBV	1010936	1037521	16.20%	4.393%
9	7.370	504	506	509	rBV	752352	730315	11.40%	3.092%
10	8.102	567	570	572	rBV	988245	976173	15.24%	4.133%
11	9.176	661	664	666	rBV	1427311	1394035	21.77%	5.902%
12	9.565	696	698	700	rVB	104271	80143	1.25%	0.339%
13	9.851	720	723	724	rBV	1025663	986096	15.40%	4.175%
14	10.628	789	791	794	rBV	783122	688992	10.76%	2.917%
15	11.325	850	852	853	rBV	876671	764433	11.94%	3.237%
16	11.394	856	858	860	rVB	79584	85562	1.34%	0.362%
17	11.931	904	905	910	rVB	61495	91129	1.42%	0.386%
18	12.525	955	957	960	rBV	324312	421043	6.57%	1.783%
19	12.754	973	977	980	rBV	368709	483424	7.55%	2.047%
20	12.902	988	990	993	rVB	862270	859579	13.42%	3.639%
21	13.085	1000	1006	1008	rBV	63572	103843	1.62%	0.440%
22	13.702	1057	1060	1061	rBV2	45047	73326	1.14%	0.310%
23	13.805	1066	1069	1073	rVB3	56146	116715	1.82%	0.494%
24	13.954	1078	1082	1083	rBV2	797400	1071425	16.73%	4.536%
25	14.960	1167	1170	1174	rBV	206573	383668	5.99%	1.624%
26	15.245	1192	1195	1197	rVB	103906	150605	2.35%	0.638%
27	15.303	1197	1200	1203	rBV	140480	227126	3.55%	0.962%
28	15.360	1203	1205	1207	rBV	481811	586745	9.16%	2.484%
29	15.497	1215	1217	1223	rVB4	56339	95733	1.49%	0.405%
30	16.023	1261	1263	1272	rVB	137946	297596	4.65%	1.260%
31	16.434	1296	1299	1304	rVB	121582	253875	3.96%	1.075%
32	16.720	1321	1324	1328	rVB2	56838	122103	1.91%	0.517%
33	16.971	1343	1346	1349	rVB	44351	84491	1.32%	0.358%
34	17.120	1357	1359	1364	rVB	41469	84459	1.32%	0.358%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

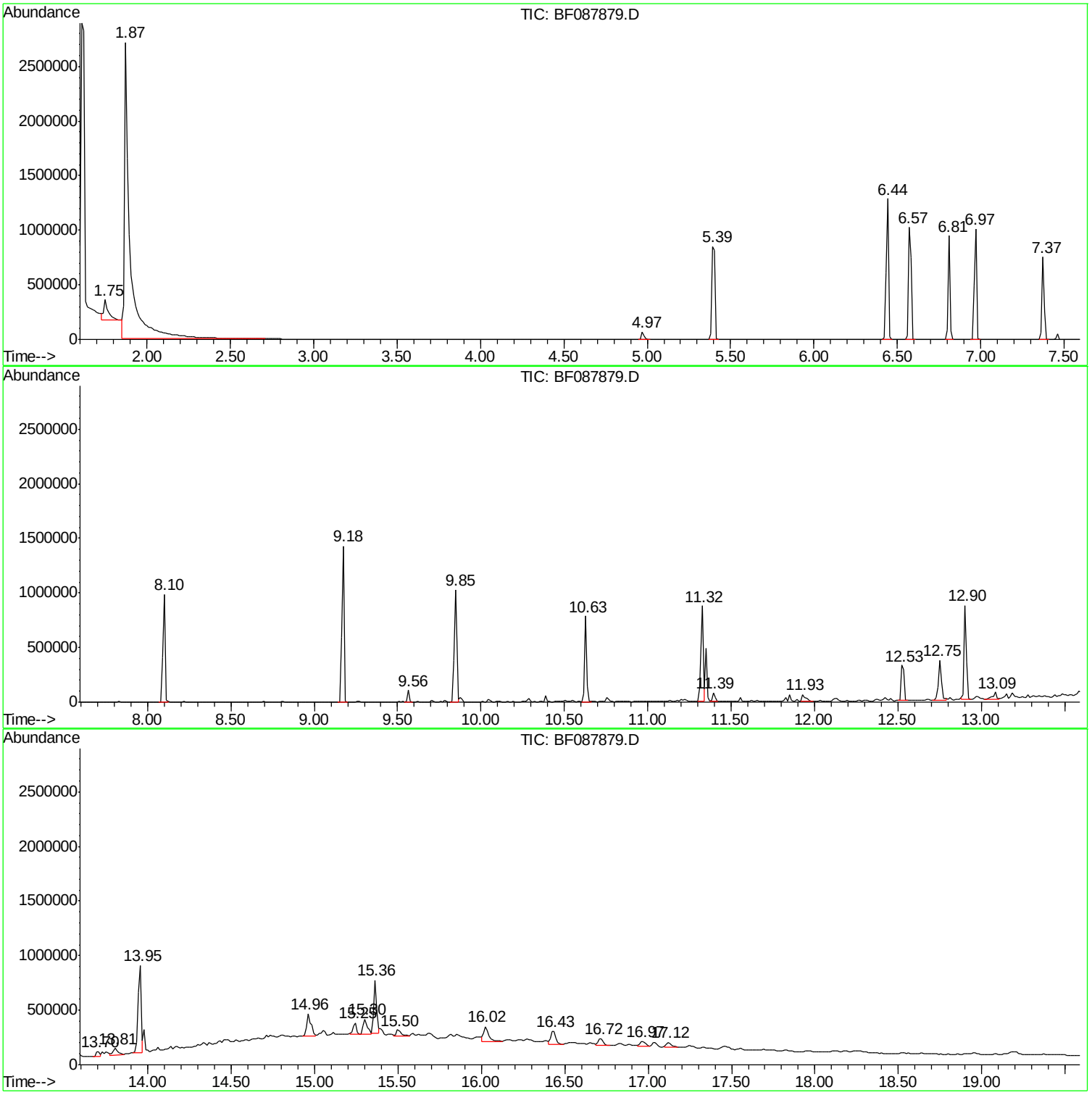
Sum of corrected areas: 23618266

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

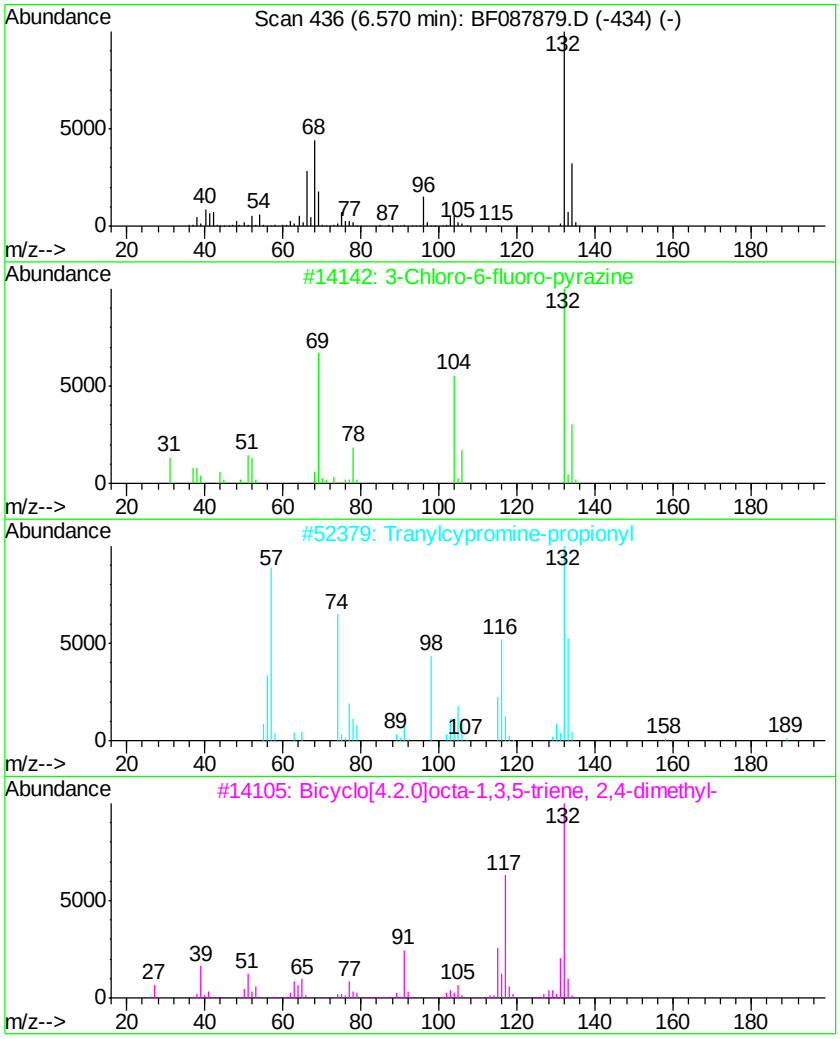
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

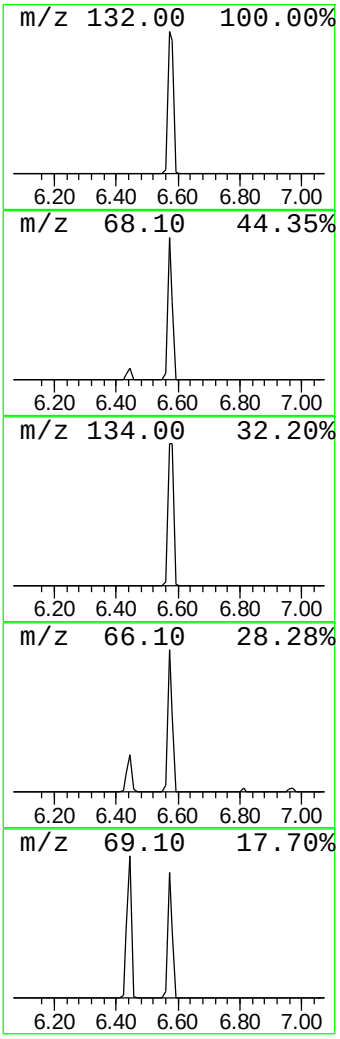
****

Peak Number 3 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	23.94 ng	1241720	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

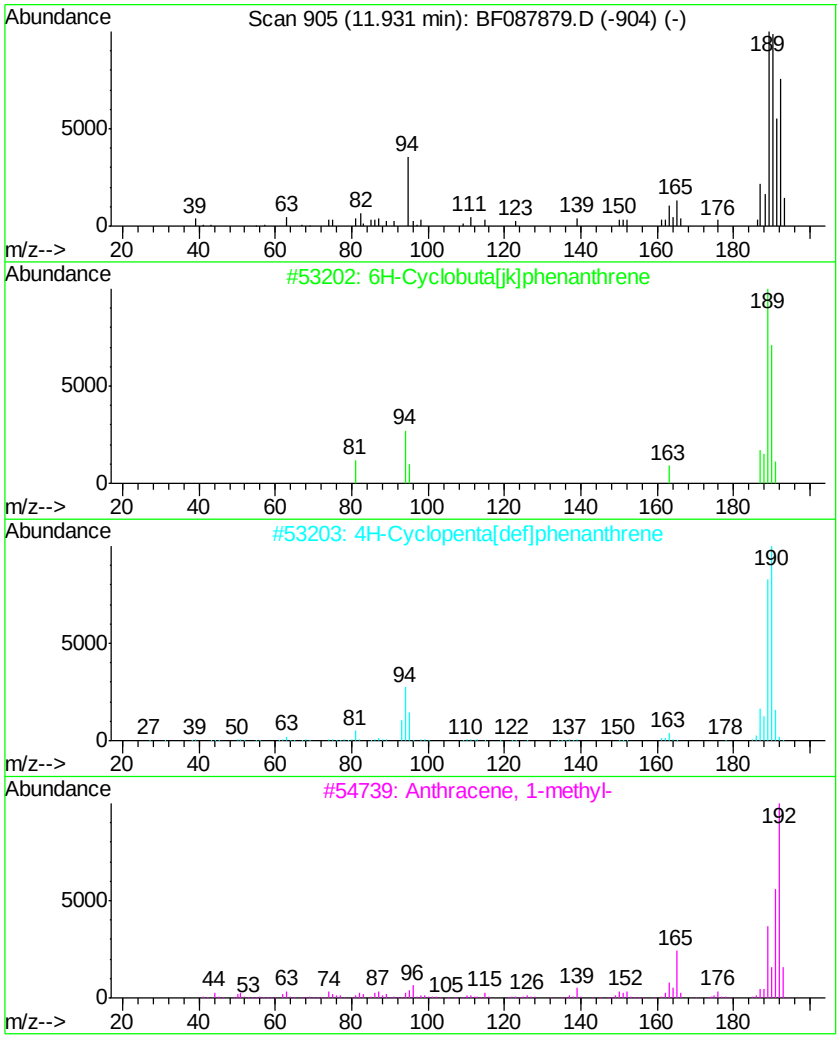
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

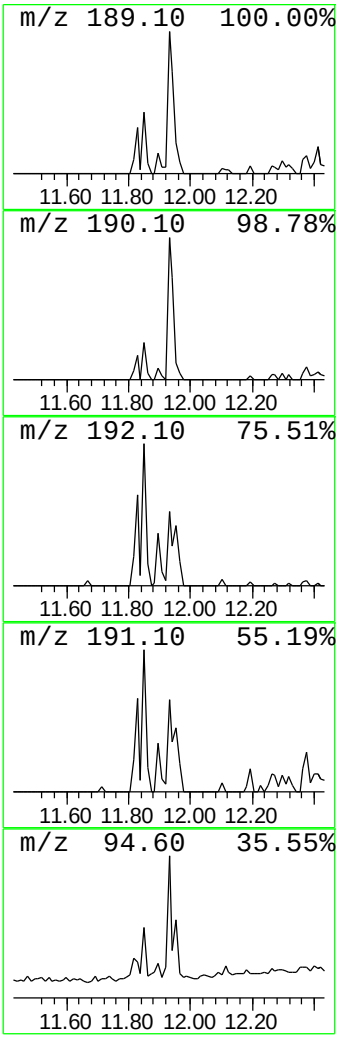
****

Peak Number 5 unknown11.93 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.38 ng	91129	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

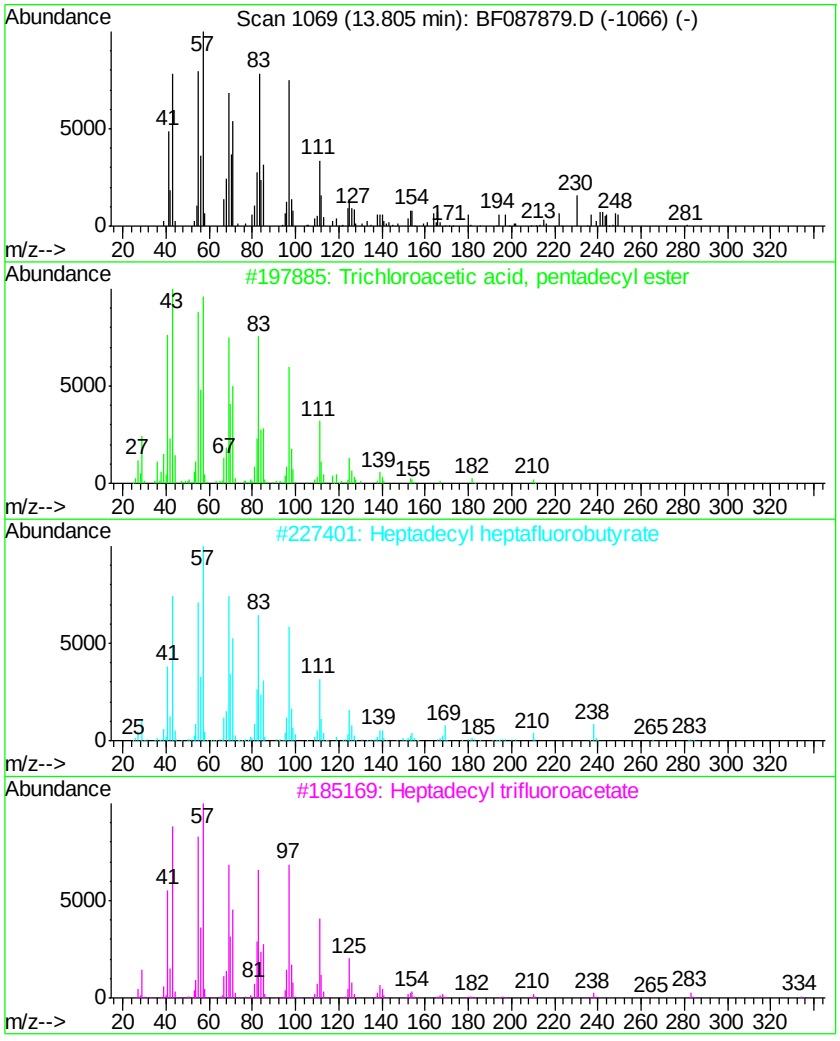
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

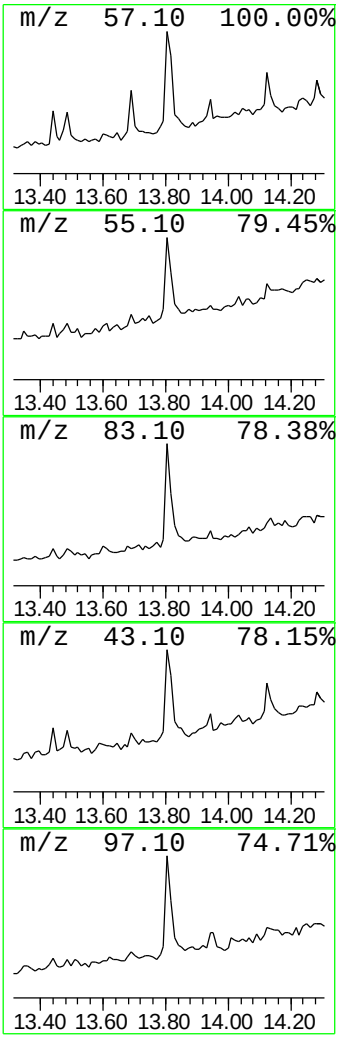
****

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.18 ng	116715	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	81





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

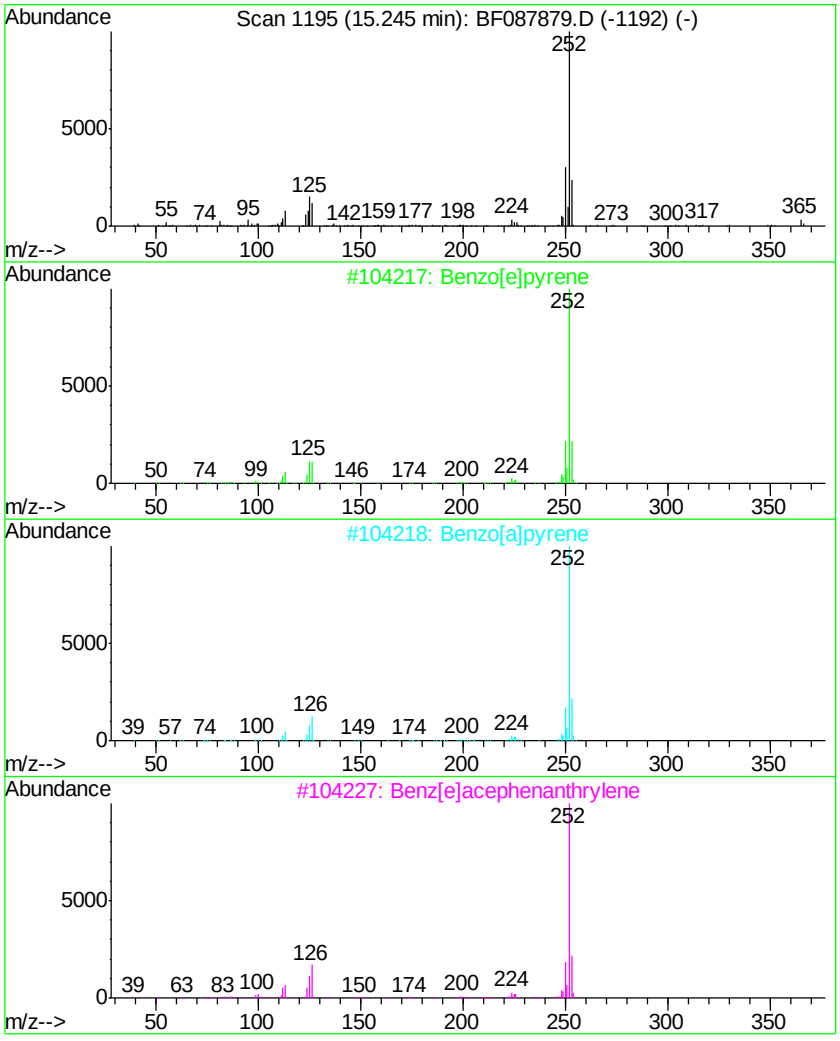
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

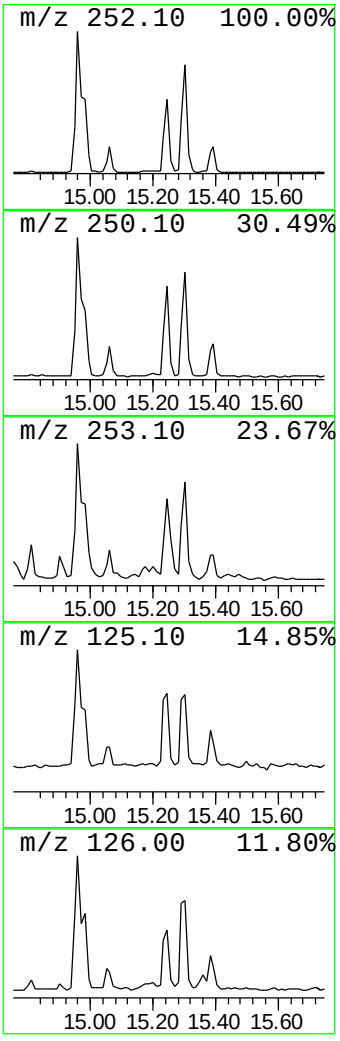
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	5.13 ng	150605	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
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Acq On : 10 Jun 2016 17:25
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Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

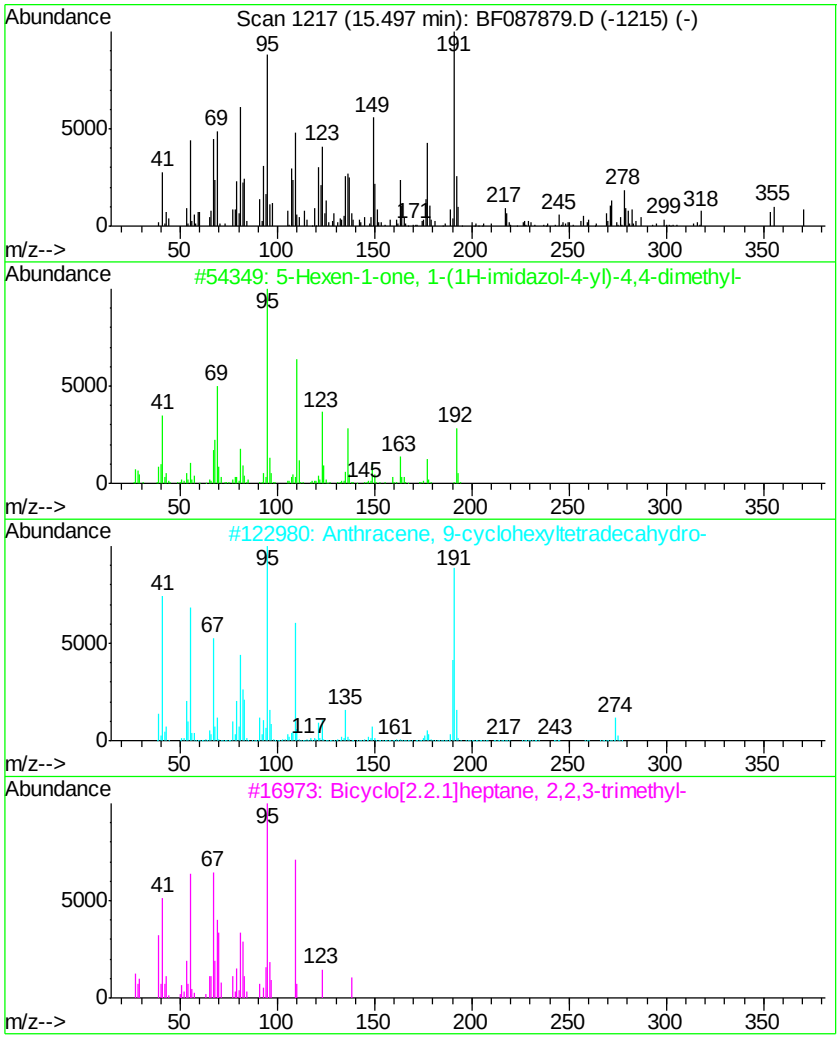
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

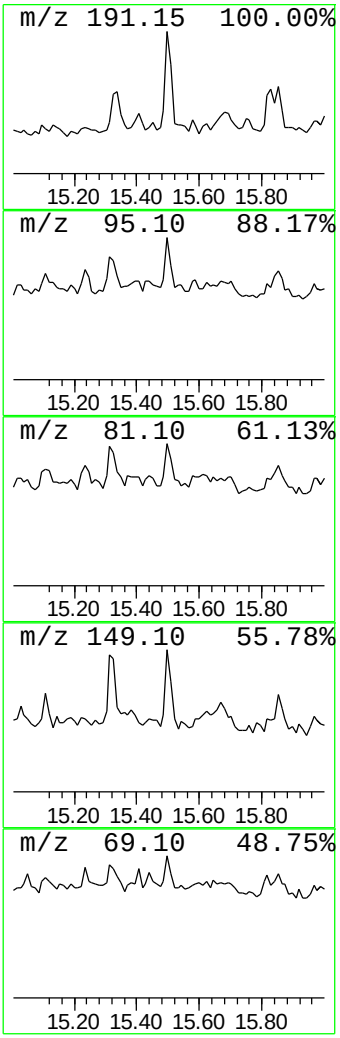
****

Peak Number 8 unknown15.50 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	3.26 ng	95733	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	38
2	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
3	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	30
4	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	18
5	Cyclopentene, 1-isopropyl-4,5-di...	138	C10H18	007712-74-5	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
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Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

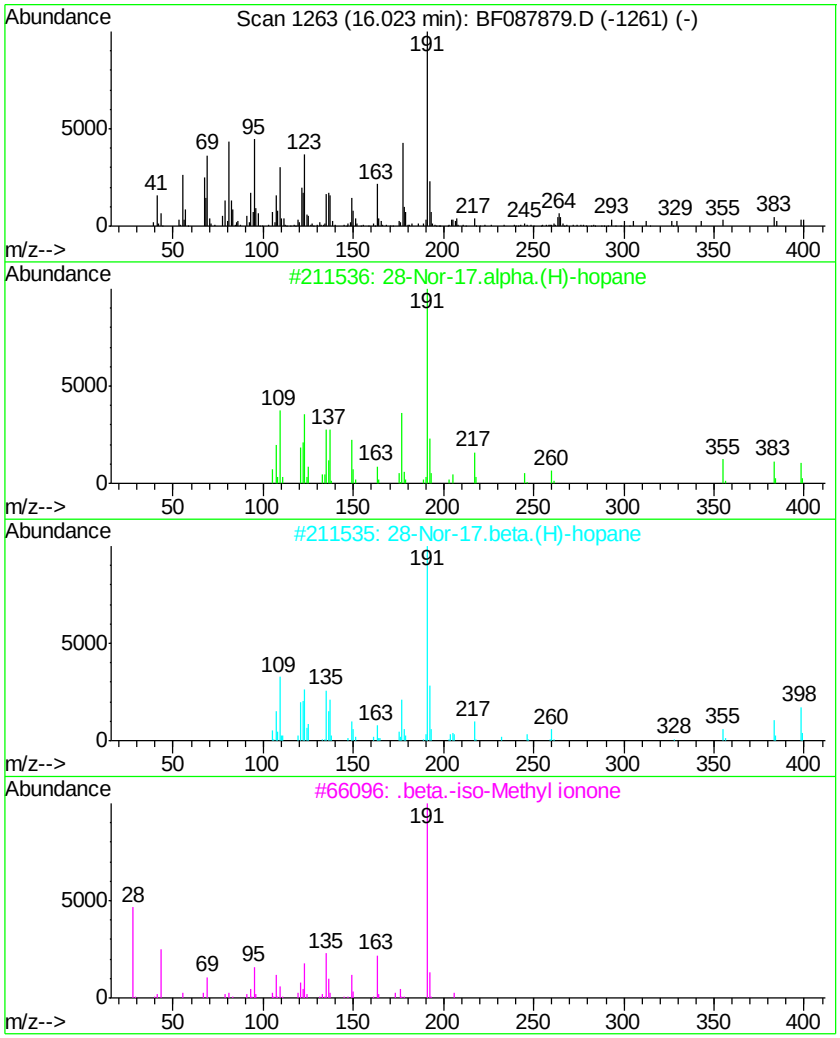
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

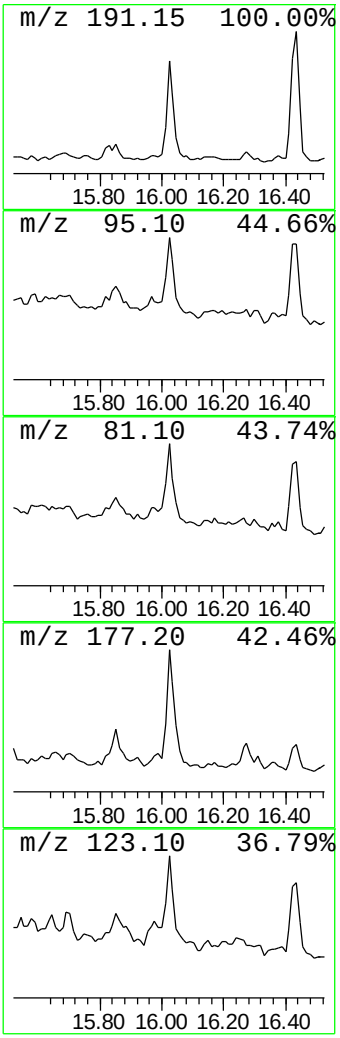
****

Peak Number 9 28-Nor-17.alpha.(H)-hopane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	10.14 ng	297596	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	80
2	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	64
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	32
5	4-Fluoro-2-trifluoromethylbenzoi...	326	C17H14F4O2	1000357-28-0	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087879.D
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Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

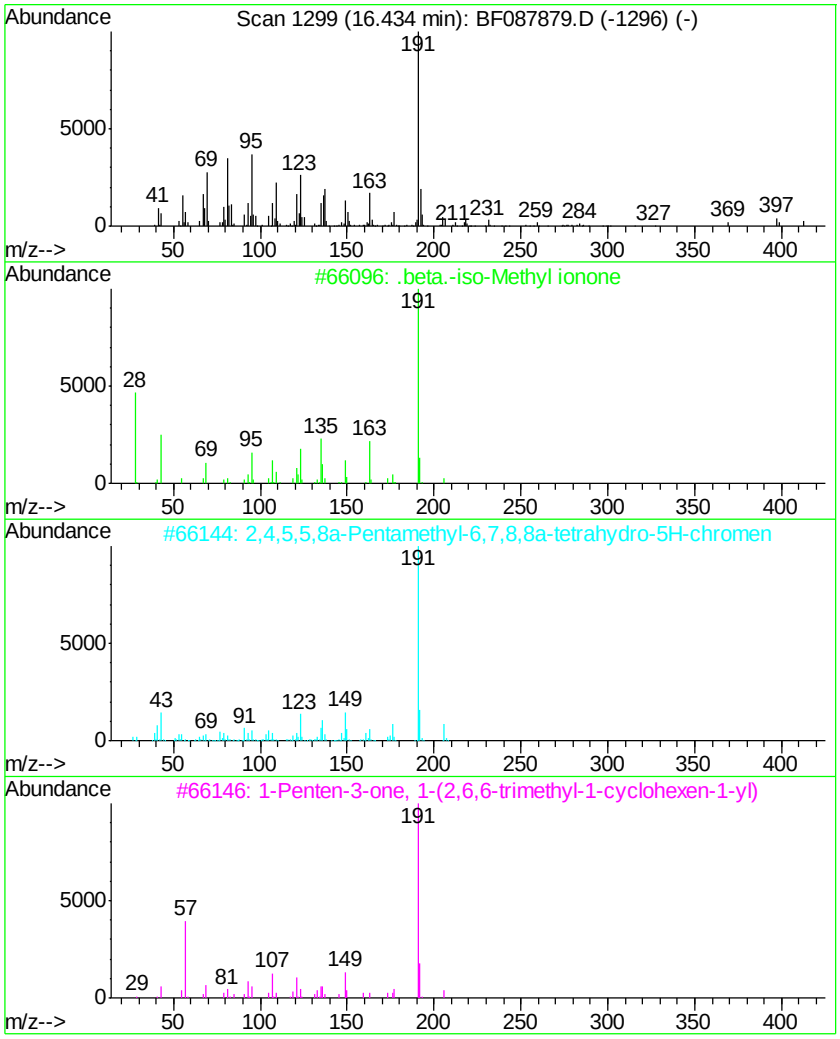
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

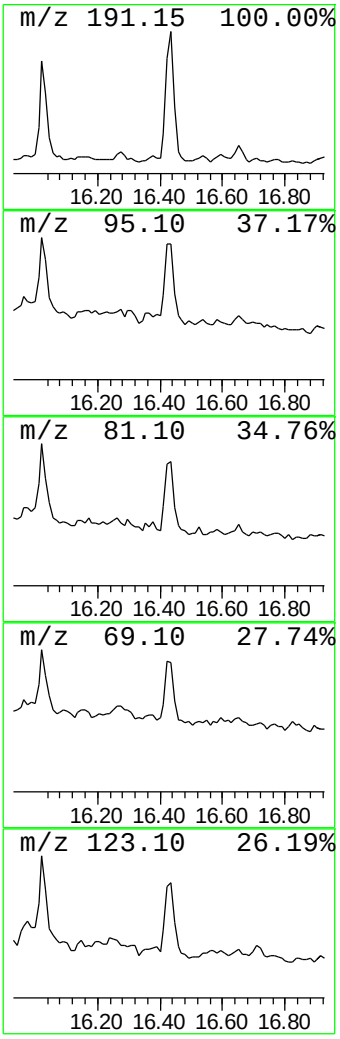
****

Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	8.65 ng	253875	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	62
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	59
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	49
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	45
5	4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	43





Library Search Compound Report

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

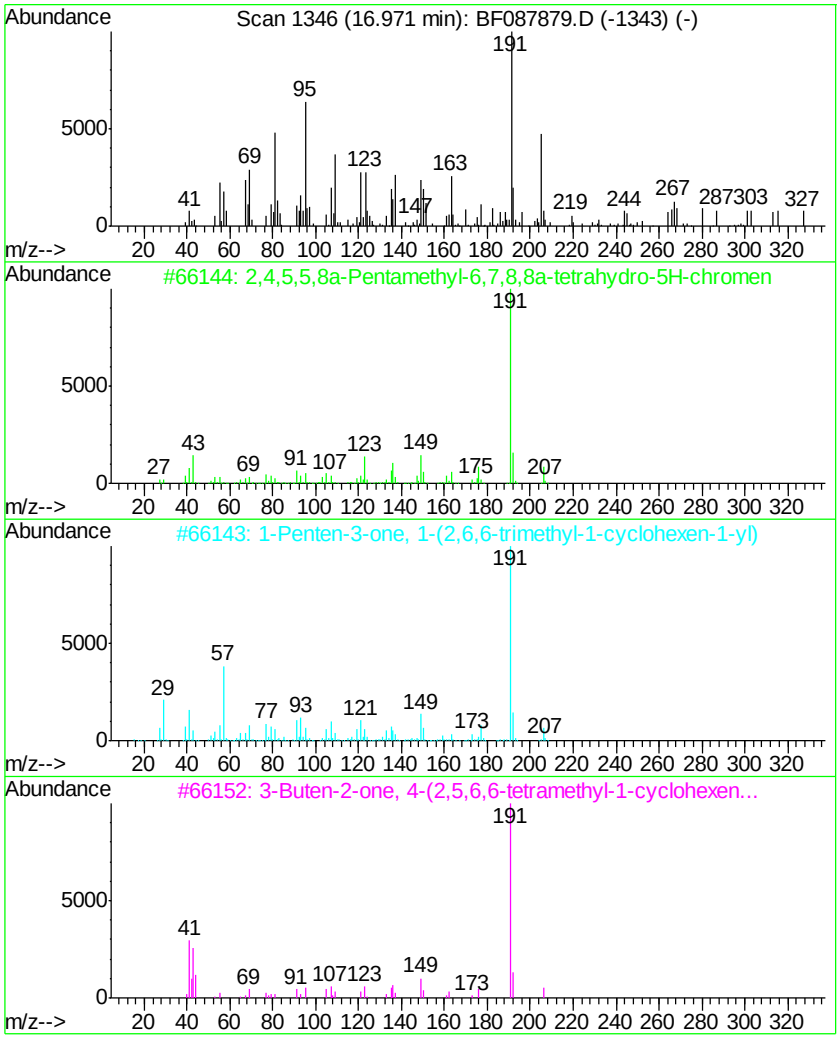
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

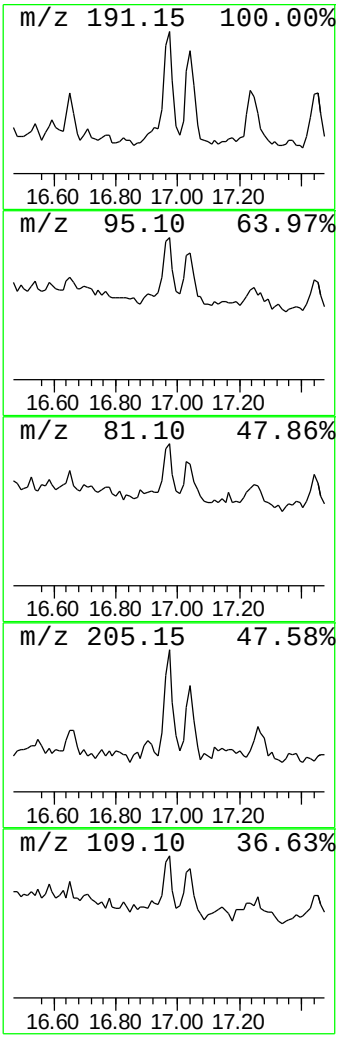
****

Peak Number 11 unknown16.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	2.88 ng	84491	Perylene-d12	15.36

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	38
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	30
3	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	27
4	Silane, diethylethoxy(2-isopropy...	266	C15H26O2Si	1000363-84-5	27
5	3-Fluoro-4-trifluoromethylbenzoi...	250	C11H10F4O2	1000357-93-2	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
Data File : BF087879.D
Acq On : 10 Jun 2016 17:25
Operator : UM/SJ
Sample : H3426-12 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-57

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
unknown6.57	6.57	23.9	ng	1241720	1	6.97	1037520	20.0
unknown11.93	11.93	2.4	ng	91129	4	11.32	764433	20.0
Trichloroacetic a...	13.81	2.2	ng	116715	5	13.95	1071430	20.0
Benzo[e]pyrene	15.25	5.1	ng	150605	6	15.36	586745	20.0
unknown15.50	15.50	3.3	ng	95733	6	15.36	586745	20.0
28-Nor-17.alpha.(...	16.02	10.1	ng	297596	6	15.36	586745	20.0
.beta.-iso-Methyl...	16.43	8.7	ng	253875	6	15.36	586745	20.0
unknown16.97	16.97	2.9	ng	84491	6	15.36	586745	20.0