LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

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-BF092415.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	2.217	5	7	32	rVB	70391	253745	7.57%	0.625%
2	5.143	259	263	265	rBV	1023991	1606687	47.96%	3.957%
3	5.543	294	298	300	rBV	2739816	3153565	94.14%	7.767%
4	6.560	384	387	390	rBV	2112984	3056579	91.25%	7.528%
5	6.709	397	400	402	rBV	2883879	3200352	95.54%	7.882%
6	6.937	418	420	422	rBV	859991	696240	20.78%	1.715%
7	7.097	431	434	436	rBV	2787303	2505971	74.81%	6.172%
8	7.509	467	470	472	rBV	2042719	2179843	65.07%	5.369%
9	8.229	530	533	537	rVB	844104	1035686	30.92%	2.551%
10	8.937	593	595	597	rBV	52303	39868	1.19%	0.098%
11	9.166	613	615	618	rBV	60522	66096	1.97%	0.163%
12	9.303	624	627	629	rBV	3791518	3349798	100.00%	8.250%
13	9.692	659	661	664	rBV	577866	603378	18.01%	1.486%
14	9.909	678	680	682	rVB	44725	41348	1.23%	0.102%
15	9.977	684	686	688	rVV2	837098	954201	28.49%	2.350%
16	10.012	688	689	691	rVB	89950	69430	2.07%	0.171%
17	10.183	702	704	706	rVB	85499	77354	2.31%	0.191%
18	10.378	719	721	724	rBV	893191	1188725	35.49%	2.928%
19	10.526	732	734	736	rVB	68804	60332	1.80%	0.149%
20	10.766	753	755	758	rBV2	1579629	2076373	61.99%	5.114%
21	10.880	763	765	768	rBV	97790	111183	3.32%	0.274%
22	11.269	797	799	801	rVB	95938	82064	2.45%	0.202%
23	11.326	801	804	805	rBV2	81007	72704	2.17%	0.179%
24	11.360	805	807	810	rVB	63269	71766	2.14%	0.177%
25	11.463	814	816	818	rBV	725748	1260371	37.63%	3.104%
26	11.498	818	819	820	rVV	592584	413894	12.36%	1.019%
27	11.543	820	823	824	rVB	182066	170480	5.09%	0.420%
28	11.635	829	831	833	rBV	62318	70269	2.10%	0.173%
29	11.692	833	836	840	rBV2	121797	178017	5.31%	0.438%
30	11.761	840	842	844	rVV2	26586	38317	1.14%	0.094%
31	11.966	858	860	861	rBV	64212	60304	1.80%	0.149%
32	12.001	861	863	864	rVV	83731	108407	3.24%	0.267%
33	12.081	868	870	874	rVV2	81402	122655	3.66%	0.302%
34	12.172	875	878	882	rVV3	23383	51009	1.52%	0.126%

LSC Area Percent Report

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Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

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-BF092415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.286	885	888	891	rVB	89417	125348	3.74%	0.309%
36	12.446	900	902	906	rBV4	18683	44273	1.32%	0.109%
37	12.515	906	908	910	rVV2	36336	49362	1.47%	0.122%
38	12.606	914	916	918	rVB	54872	67281	2.01%	0.166%
39	12.686	920	923	925	rVB	655012	820281	24.49%	2.020%
40	12.869	937	939	940	rBV	85940	87294	2.61%	0.215%
41	12.915	940	943	945	rVV	507779	744530	22.23%	1.834%
42	12.949	945	946	949	rVB2	30123	43808	1.31%	0.108%
43	13.063	953	956	958	rVB	2125670	3009755	89.85%	7.413%
44	13.132	958	962	963	rBV2	33566	47930	1.43%	0.118%
45	13.235	966	971	973	rBV3	37714	80649	2.41%	0.199%
46	13.338	978	980	982	rBV	52367	60709	1.81%	0.150%
47	13.532	995	997	999	rBV	110169	103794	3.10%	0.256%
48	13.578	999	1001	1003	rVV2	57084	68572	2.05%	0.169%
49	13.624	1003	1005	1012	rVB5	39948	73541	2.20%	0.181%
50	13.738	1013	1015	1018	rBV	65180	91825	2.74%	0.226%
51	13.852	1022	1025	1027	rBV2	57837	90750	2.71%	0.224%
52	13.909	1029	1030	1031	rVV	47127	56246	1.68%	0.139%
53	13.944	1031	1033	1036	rVV2	333598	368580	11.00%	0.908%
54	14.024	1038	1040	1042	rBV	23875	38589	1.15%	0.095%
55	14.104	1043	1047	1053	rVV3	806369	1562342	46.64%	3.848%
56	14.264	1058	1061	1065	rBV5	36386	96980	2.90%	0.239%
57	14.332	1065	1067	1069	rBV2	35078	45654	1.36%	0.112%
58	14.492	1079	1081	1083	rBV	45378	45794	1.37%	0.113%
59	14.527	1083	1084	1086	rBV	30554	38595	1.15%	0.095%
60	14.584	1086	1089	1090	rBV2	46105	80305	2.40%	0.198%
61	14.675	1095	1097	1101	rVB2	59759	122998	3.67%	0.303%
62	14.732	1101	1102	1104	rBV	30399	49644	1.48%	0.122%
63	14.881	1113	1115	1120	rVB4	57093	124811	3.73%	0.307%
64	14.972	1120	1123	1126	rVV3	33870	103133	3.08%	0.254%
65	15.052	1129	1130	1133	rBV2	21490	38137	1.14%	0.094%
66	15.144	1136	1138	1143	rBV	249678	546289	16.31%	1.345%
67	15.258	1146	1148	1150	rVB	36067	41736	1.25%	0.103%
68	15.452	1162	1165	1168	rVB	149589	202223	6.04%	0.498%
69	15.509	1168	1170	1173	rVV	169630	233960	6.98%	0.576%
70	15.578	1173	1176	1183	rVB	583434	920988	27.49%	2.268%
71	16.047	1214	1217	1219	rBV	21827	42838	1.28%	0.106%

LSC Area Percent Report

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Operator : UM/IZ
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Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

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-BF092415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.092	1219	1221	1224	rVB2	56997	89773	2.68%	0.221%
73	16.287	1236	1238	1245	rVB6	29838	69659	2.08%	0.172%
74	16.721	1273	1276	1282	rVB6	30714	71883	2.15%	0.177%
75	16.870	1284	1289	1293	rVV4	25189	91886	2.74%	0.226%
76	17.041	1300	1304	1308	rVB2	90077	185954	5.55%	0.458%
77	17.144	1310	1313	1316	rVB4	20070	45579	1.36%	0.112%
78	17.224	1317	1320	1323	rBV2	37522	89717	2.68%	0.221%
79	17.475	1339	1342	1347	rVB	64133	149077	4.45%	0.367%
80	17.624	1353	1355	1360	rVB5	17791	39809	1.19%	0.098%
81	18.961	1467	1472	1479	rBV	118289	372203	11.11%	0.917%

Sum of corrected areas: 40602095

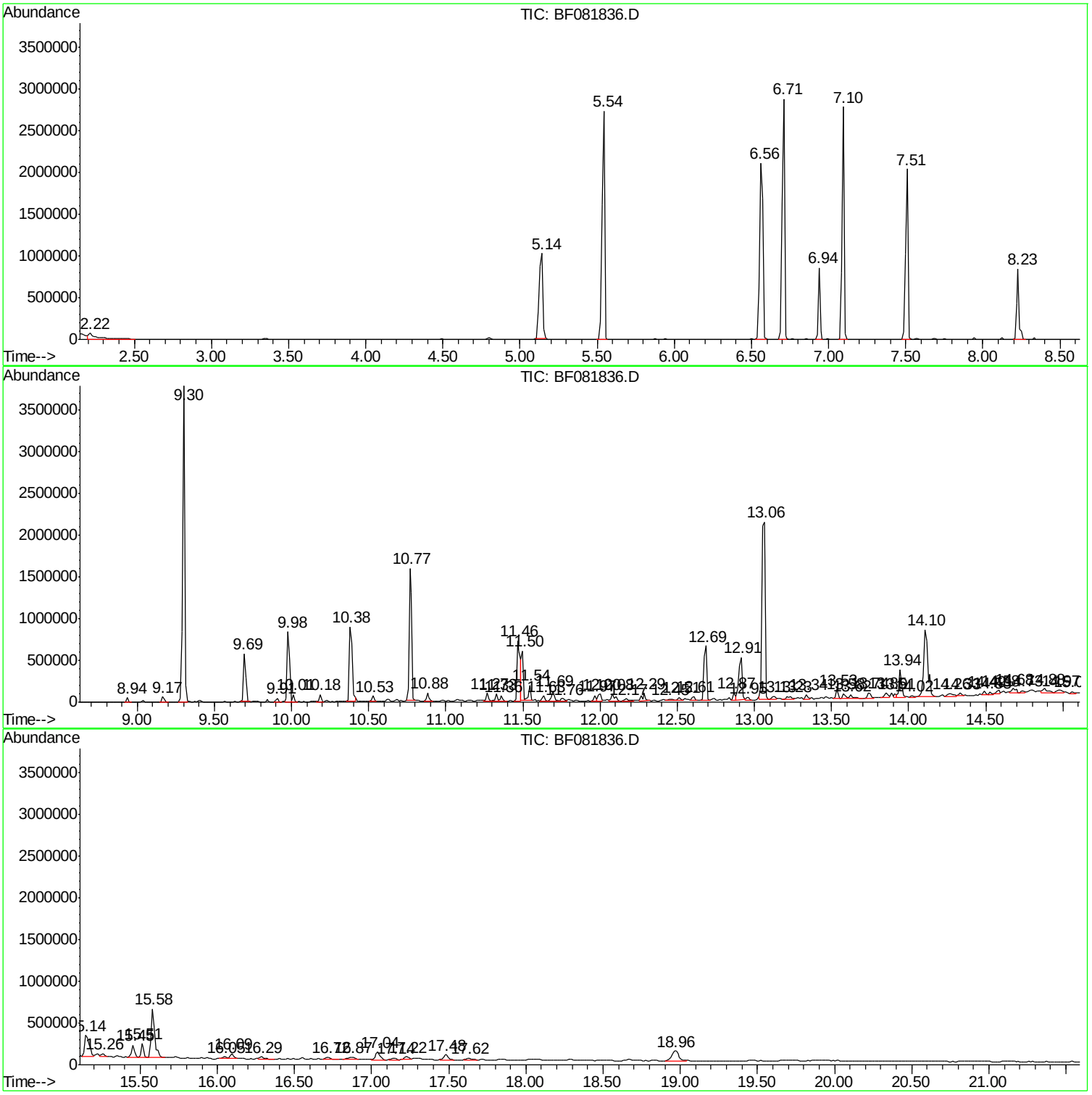
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

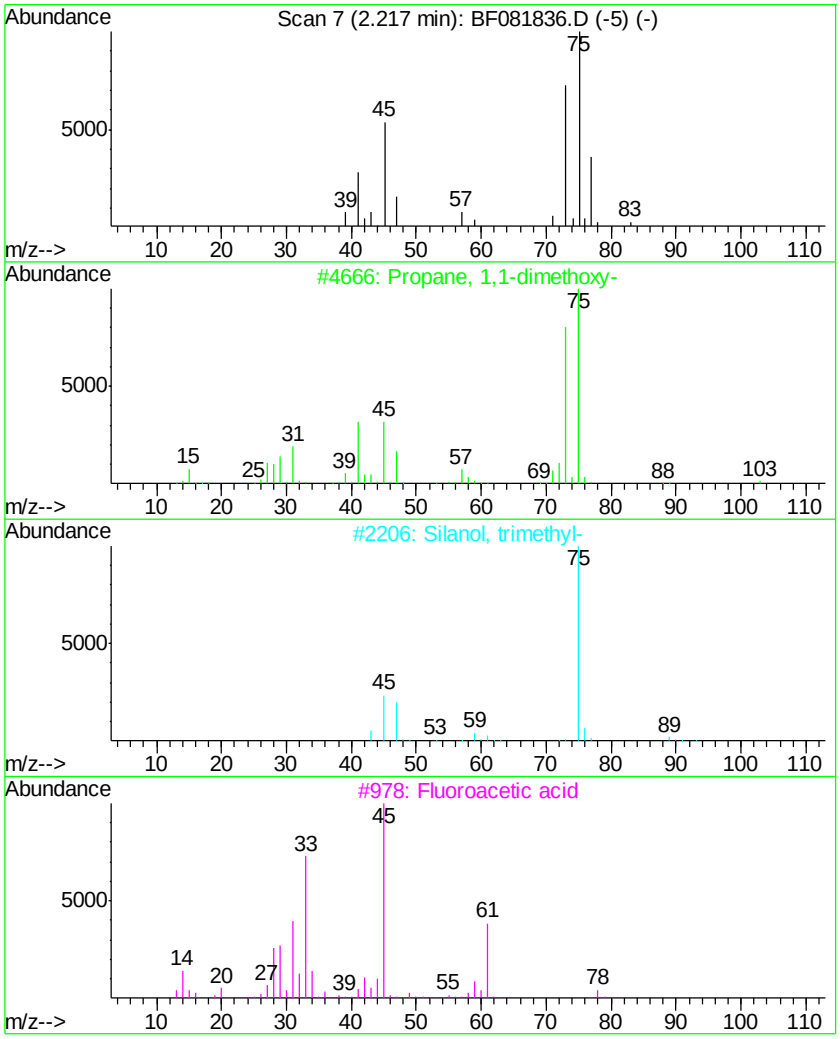
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

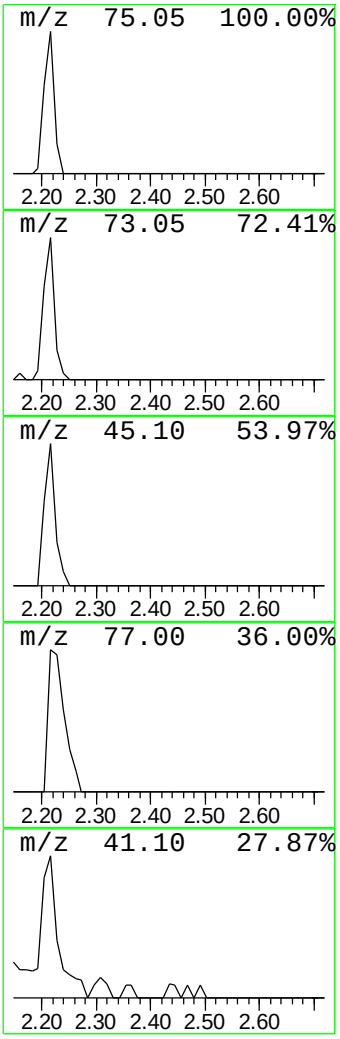
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	7.29 ng	253745	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	59
2	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	28
3	Fluoroacetic acid	78	C2H3FO2	000144-49-0	7
4	Glycine	75	C2H5NO2	000056-40-6	7
5	Formamide, N-methylthio	75	C2H5NS	018952-41-5	5





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Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

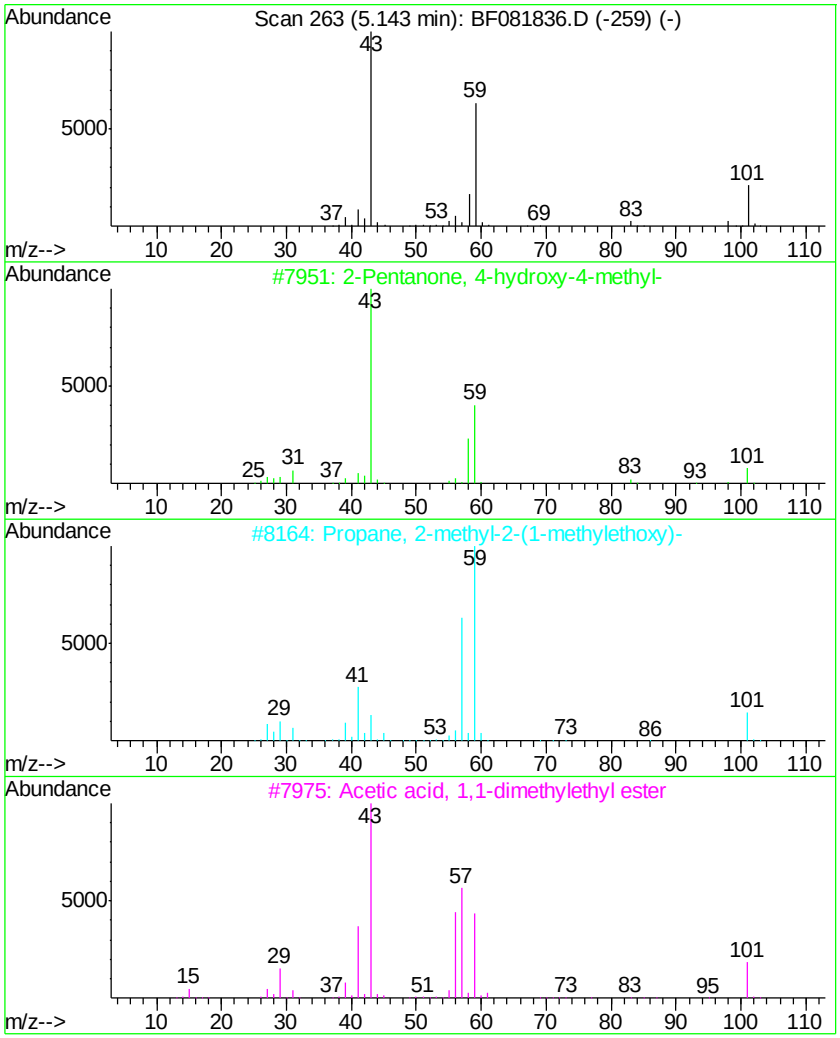
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

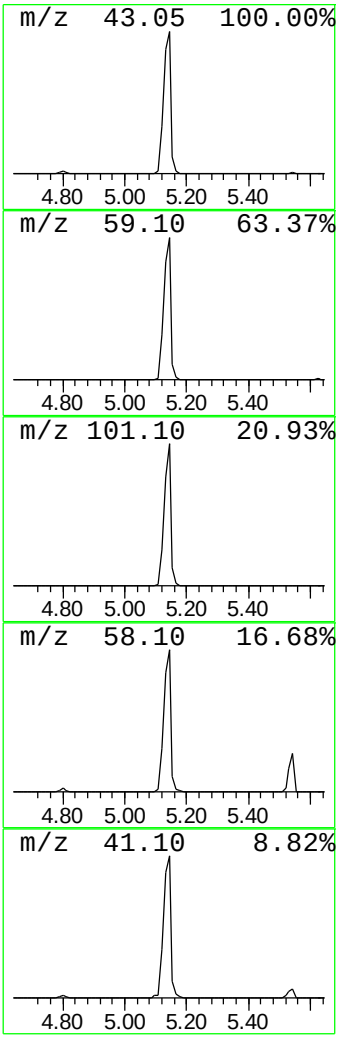
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	46.15 ng	1606690	1,4-Dichlorobenzene-d4	6.94

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	42
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	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

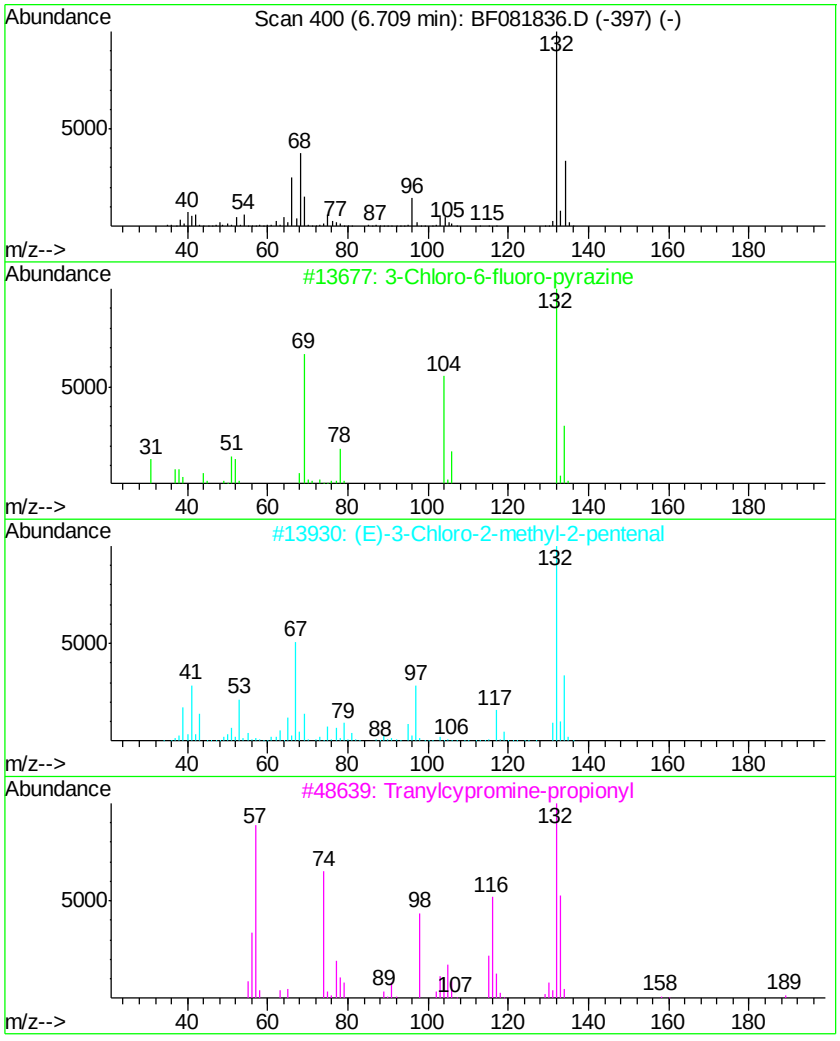
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

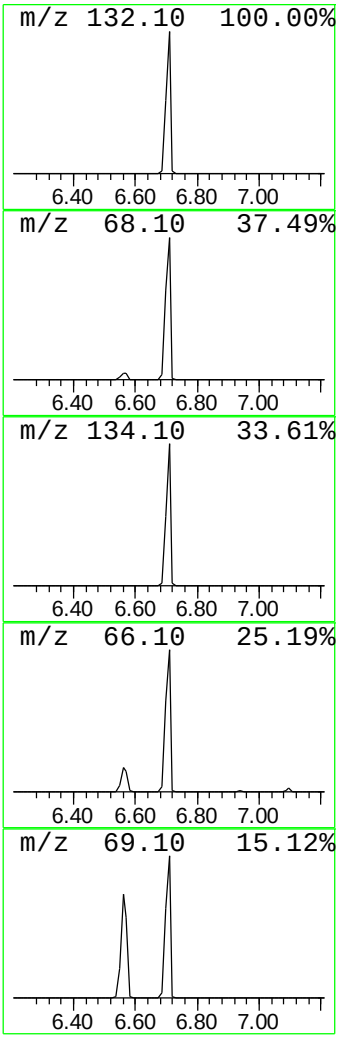
****

Peak Number 3 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	91.93 ng	3200350	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
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TIC Library : C:\DATABASE\NIST02.L
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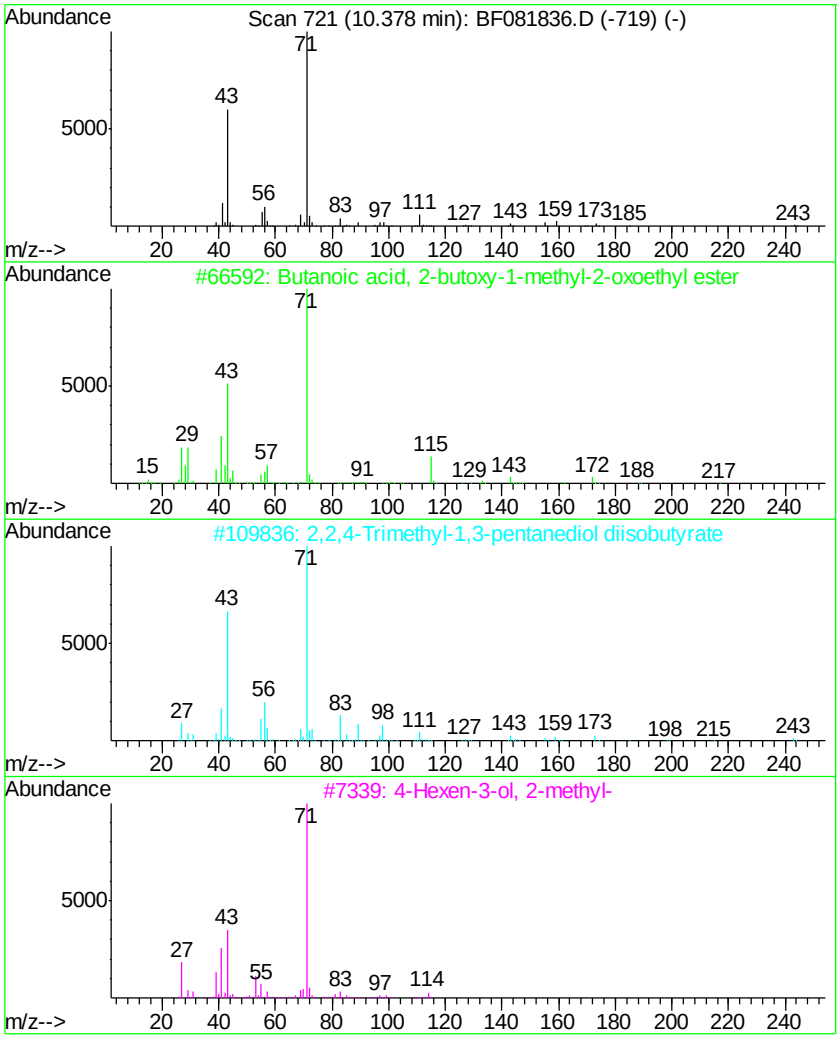
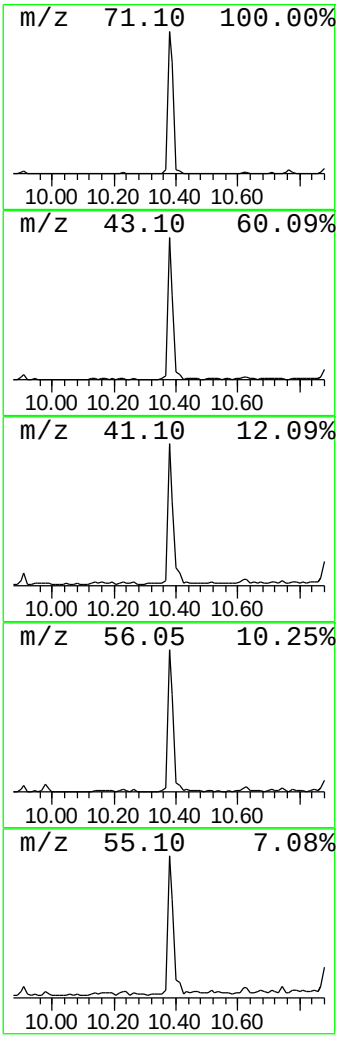
****

Peak Number 5 Butanoic acid, 2-butoxy-1-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	24.92 ng	1188730	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
3	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	45
4	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	38
5	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	38





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Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

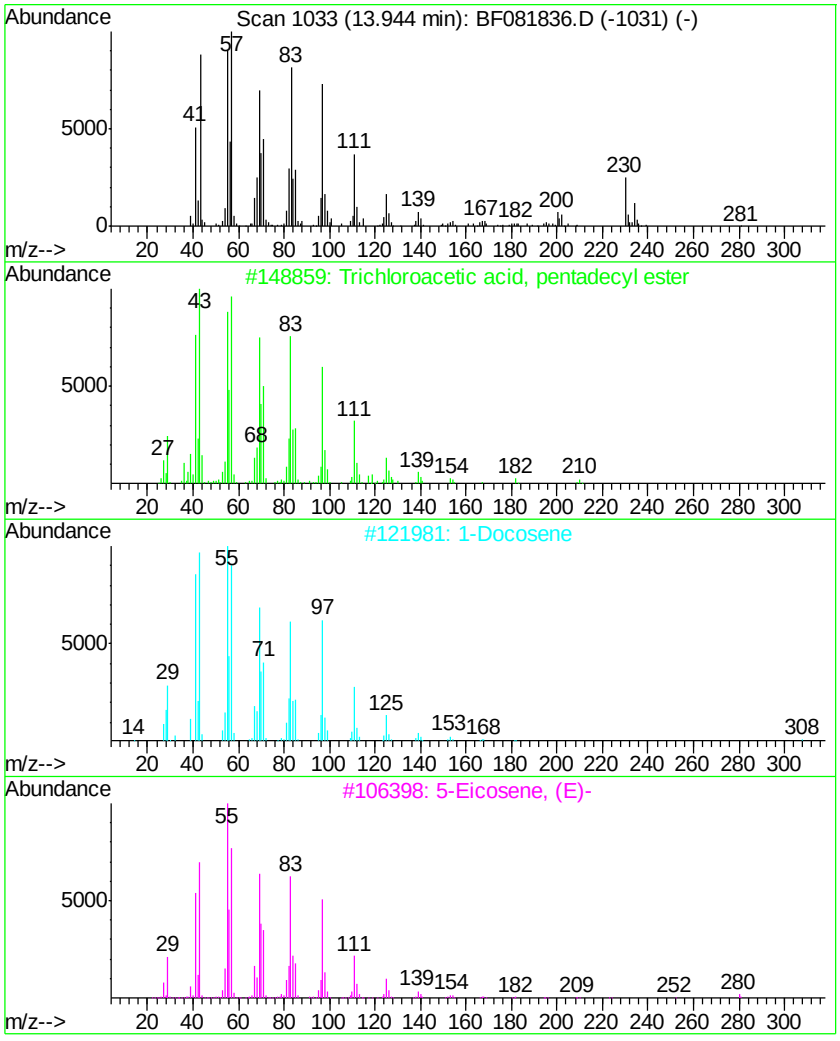
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

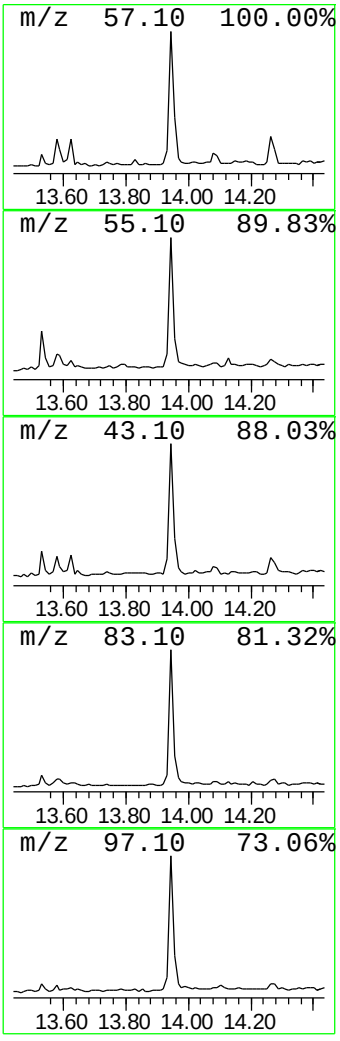
****

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	4.72 ng	368580	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2	1-Docosene	308	C22H44	001599-67-3	93
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	90





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Data File : BF081836.D
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Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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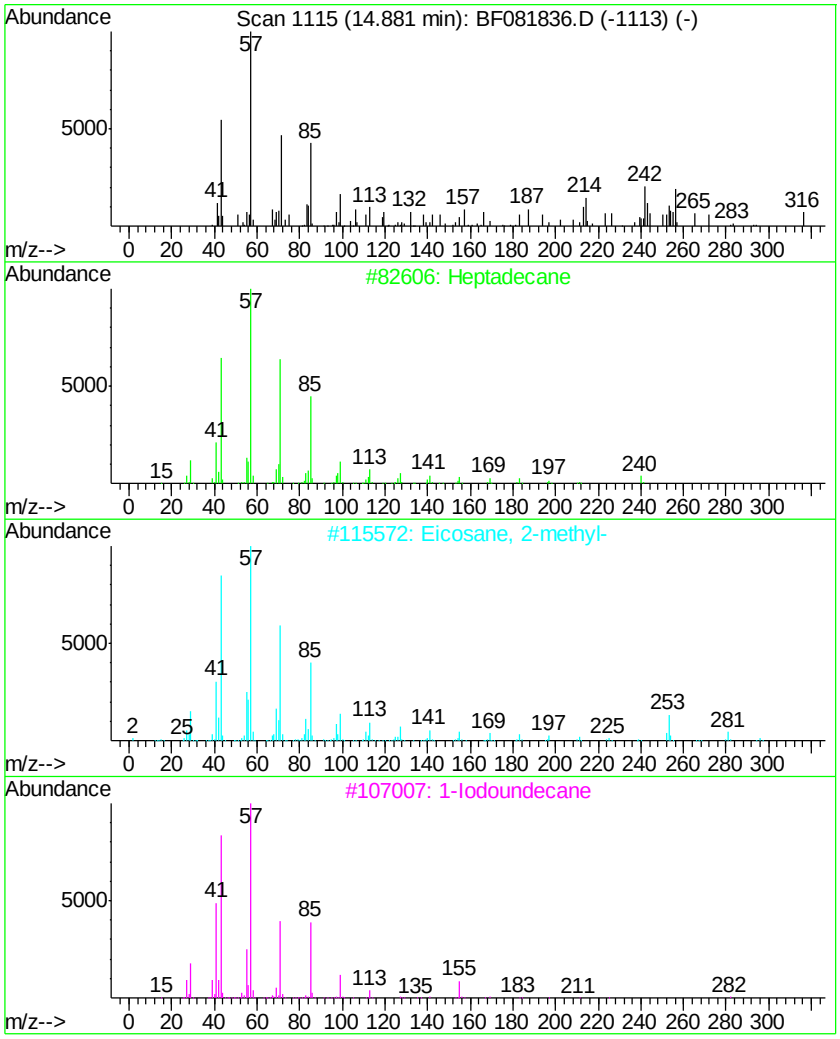
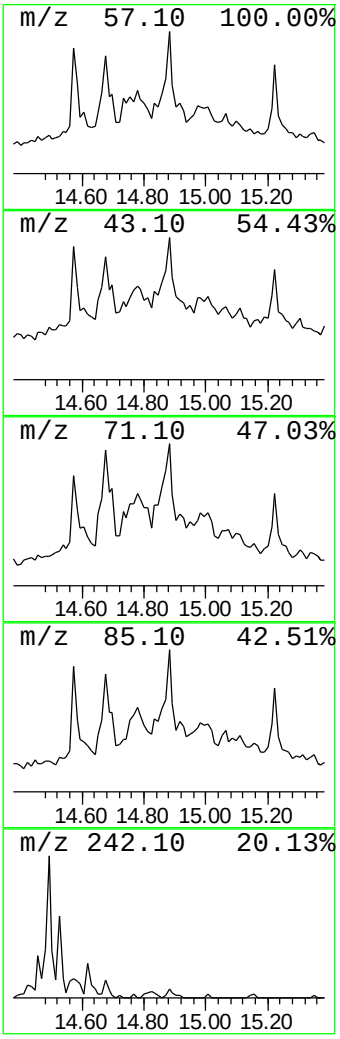
Peak Number 7 unknown14.88 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	2.71 ng	124811	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	45
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	43
3	1-Iodoundecane	282	C11H23I	004282-44-4	38
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	38
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

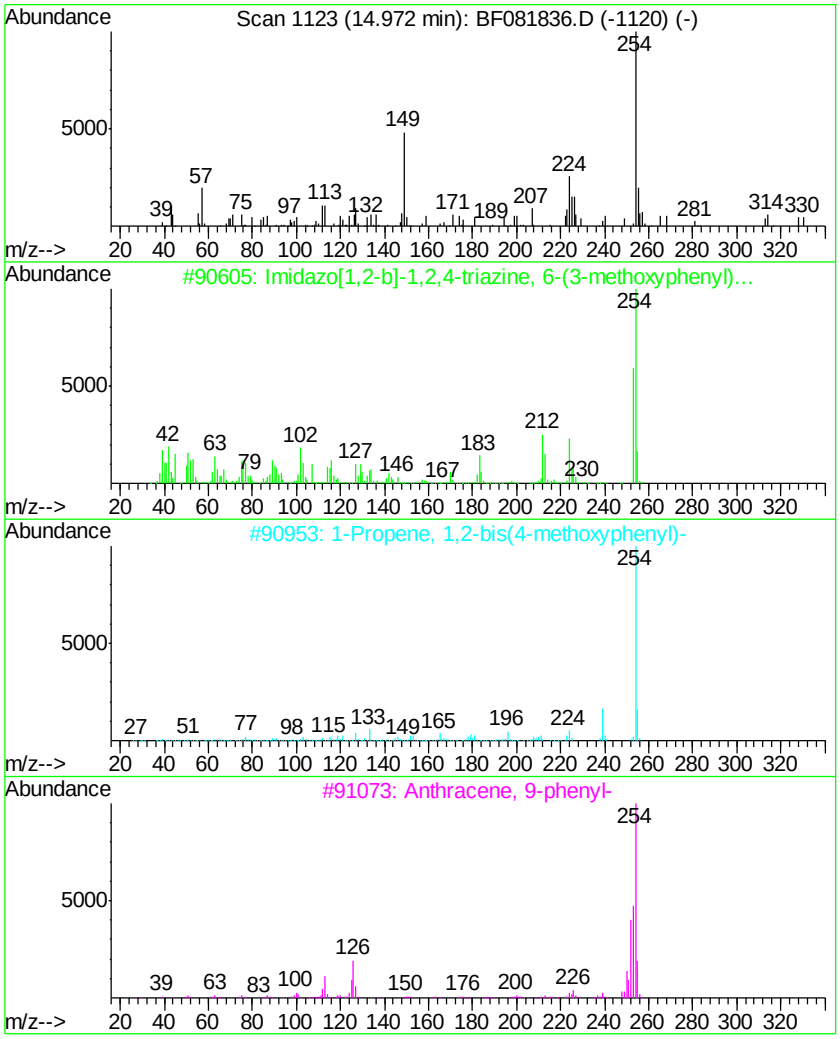
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

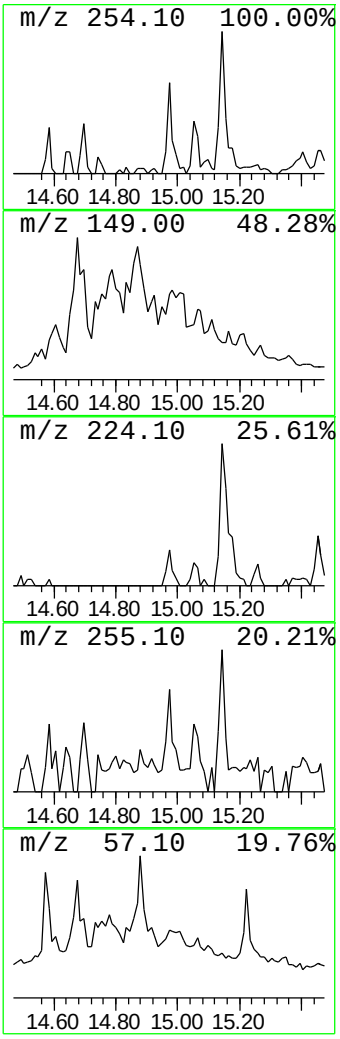
****

Peak Number 8 unknown14.97 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.24 ng	103133	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazo[1,2-b]-1,2,4-triazine, 6...	254	C14H14N4O	1000277-24-4	47
2	1-Propene, 1,2-bis(4-methoxyphen...	254	C17H18O2	020802-02-2	43
3	Anthracene, 9-phenyl-	254	C20H14	000602-55-1	43
4	2,2'-Binaphthalene	254	C20H14	000612-78-2	43
5	1,2'-Binaphthalene	254	C20H14	004325-74-0	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081836.D
Acq On : 26 Sep 2015 19:27
Operator : UM/IZ
Sample : G3779-02
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S1-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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
Propane, 1,1-dime...	2.22	7.3	ng	253745	1	6.94	696240	20.0
2-Pentanone, 4-hy...	5.14	46.1	ng	1606690	1	6.94	696240	20.0
unknown6.71	6.71	91.9	ng	3200350	1	6.94	696240	20.0
Butanoic acid, 2-...	10.38	24.9	ng	1188730	3	9.98	954201	20.0
Trichloroacetic a...	13.94	4.7	ng	368580	5	14.12	1562340	20.0
unknown14.88	14.88	2.7	ng	124811	6	15.58	920988	20.0
unknown14.97	14.97	2.2	ng	103133	6	15.58	920988	20.0