LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090178.D
Acq On : 22 Sep 2016 00:06
Operator : UM/SJ
Sample : H4856-03 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

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-BF092016.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	1.667	6	7	36	rVB	1532153	3648190	100.00%	16.189%
2	4.582	260	262	272	rVB	198299	297928	8.17%	1.322%
3	5.062	302	304	307	rBV	1018009	1119296	30.68%	4.967%
4	6.159	397	400	402	rBV	1253906	1249222	34.24%	5.544%
5	6.273	407	410	412	rBV	1188373	1309612	35.90%	5.812%
6	6.502	428	430	433	rBV	935756	940633	25.78%	4.174%
7	6.662	441	444	446	rBV	1111050	1012460	27.75%	4.493%
8	7.073	478	480	484	rBV	811361	743381	20.38%	3.299%
9	7.793	541	543	545	rBV	1466493	1293490	35.46%	5.740%
10	8.868	635	637	640	rBV	838777	1153557	31.62%	5.119%
11	9.279	671	673	675	rVV	291637	363428	9.96%	1.613%
12	9.542	693	696	697	rVV	1121774	1358877	37.25%	6.030%
13	9.942	729	731	734	rVV2	23105	38554	1.06%	0.171%
14	10.319	761	764	766	rBV	702060	703985	19.30%	3.124%
15	10.479	773	778	781	rVV	61541	103106	2.83%	0.458%
16	10.914	814	816	817	rVB2	45155	45216	1.24%	0.201%
17	11.005	821	824	825	rBV	1387918	1239892	33.99%	5.502%
18	11.074	828	830	832	rVB2	29069	39566	1.08%	0.176%
19	11.508	865	868	869	rBV	42452	63656	1.74%	0.282%
20	11.531	869	870	872	rVV	68569	64174	1.76%	0.285%
21	11.565	872	873	875	rVV2	53285	70732	1.94%	0.314%
22	11.611	875	877	881	rVB	70775	118960	3.26%	0.528%
23	11.817	891	895	897	rBV2	21738	53488	1.47%	0.237%
24	11.954	905	907	908	rBV	50802	43299	1.19%	0.192%
25	12.057	913	916	917	rBV	28524	41275	1.13%	0.183%
26	12.079	917	918	921	rVV2	20107	37404	1.03%	0.166%
27	12.125	921	922	926	rVB2	38719	46776	1.28%	0.208%
28	12.205	926	929	931	rBV	216443	224665	6.16%	0.997%
29	12.342	939	941	945	rBV3	17026	37942	1.04%	0.168%
30	12.422	945	948	950	rBV	254048	250837	6.88%	1.113%
31	12.491	952	954	957	rVB4	25909	42068	1.15%	0.187%
32	12.582	960	962	965	rBV	820193	811696	22.25%	3.602%
33	12.754	976	977	980	rVB	49584	49955	1.37%	0.222%
34	12.857	984	986	990	rVB2	36858	47635	1.31%	0.211%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090178.D
Acq On : 22 Sep 2016 00:06
Operator : UM/SJ
Sample : H4856-03 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

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-BF092016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.508	1039	1043	1046	rBV2	202211	314127	8.61%	1.394%
36	13.611	1049	1052	1059	rVV	932577	1341834	36.78%	5.955%
37	13.828	1069	1071	1076	rBV3	29762	38565	1.06%	0.171%
38	14.137	1095	1098	1101	rBV2	49655	117898	3.23%	0.523%
39	14.594	1136	1138	1142	rBV	130115	303378	8.32%	1.346%
40	14.845	1158	1160	1162	rVB2	70740	100459	2.75%	0.446%
41	14.891	1162	1164	1166	rBV	88015	136888	3.75%	0.607%
42	14.948	1166	1169	1171	rBV	649164	939704	25.76%	4.170%
43	15.508	1216	1218	1224	rVB	153866	283114	7.76%	1.256%
44	15.851	1246	1248	1254	rVB	111325	197858	5.42%	0.878%
45	16.308	1285	1288	1290	rVB2	52218	95558	2.62%	0.424%

Sum of corrected areas: 22534338

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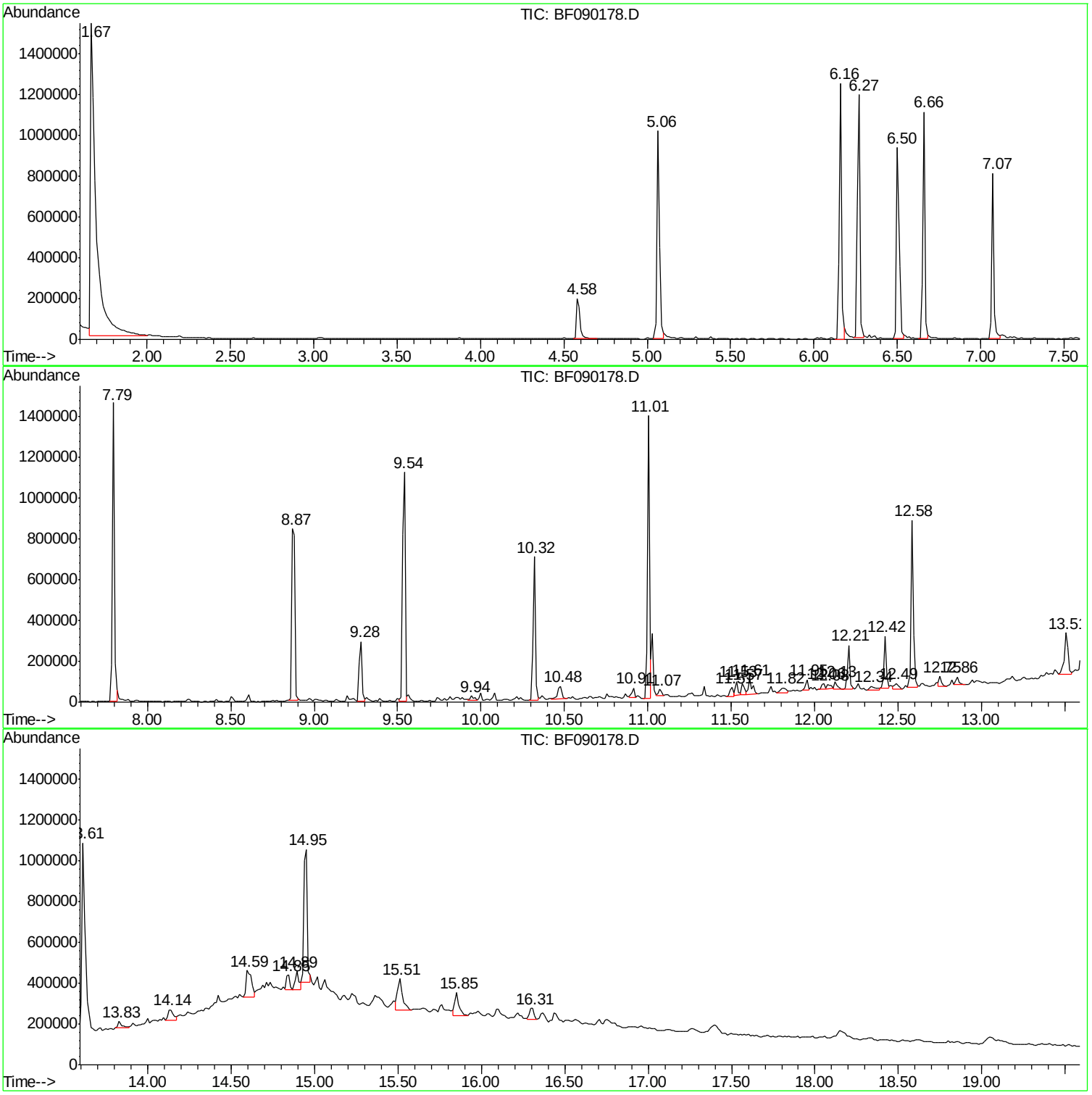
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090178.D
Acq On : 22 Sep 2016 00:06
Operator : UM/SJ
Sample : H4856-03 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

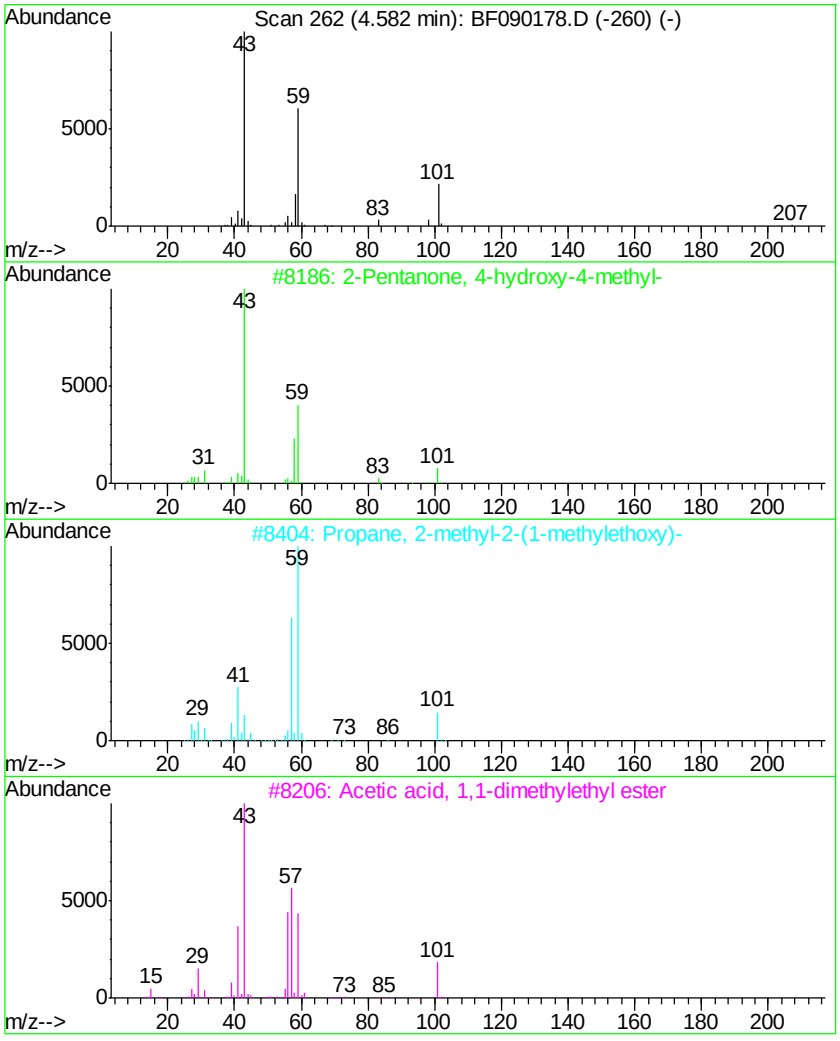
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

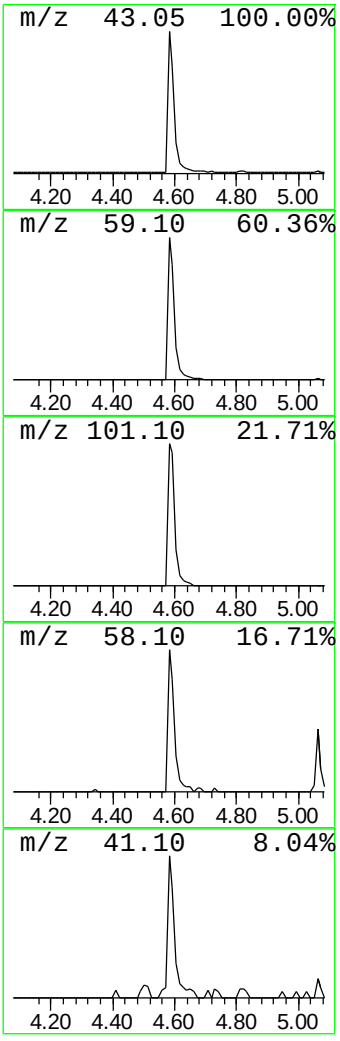
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	6.33 ng	297928	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090178.D
Acq On : 22 Sep 2016 00:06
Operator : UM/SJ
Sample : H4856-03 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

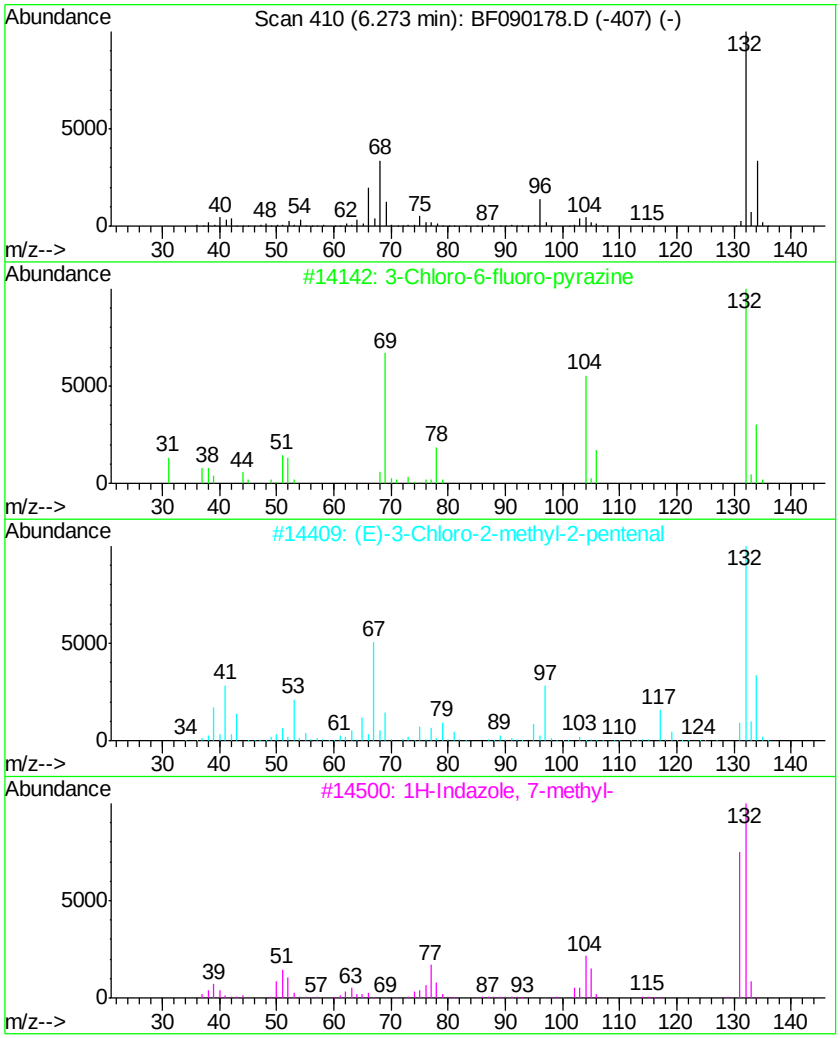
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

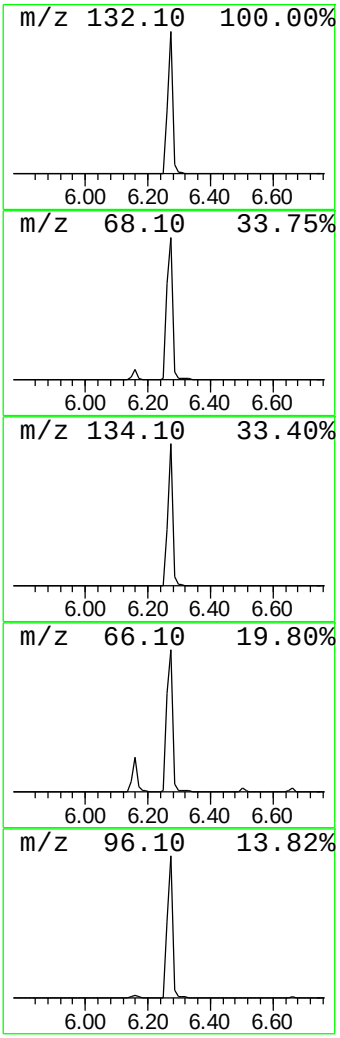
****

Peak Number 3 unknown6.27 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	27.85 ng	1309610	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092116\
Data File : BF090178.D
Acq On : 22 Sep 2016 00:06
Operator : UM/SJ
Sample : H4856-03 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

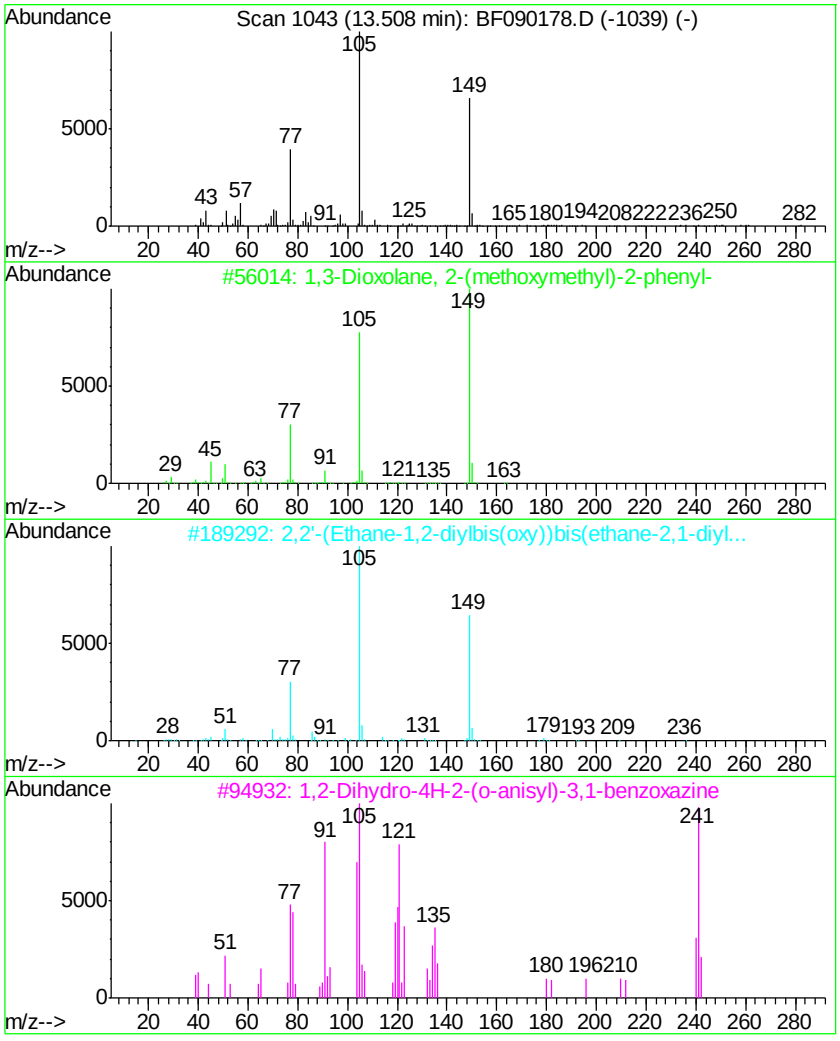
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

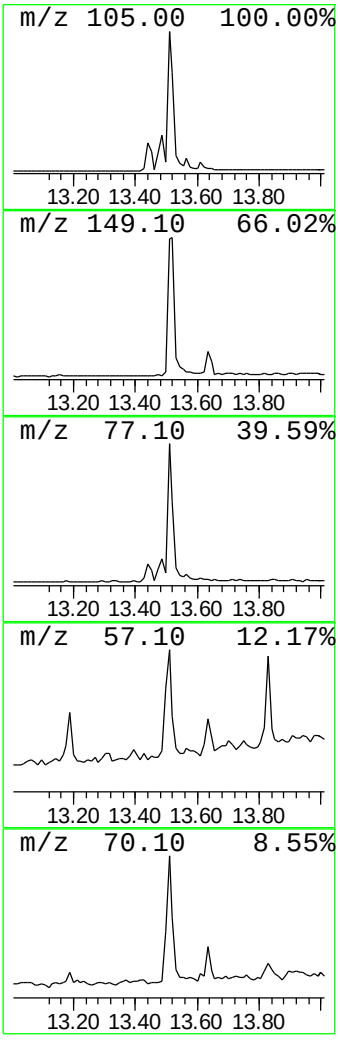
****

Peak Number 5 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	4.68 ng	314127	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	50
3	1,2-Dihydro-4H-2-(o-anisyl)-3,1-...	241	C15H15NO2	090284-41-6	42
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	38
5	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	38





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ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

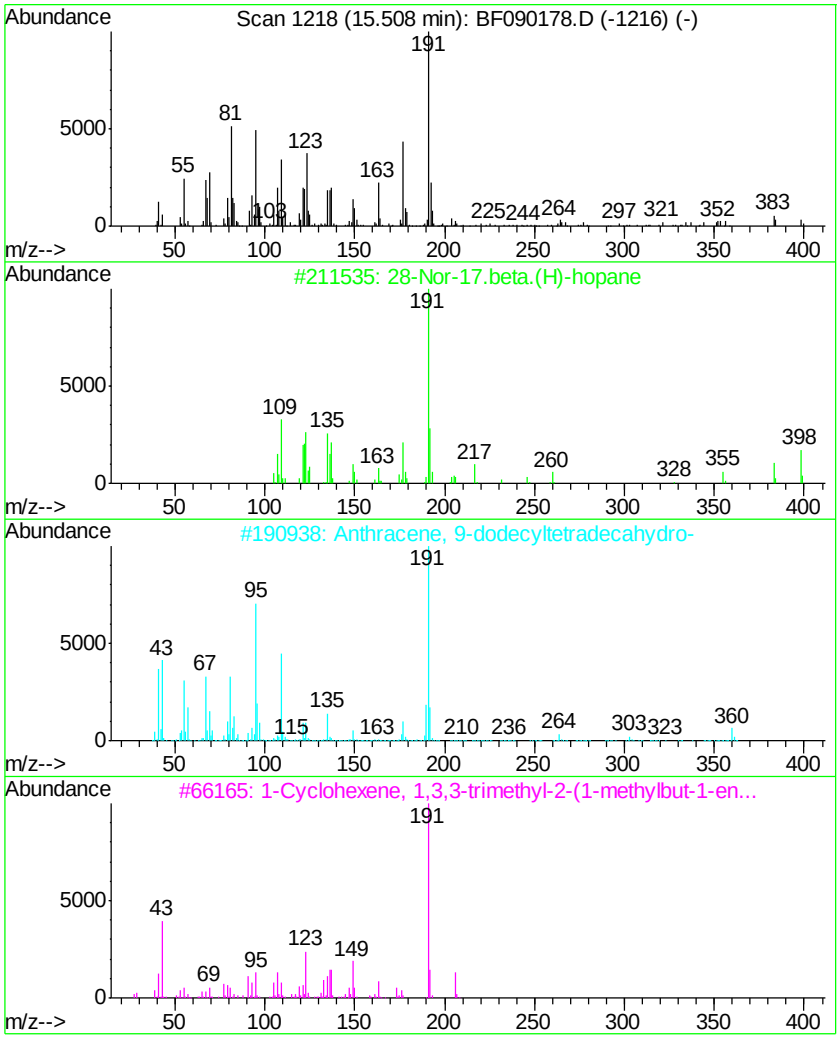
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

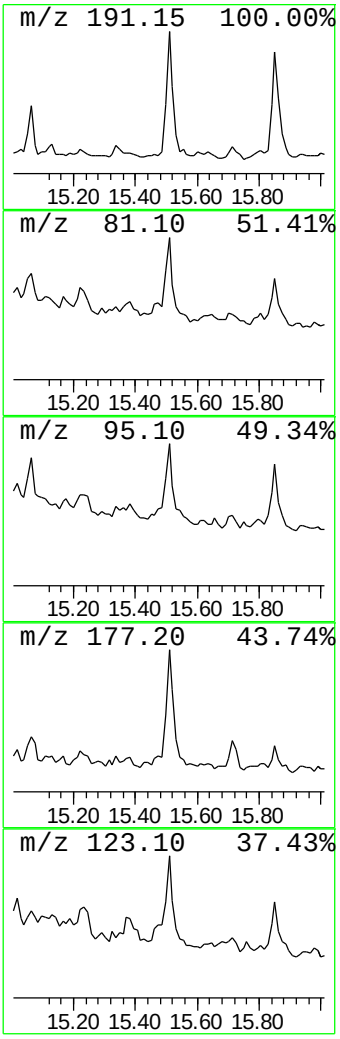
****

Peak Number 6 28-Nor-17.beta.(H)-hopane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	6.03 ng	283114	Perylene-d12	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	68
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	37
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	37
4	Pentanoic acid, 4-methyl-2-(2,5-...	278	C13H18N4O3	1000294-63-5	32
5	3-Fluoro-5-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-34-4	22





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Operator : UM/SJ
Sample : H4856-03 2X
Misc :
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Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

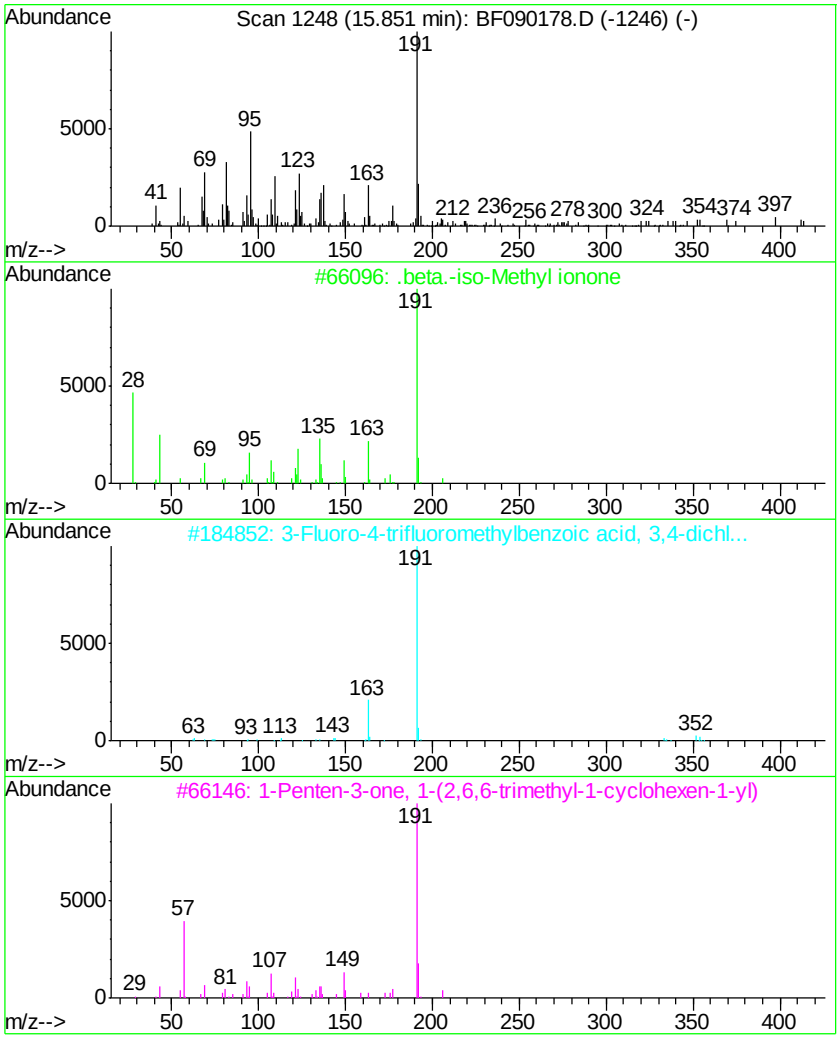
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

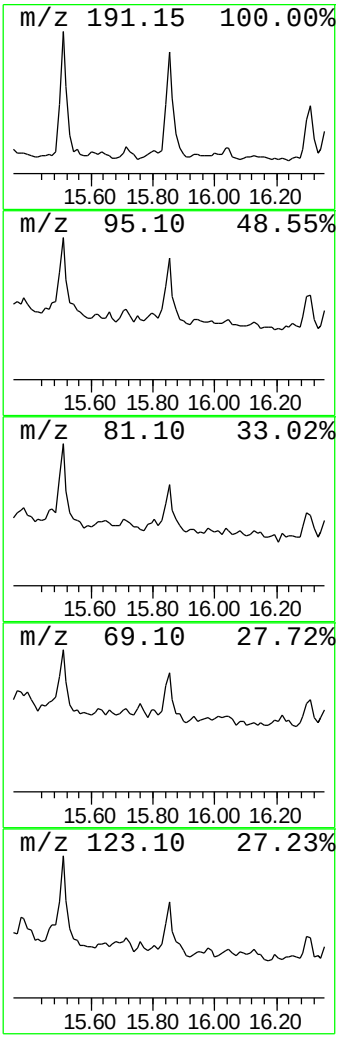
****

Peak Number 7 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	4.21 ng	197858	Perylene-d12	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	68
2	3-Fluoro-4-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-94-6	38
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
4	4-Fluoro-2-trifluoromethylbenzam...	335	C14H7ClF5NO	1000358-09-2	35
5	3-Fluoro-5-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-34-4	35





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Misc :
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Instrument : BNA_F
ClientSampleId : BH-3-4-5FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

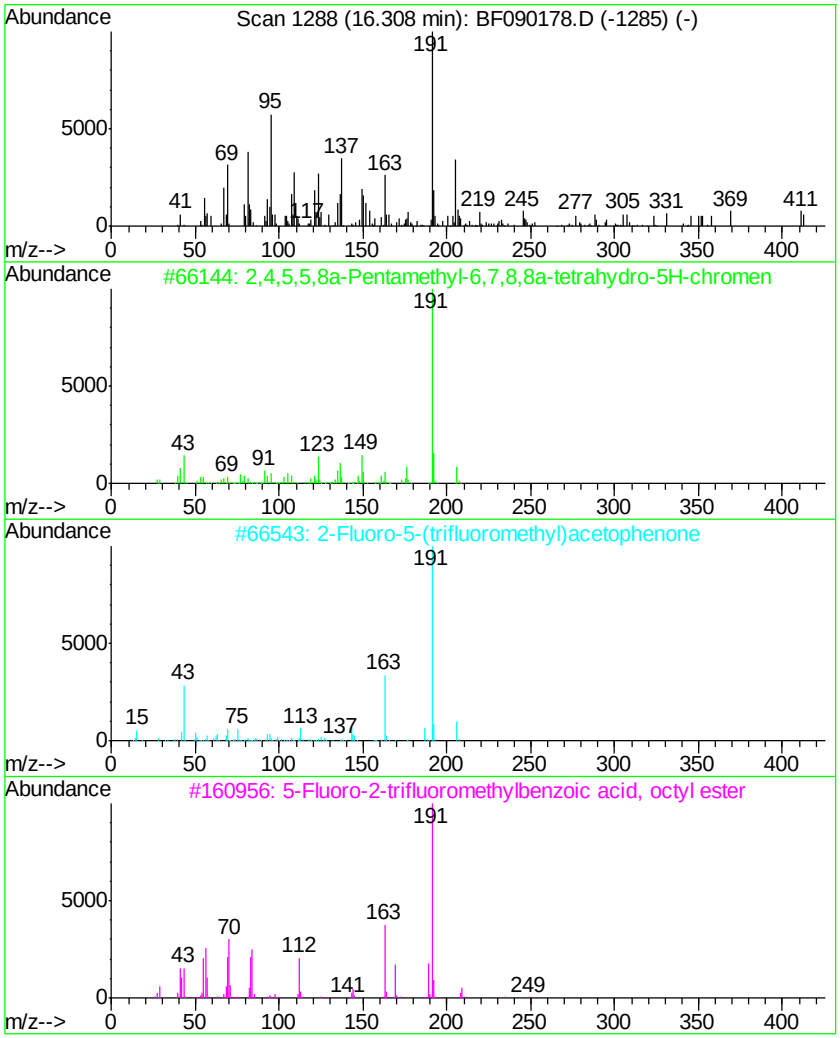
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

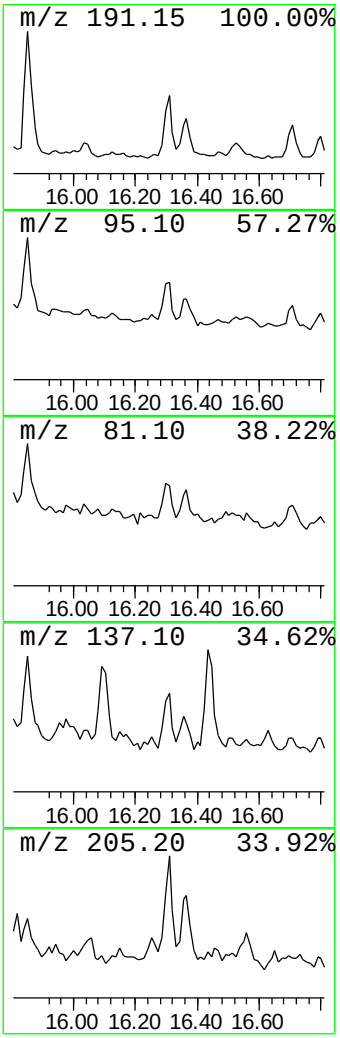
****

Peak Number 8 unknown16.31 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	2.03 ng	95558	Perylene-d12	14.95

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	2-Fluoro-5-(trifluoromethyl)acet...	206	C9H6F4O	202664-53-7	35
3	5-Fluoro-2-trifluoromethylbenzoi...	320	C16H20F4O2	1000338-74-4	35
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	30
5	2,3-Dimethyl-6-(3-methyl-butyryl...	248	C15H20O3	071940-30-2	27





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.58	6.3	ng	297928	1	6.50	940633	20.0
unknown6.27	6.27	27.9	ng	1309610	1	6.50	940633	20.0
1,3-Dioxolane, 2-...	13.51	4.7	ng	314127	5	13.61	1341830	20.0
28-Nor-17.beta.(H...	15.51	6.0	ng	283114	6	14.95	939704	20.0
.beta.-iso-Methyl...	15.85	4.2	ng	197858	6	14.95	939704	20.0
unknown16.31	16.31	2.0	ng	95558	6	14.95	939704	20.0