LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
Data File : BF084686.D
Acq On : 30 Jan 2016 15:17
Operator : SJ/IZ
Sample : H1273-07 5X
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

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-BF012916.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	3.516	122	125	130	rBV	12560	21505	1.51%	0.103%
2	4.178	181	183	188	rVB	41966	53631	3.76%	0.258%
3	4.864	241	243	246	rBV	592686	842164	59.10%	4.044%
4	5.264	276	278	281	rBV	9725	18167	1.27%	0.087%
5	5.321	281	283	285	rBV	709610	972859	68.28%	4.672%
6	5.721	317	318	321	rVB	46896	42023	2.95%	0.202%
7	5.984	338	341	343	rBV	1118435	961497	67.48%	4.617%
8	6.156	352	356	358	rBV	42729	42884	3.01%	0.206%
9	6.373	372	375	377	rBV	989103	1021303	71.68%	4.904%
10	6.419	377	379	381	rVV	371734	307601	21.59%	1.477%
11	6.487	383	385	388	rBV	973839	1034696	72.62%	4.969%
12	6.567	388	392	396	rVB3	7833	20586	1.44%	0.099%
13	6.727	403	406	408	rBV	1117870	1121640	78.72%	5.386%
14	6.842	414	416	417	rBV	134422	109064	7.65%	0.524%
15	6.876	417	419	422	rVB	882701	779659	54.72%	3.744%
16	7.287	453	455	457	rBV	799063	651644	45.73%	3.129%
17	7.402	461	465	468	rBV	13368	18681	1.31%	0.090%
18	7.539	476	477	480	rBV	36041	50425	3.54%	0.242%
19	7.722	488	493	495	rBV3	14940	23529	1.65%	0.113%
20	7.756	495	496	499	rVV3	12345	16663	1.17%	0.080%
21	7.916	508	510	512	rBV	55645	65933	4.63%	0.317%
22	8.007	516	518	520	rBV	1411618	1424882	100.00%	6.842%
23	8.042	520	521	523	rVB	507117	376049	26.39%	1.806%
24	8.145	528	530	531	rBV2	21002	15723	1.10%	0.076%
25	9.093	610	613	615	rBV	772613	955290	67.04%	4.587%
26	9.425	638	642	645	rBV2	13162	20213	1.42%	0.097%
27	9.482	645	647	650	rBV	125224	167227	11.74%	0.803%
28	9.710	664	667	669	rVB	20304	24034	1.69%	0.115%
29	9.768	669	672	674	rBV	1090344	1416104	99.38%	6.800%
30	10.202	709	710	712	rVB	41308	33609	2.36%	0.161%
31	10.305	718	719	723	rVB4	15970	15153	1.06%	0.073%
32	10.419	727	729	732	rVV	16866	24154	1.70%	0.116%
33	10.545	738	740	742	rBV	570352	504110	35.38%	2.421%
34	10.671	750	751	756	rVB	37814	57534	4.04%	0.276%

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Misc :
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Instrument : BNA_F
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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.773	758	760	763	rVB4	9187	14971	1.05%	0.072%
36	10.876	765	769	771	rBV4	8565	25233	1.77%	0.121%
37	11.116	789	790	796	rVB3	26024	51882	3.64%	0.249%
38	11.242	799	801	802	rBV	1465042	1244682	87.35%	5.977%
39	11.265	802	803	805	rVB	209733	149851	10.52%	0.720%
40	11.311	805	807	809	rBV	36212	40205	2.82%	0.193%
41	11.482	819	822	825	rBV5	19417	39470	2.77%	0.190%
42	11.551	825	828	829	rVV	26597	34696	2.44%	0.167%
43	11.573	829	830	833	rVB	94240	112654	7.91%	0.541%
44	11.745	839	845	846	rBV4	41351	58716	4.12%	0.282%
45	11.768	846	847	849	rVB	49011	42343	2.97%	0.203%
46	11.813	849	851	852	rBV	19879	18738	1.32%	0.090%
47	11.848	852	854	860	rVB	53301	86431	6.07%	0.415%
48	11.962	860	864	868	rBV2	53754	112990	7.93%	0.543%
49	12.042	868	871	872	rBV3	17950	41866	2.94%	0.201%
50	12.111	876	877	879	rBV2	9379	17006	1.19%	0.082%
51	12.236	886	888	891	rVB4	19829	28757	2.02%	0.138%
52	12.294	891	893	895	rBV	77587	109863	7.71%	0.528%
53	12.339	895	897	898	rVV2	24452	41835	2.94%	0.201%
54	12.374	898	900	904	rVB	317001	297553	20.88%	1.429%
55	12.454	904	907	908	rBV	169462	234627	16.47%	1.127%
56	12.602	916	920	922	rBV5	19065	53284	3.74%	0.256%
57	12.671	923	926	928	rVV2	232431	382192	26.82%	1.835%
58	12.739	928	932	934	rVB3	50078	72317	5.08%	0.347%
59	12.819	937	939	942	rVB	447067	604203	42.40%	2.901%
60	12.899	942	946	947	rBV	24417	42302	2.97%	0.203%
61	12.934	947	949	952	rBV	81391	153629	10.78%	0.738%
62	13.071	959	961	962	rBV2	42660	37756	2.65%	0.181%
63	13.105	962	964	965	rBV	41961	38504	2.70%	0.185%
64	13.196	970	972	974	rBV	235258	266942	18.73%	1.282%
65	13.368	985	987	989	rBV	116474	114821	8.06%	0.551%
66	13.414	989	991	992	rVV	40492	41585	2.92%	0.200%
67	13.734	1017	1019	1022	rVB2	134667	165268	11.60%	0.794%
68	13.871	1028	1031	1037	rBV	1139072	1242193	87.18%	5.965%
69	14.054	1045	1047	1049	rBV2	46253	60626	4.25%	0.291%
70	14.877	1117	1119	1123	rBV	95783	184723	12.96%	0.887%
71	15.197	1145	1147	1150	rVB	77078	113442	7.96%	0.545%

LSC Area Percent Report

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Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	15.265	1150	1153	1155	rBV	727879	1046707	73.46%	5.026%
73	15.300	1155	1156	1160	rVB3	50599	87765	6.16%	0.421%
74	16.500	1258	1261	1264	rVB	57365	102119	7.17%	0.490%

Sum of corrected areas: 20824983

LSC Report - Integrated Chromatogram

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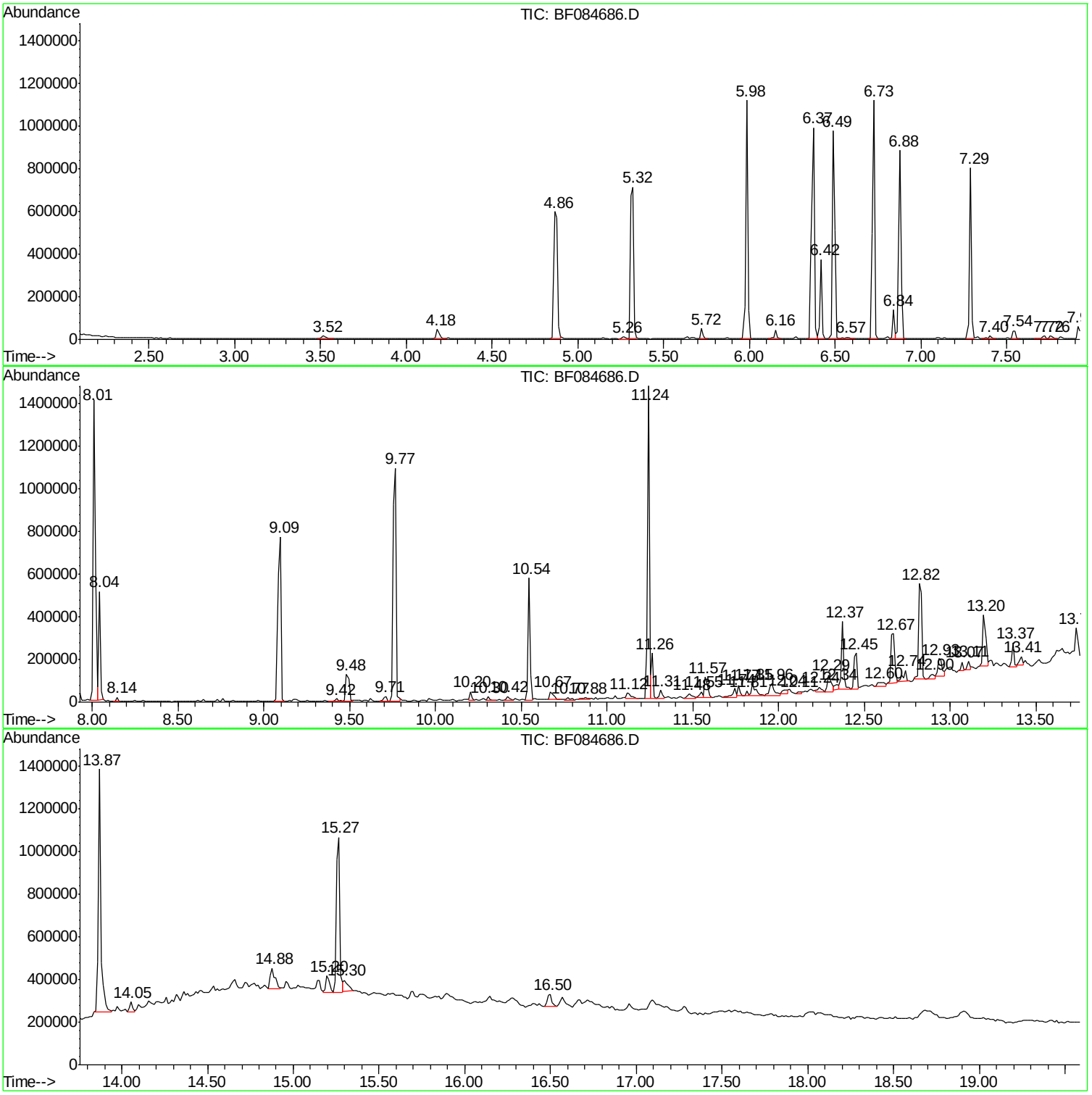
Sample : H1273-07 5X
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
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Operator : SJ/IZ
Sample : H1273-07 5X
Misc :
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Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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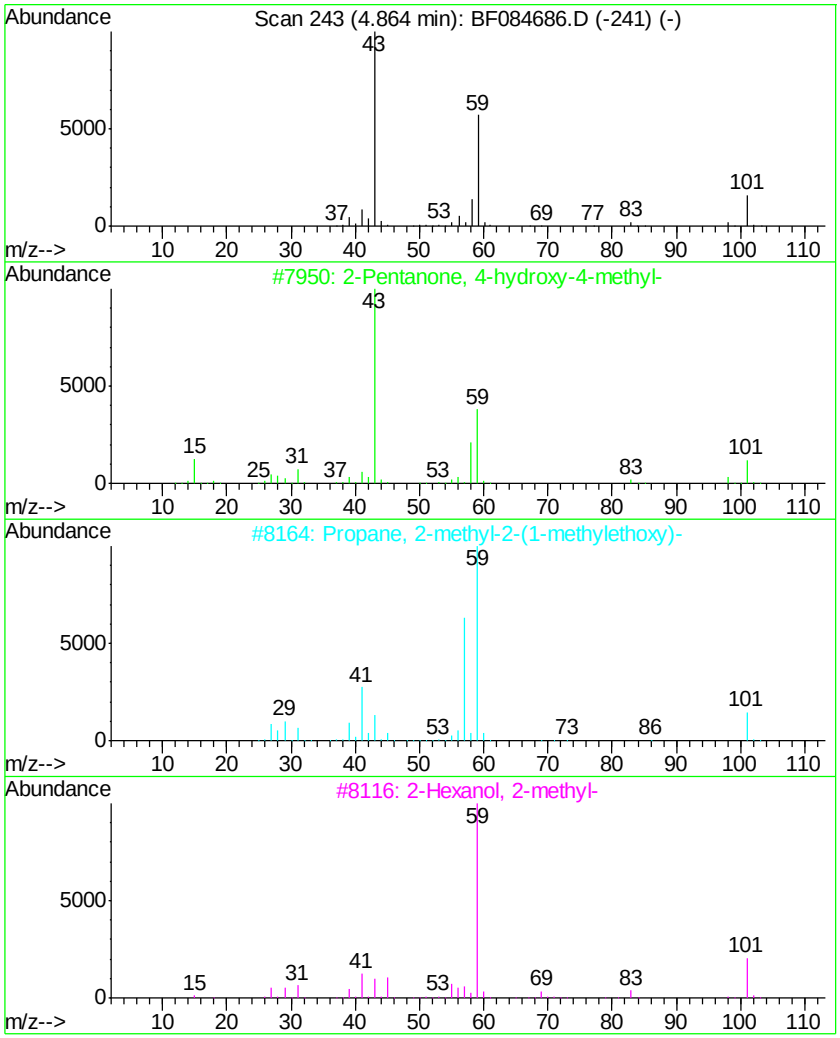
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

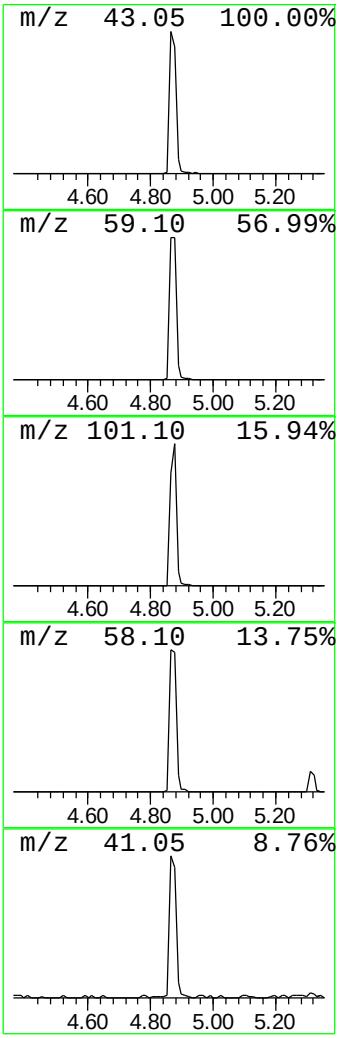
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	15.02 ng	842164	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
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Acq On : 30 Jan 2016 15:17
Operator : SJ/IZ
Sample : H1273-07 5X
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

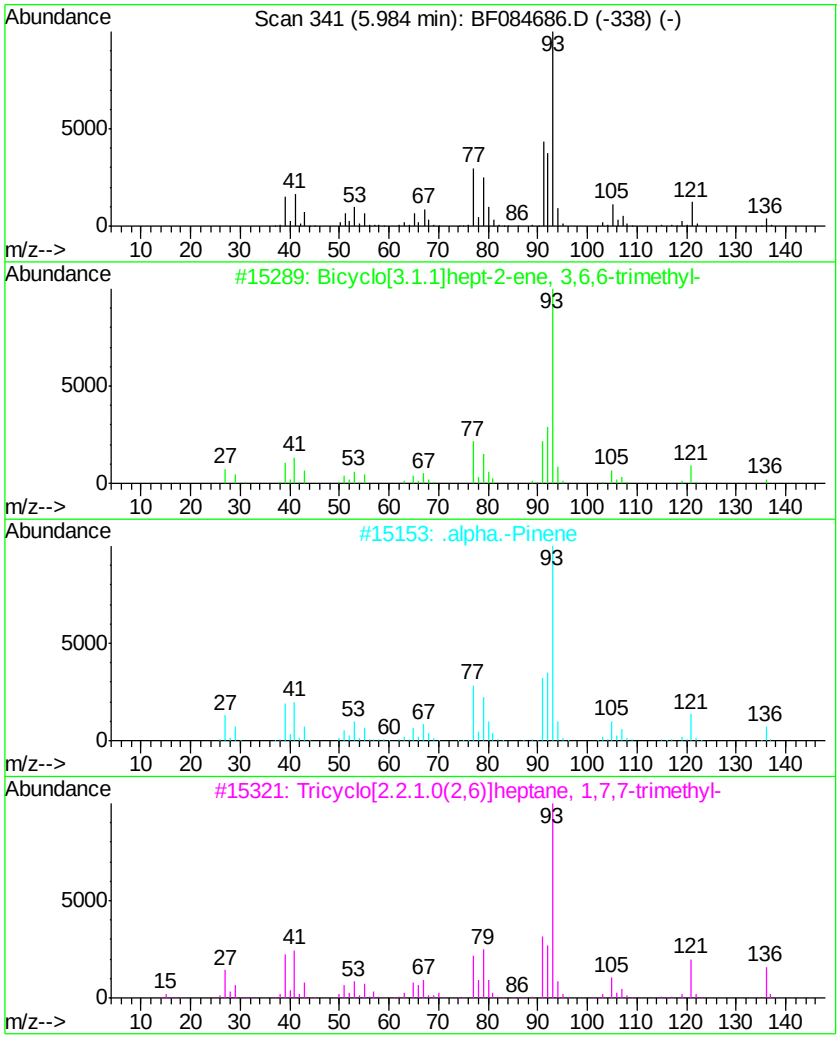
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

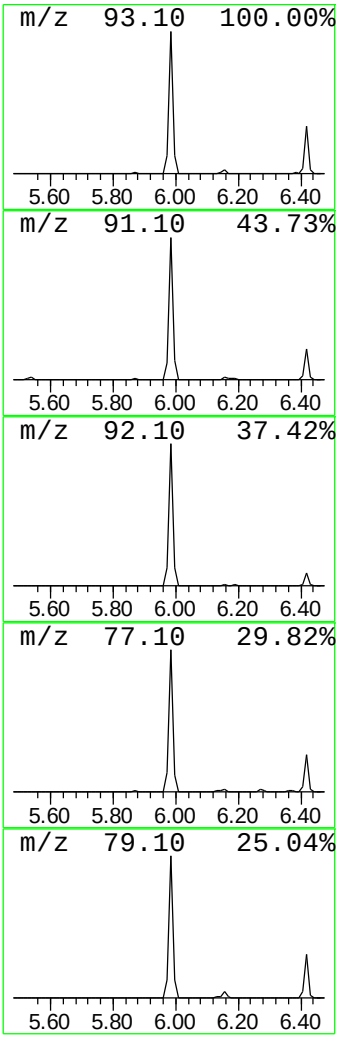
****

Peak Number 2 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.98	17.14 ng	961497	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	Bicyclo[4.1.0]hept-3-ene, 3,7,7-...	136	C10H16	000498-15-7	91
5	1,4-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-85-4	90





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Sample : H1273-07 5X
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

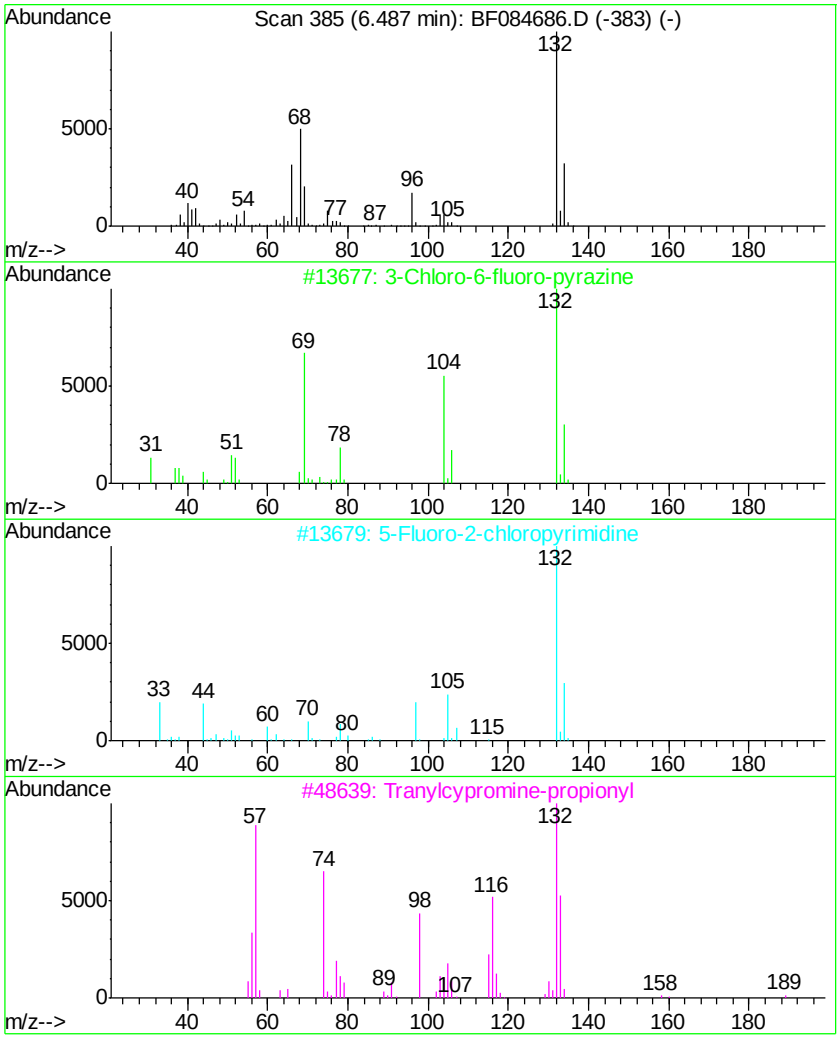
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

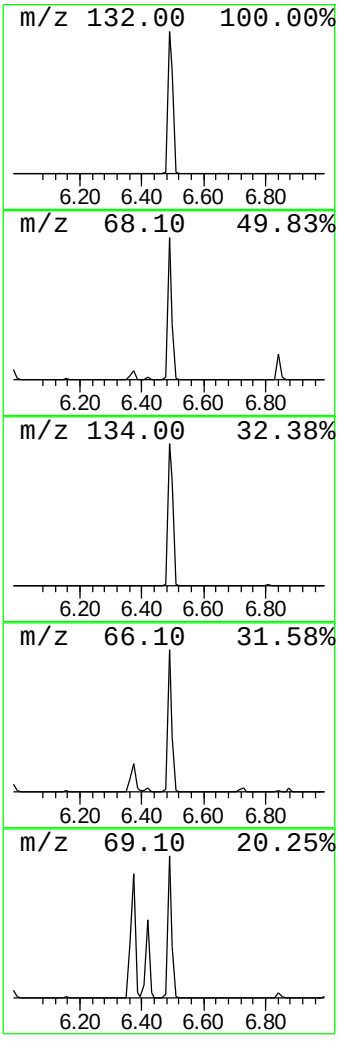
****

Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	18.45 ng	1034700	1,4-Dichlorobenzene-d4	6.73

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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TIC Library : C:\DATABASE\NIST02.L
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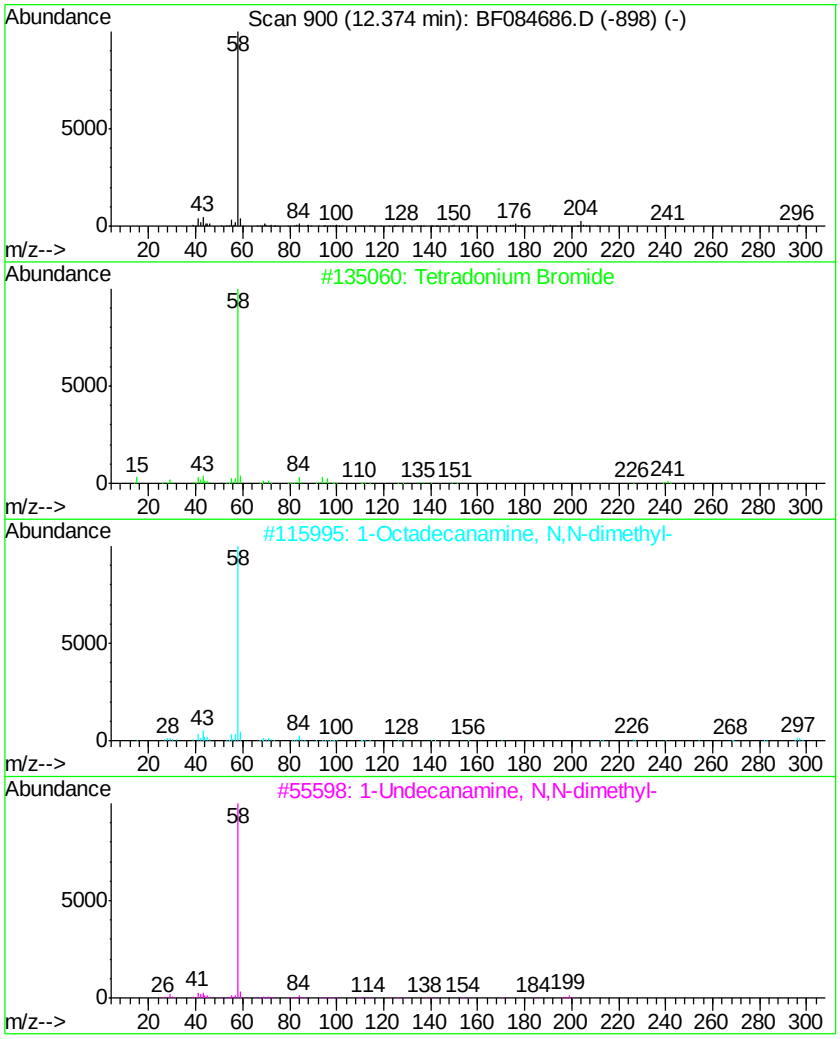
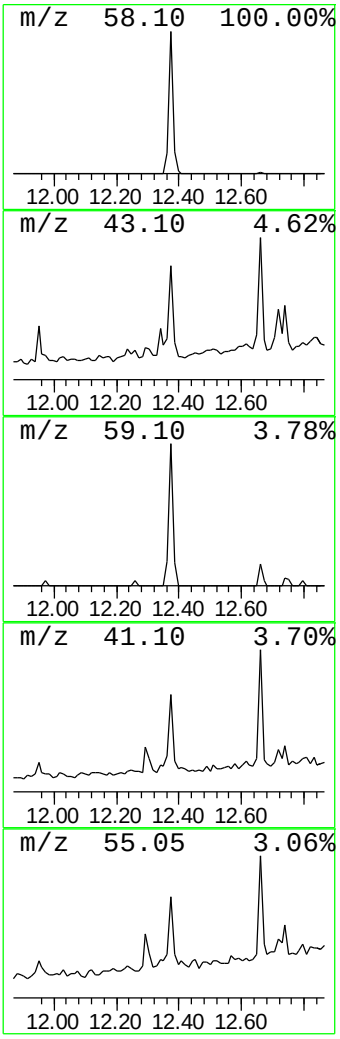
****

Peak Number 5 Tetradonium Bromide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	4.78 ng	297553	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradonium Bromide	335	C17H38BrN	001119-97-7	64
2	1-Octadecanamine, N,N-dimethyl-	297	C20H43N	000124-28-7	64
3	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	56
4	Stearyltrimethylammonium chloride	347	C21H46ClN	000112-03-8	56
5	1-Hexadecanamine, N,N-dimethyl-	269	C18H39N	000112-69-6	56





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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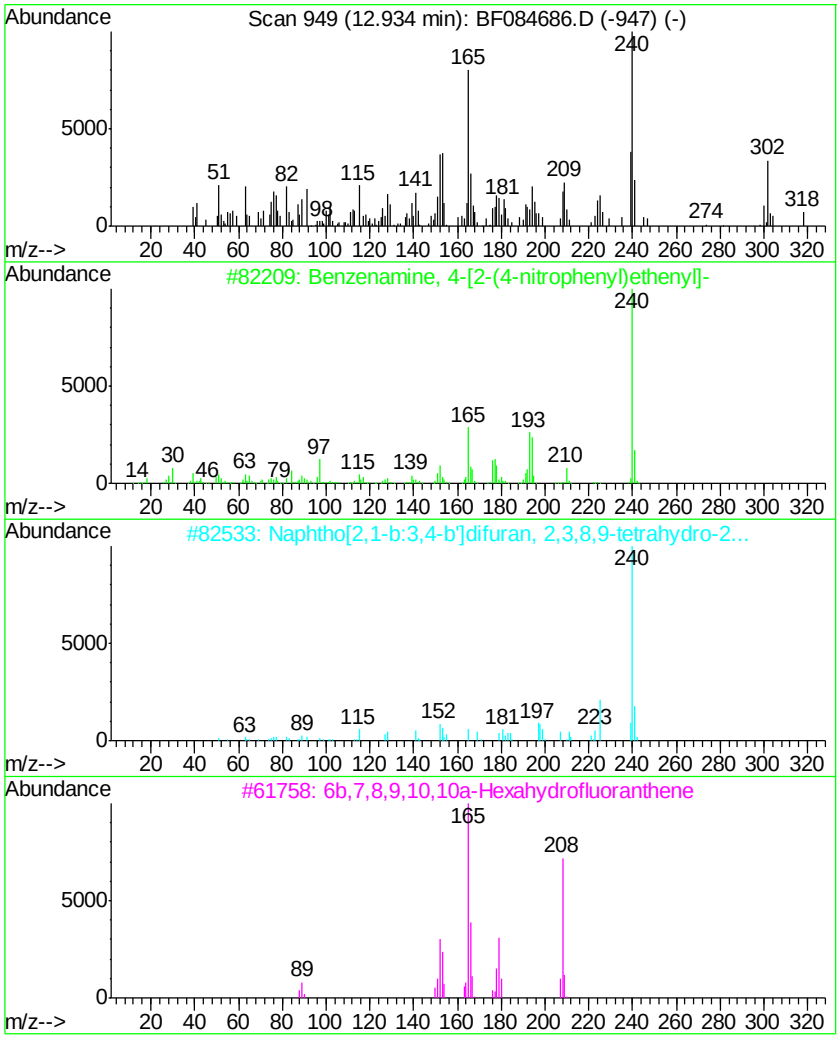
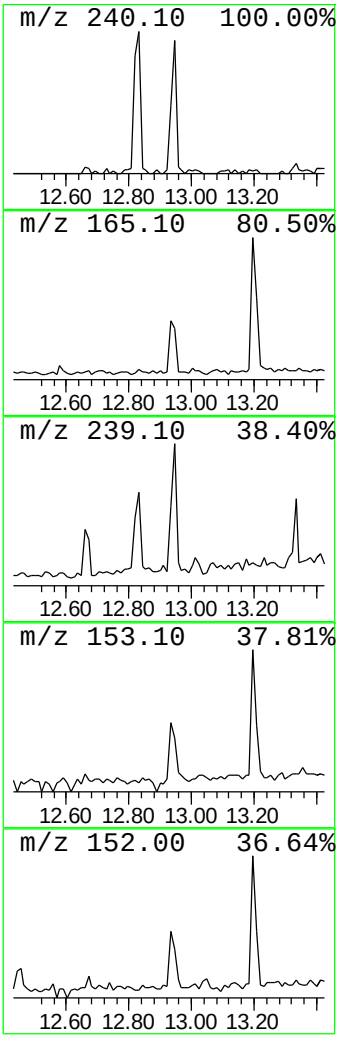
****

Peak Number 6 unknown12.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	2.47 ng	153629	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 4-[2-(4-nitrophenyl...	240	C14H12N2O2	004629-58-7	38
2	Naphtho[2,1-b:3,4-b']difuran, 2,...	240	C16H16O2	068873-19-8	38
3	6b,7,8,9,10,10a-Hexahydrofluoran...	208	C16H16	022187-09-3	35
4	Pyridine, 1-acetyl-1,2,3,4-tetra...	208	C12H20N2O	054966-22-2	35
5	Benzenamine, N-[(4-methylphenyl)...	240	C14H12N2O2	020192-50-1	27





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Sample : H1273-07 5X
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

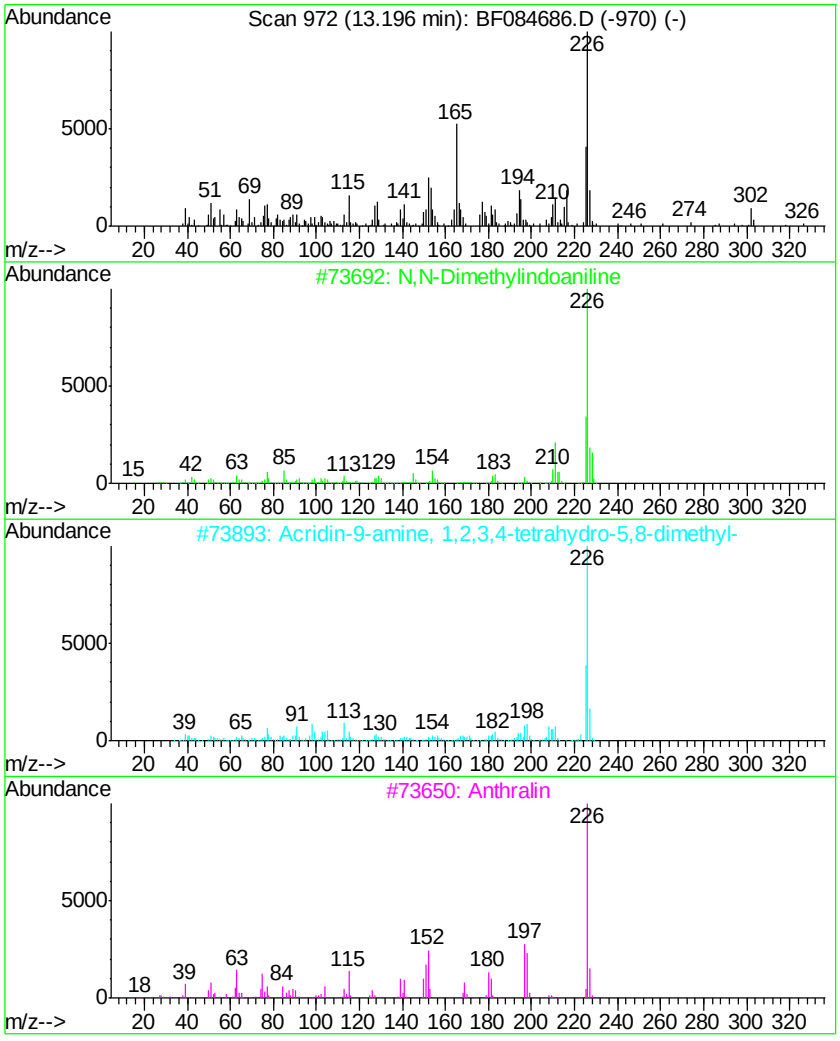
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

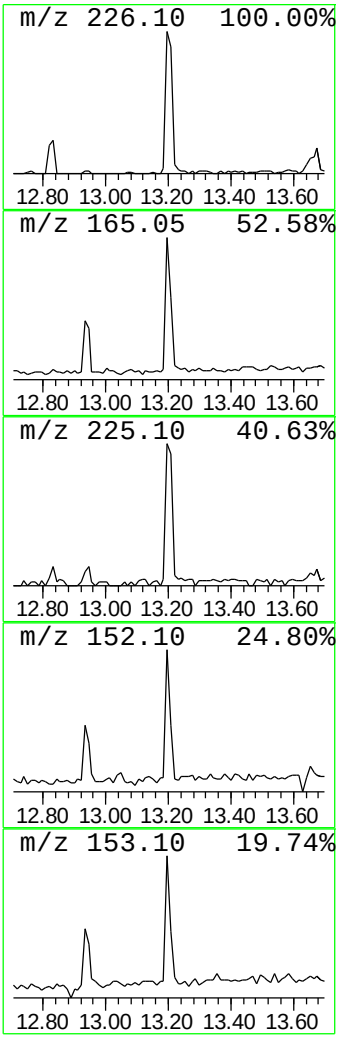
****

Peak Number 7 N,N-Dimethylindoaniline Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	4.30 ng	266942	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Dimethylindoaniline	226	C14H14N2O	002150-58-5	87
2	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	55
3	Anthralin	226	C14H10O3	000480-22-8	46
4	9(10H)-Anthracenone, 1,8-dihydroxy-	226	C14H10O3	001143-38-0	46
5	Benzenamine, N-[(4-nitrophenyl)m...	226	C13H10N2O2	000785-80-8	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013016\
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Operator : SJ/IZ
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

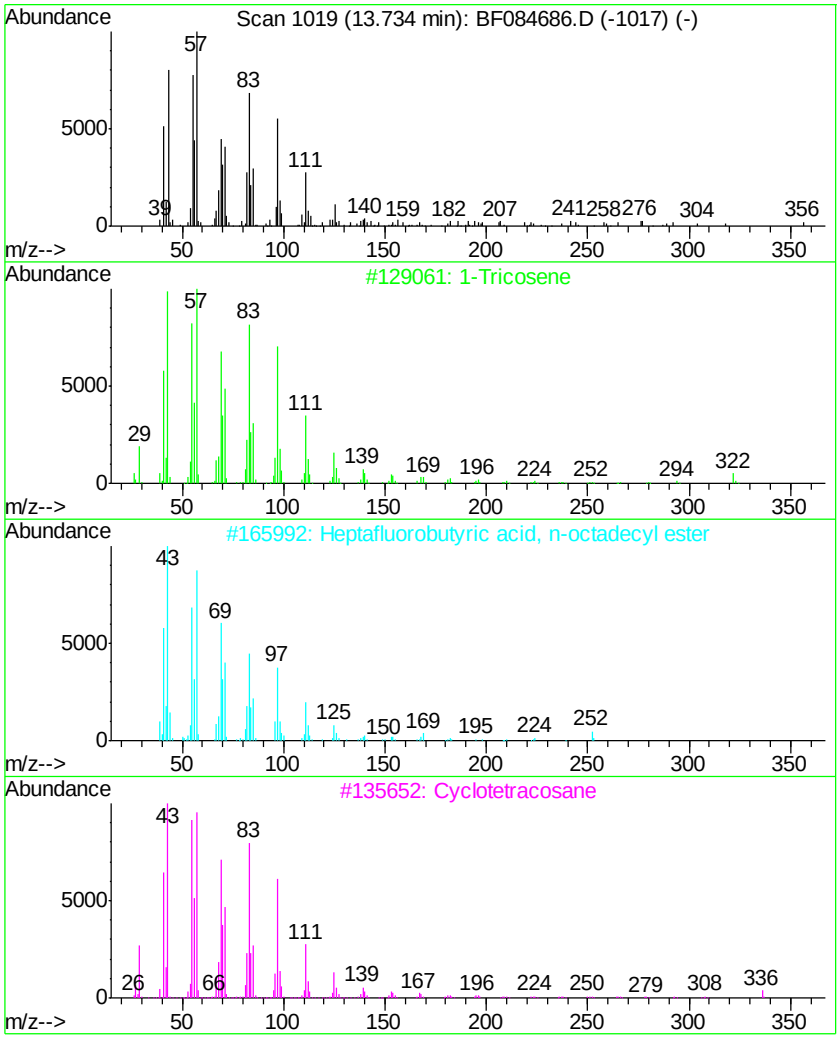
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

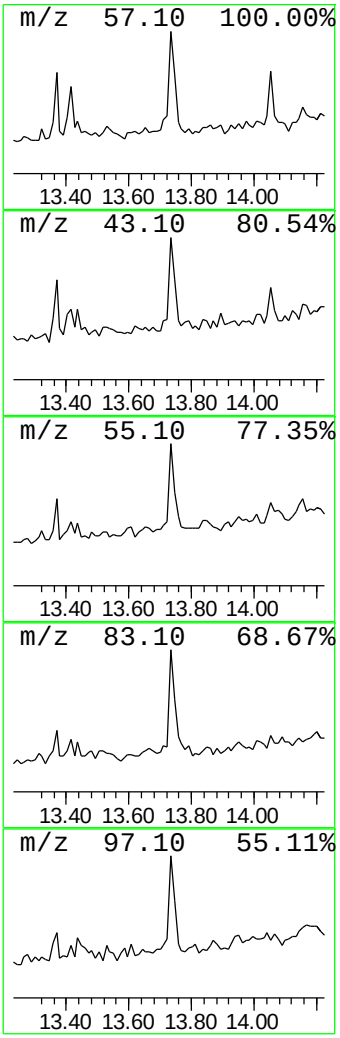
****

Peak Number 8 1-Tricosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.66 ng	165268	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Cyclotetracosane	336	C24H48	000297-03-0	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013016\
Data File : BF084686.D
Acq On : 30 Jan 2016 15:17
Operator : SJ/IZ
Sample : H1273-07 5X
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B010(15-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.86	15.0	ng	842164	1	6.73	1121640	20.0
Bicyclo[3.1.1]hep...	5.98	17.1	ng	961497	1	6.73	1121640	20.0
unknown6.49	6.49	18.4	ng	1034700	1	6.73	1121640	20.0
Tetradonium Bromide	12.37	4.8	ng	297553	4	11.24	1244680	20.0
unknown12.93	12.93	2.5	ng	153629	5	13.87	1242190	20.0
N,N-Dimethylindoa...	13.20	4.3	ng	266942	5	13.87	1242190	20.0
1-Tricosene	13.73	2.7	ng	165268	5	13.87	1242190	20.0