LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
Data File : BF086137.D
Acq On : 7 Apr 2016 18:38
Operator : UM/SJ
Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

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-BF040216.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	4.898	244	246	259	rBV	243097	387768	12.64%	0.843%
2	5.333	281	284	299	rBV	2269454	2451950	79.90%	5.330%
3	5.733	318	319	322	rBV	25886	32643	1.06%	0.071%
4	6.384	373	376	378	rBV	2296701	2522767	82.20%	5.484%
5	6.499	384	386	389	rBV	1910717	2490433	81.15%	5.413%
6	6.739	404	407	409	rBV	518388	659884	21.50%	1.434%
7	6.887	418	420	423	rBV	2059193	1934672	63.04%	4.205%
8	7.310	454	457	459	rBV	1190050	1664793	54.25%	3.619%
9	7.424	464	467	472	rVB	31037	43509	1.42%	0.095%
10	8.019	517	519	522	rBV	977780	899481	29.31%	1.955%
11	9.093	611	613	616	rBV	2191584	2903035	94.60%	6.310%
12	9.493	646	648	651	rBV	445703	440297	14.35%	0.957%
13	9.710	664	667	668	rBV	56680	48163	1.57%	0.105%
14	9.768	670	672	675	rVB	827662	966577	31.50%	2.101%
15	9.939	684	687	691	rBV2	11514	32429	1.06%	0.070%
16	10.202	709	710	712	rVB	54883	66433	2.16%	0.144%
17	10.293	716	718	724	rVB4	14648	40498	1.32%	0.088%
18	10.419	726	729	731	rBV	28661	44057	1.44%	0.096%
19	10.568	739	742	744	rBV2	1586370	1908061	62.17%	4.148%
20	10.682	750	752	756	rVB	73794	95897	3.12%	0.208%
21	10.831	761	765	767	rBV2	87574	177042	5.77%	0.385%
22	10.876	767	769	771	rVV	156550	186867	6.09%	0.406%
23	10.911	771	772	773	rVB	49712	34102	1.11%	0.074%
24	10.956	773	776	779	rVB3	131759	180961	5.90%	0.393%
25	11.013	779	781	783	rVB2	57627	75854	2.47%	0.165%
26	11.059	783	785	786	rBV	294651	444341	14.48%	0.966%
27	11.105	786	789	792	rVB	232615	617120	20.11%	1.341%
28	11.185	792	796	800	rVB5	297383	868939	28.31%	1.889%
29	11.253	800	802	805	rBV	1265623	1089063	35.49%	2.367%
30	11.322	805	808	810	rBV3	172556	351511	11.45%	0.764%
31	11.368	810	812	814	rVB3	347758	428686	13.97%	0.932%
32	11.413	814	816	818	rVB2	266479	385795	12.57%	0.839%
33	11.459	818	820	822	rBV2	67843	157238	5.12%	0.342%
34	11.505	822	824	826	rBV3	39675	57530	1.87%	0.125%

LSC Area Percent Report

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Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

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-BF040216.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.551	826	828	829	rBV	68083	82262	2.68%	0.179%
36	11.619	832	834	835	rBV2	43965	53294	1.74%	0.116%
37	11.653	835	837	841	rVB4	52769	108670	3.54%	0.236%
38	11.756	841	846	848	rVB6	133473	327900	10.68%	0.713%
39	11.791	848	849	855	rBV2	94998	186824	6.09%	0.406%
40	11.893	855	858	862	rVB5	36328	127849	4.17%	0.278%
41	11.951	862	863	866	rVB	42614	48146	1.57%	0.105%
42	12.031	866	870	872	rBV3	53956	152111	4.96%	0.331%
43	12.088	872	875	877	rVB4	45690	73972	2.41%	0.161%
44	12.145	877	880	882	rBV3	63489	115712	3.77%	0.252%
45	12.179	882	883	887	rVB2	65021	145708	4.75%	0.317%
46	12.236	887	888	889	rBV	48474	51664	1.68%	0.112%
47	12.259	889	890	892	rBV2	25361	32674	1.06%	0.071%
48	12.294	892	893	895	rBV2	68678	101320	3.30%	0.220%
49	12.374	895	900	901	rBV5	85499	218288	7.11%	0.474%
50	12.419	903	904	907	rVB3	43011	56436	1.84%	0.123%
51	12.476	907	909	912	rBV4	114431	321071	10.46%	0.698%
52	12.522	912	913	916	rBV3	56451	85688	2.79%	0.186%
53	12.579	916	918	919	rVB2	40650	52547	1.71%	0.114%
54	12.648	922	924	926	rBV2	204805	460177	14.99%	1.000%
55	12.762	928	934	936	rBV7	216992	893287	29.11%	1.942%
56	12.842	938	941	943	rVV	3136882	3068909	100.00%	6.671%
57	12.899	943	946	949	rVB5	31322	82337	2.68%	0.179%
58	13.014	955	956	957	rBV	170834	172432	5.62%	0.375%
59	13.059	957	960	964	rVV2	206048	676561	22.05%	1.471%
60	13.116	964	965	969	rVV4	105881	313830	10.23%	0.682%
61	13.219	973	974	975	rBV	225710	188106	6.13%	0.409%
62	13.254	975	977	980	rVB2	231415	573246	18.68%	1.246%
63	13.322	980	983	984	rBV	229014	447112	14.57%	0.972%
64	13.414	989	991	992	rVB	173746	199628	6.50%	0.434%
65	13.448	992	994	995	rVB2	117234	156318	5.09%	0.340%
66	13.471	995	996	999	rVB3	157545	200239	6.52%	0.435%
67	13.528	999	1001	1004	rBV4	220571	468562	15.27%	1.019%
68	13.585	1004	1006	1009	rVB3	163457	313903	10.23%	0.682%
69	13.665	1009	1013	1014	rBV3	206864	421266	13.73%	0.916%
70	13.699	1014	1016	1017	rVB2	90959	94776	3.09%	0.206%
71	13.745	1017	1020	1022	rBV	250945	639568	20.84%	1.390%

LSC Area Percent Report

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Sample : H2345-01
Misc :
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Instrument : BNA_F
ClientSampleId : EP003

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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.814	1025	1026	1030	rVB3	172457	342835	11.17%	0.745%
73	13.894	1030	1033	1035	rBV	860848	961915	31.34%	2.091%
74	13.951	1035	1038	1041	rVB3	170578	354420	11.55%	0.770%
75	14.054	1043	1047	1048	rBV	326571	402691	13.12%	0.875%
76	14.122	1051	1053	1054	rBV	118484	128946	4.20%	0.280%
77	14.179	1054	1058	1060	rBV5	172814	562403	18.33%	1.223%
78	14.248	1060	1064	1065	rBV4	149514	351833	11.46%	0.765%
79	14.351	1070	1073	1076	rVB	365918	896338	29.21%	1.948%
80	14.442	1079	1081	1083	rVB2	199083	286712	9.34%	0.623%
81	14.522	1083	1088	1089	rBV3	378468	1038961	33.85%	2.258%
82	14.614	1095	1096	1098	rBV2	114893	179538	5.85%	0.390%
83	14.659	1098	1100	1103	rVB	455957	836145	27.25%	1.818%
84	14.728	1103	1106	1108	rBV2	132171	130906	4.27%	0.285%
85	14.774	1108	1110	1111	rBV2	188244	150839	4.92%	0.328%
86	14.808	1111	1113	1115	rBV3	204023	301473	9.82%	0.655%
87	14.865	1115	1118	1119	rBV3	343571	637741	20.78%	1.386%
88	14.911	1119	1122	1129	rVB	326327	1222066	39.82%	2.656%
89	15.288	1153	1155	1161	rBV	547051	710603	23.15%	1.545%
90	15.688	1188	1190	1193	rBV	30886	46582	1.52%	0.101%
91	15.837	1196	1203	1206	rBV5	17767	60418	1.97%	0.131%

Sum of corrected areas: 46004154

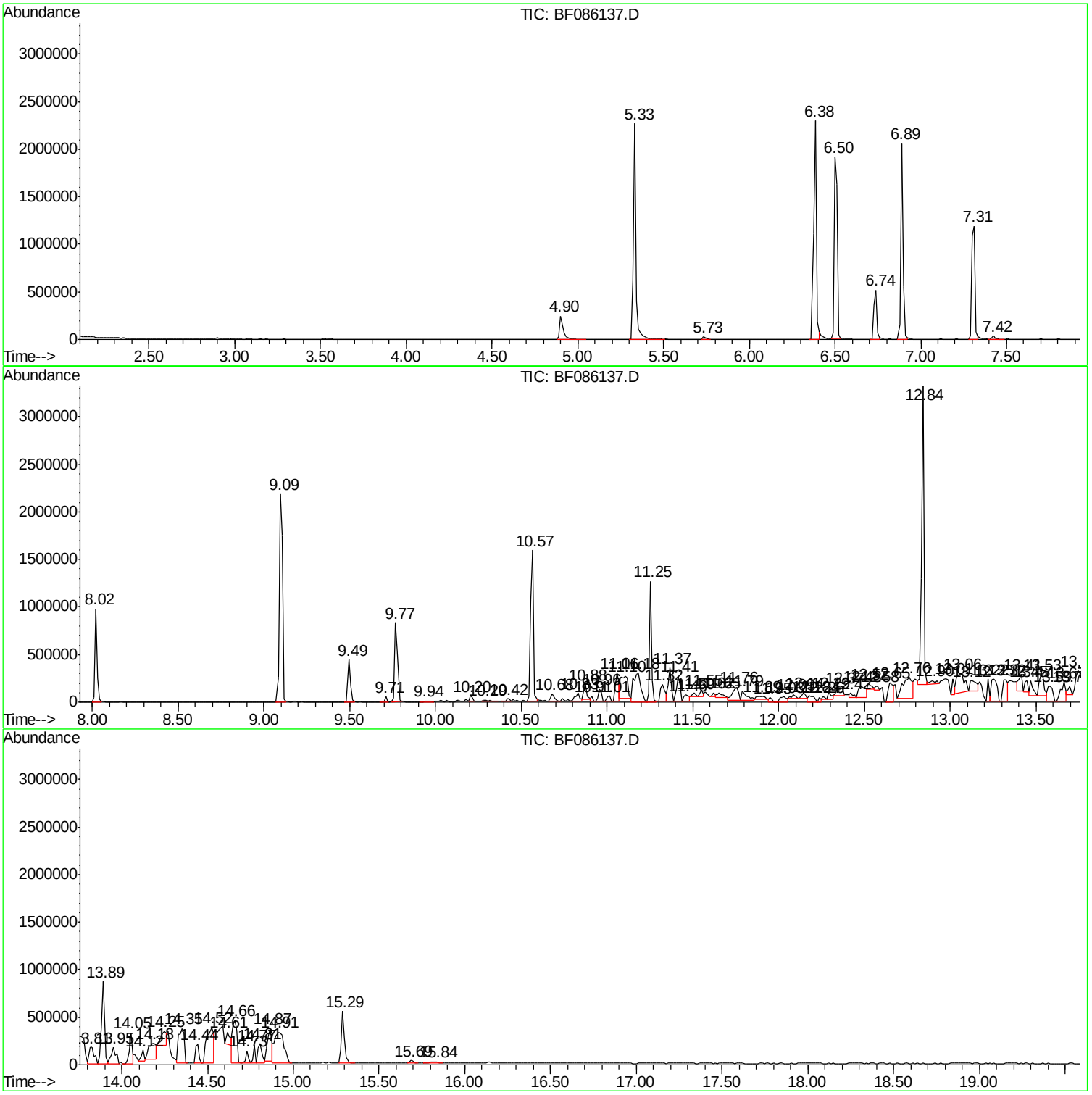
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
Data File : BF086137.D
Acq On : 7 Apr 2016 18:38
Operator : UM/SJ
Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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\BF040716\
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Operator : UM/SJ
Sample : H2345-01
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

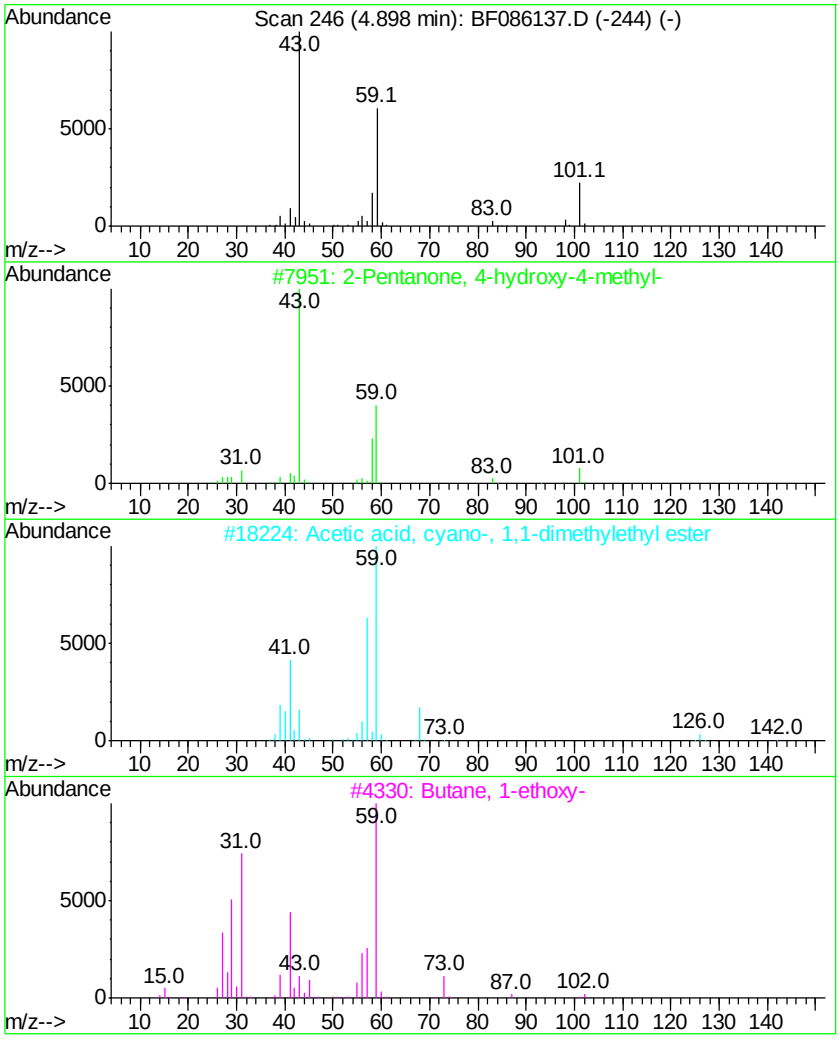
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

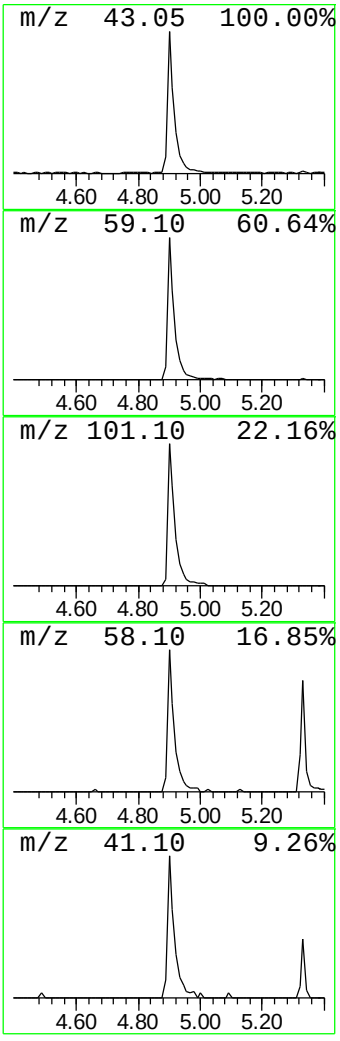
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	11.75 ng	387768	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
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\BF040716\
Data File : BF086137.D
Acq On : 7 Apr 2016 18:38
Operator : UM/SJ
Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

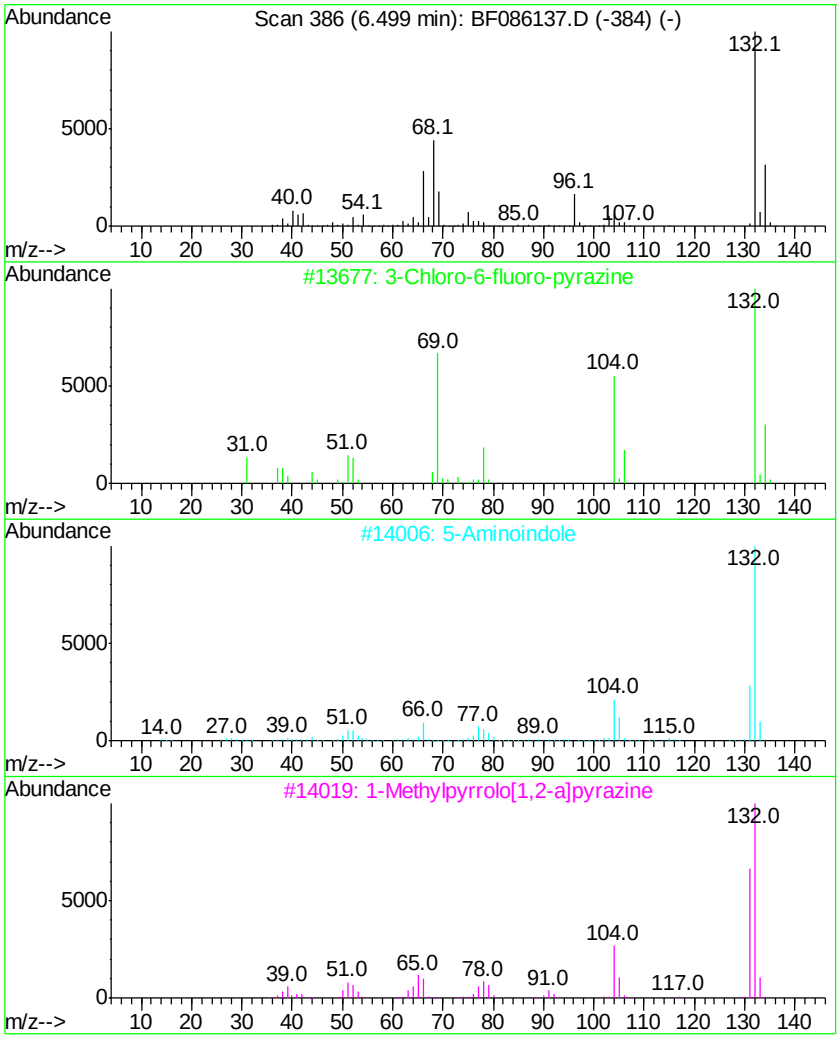
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

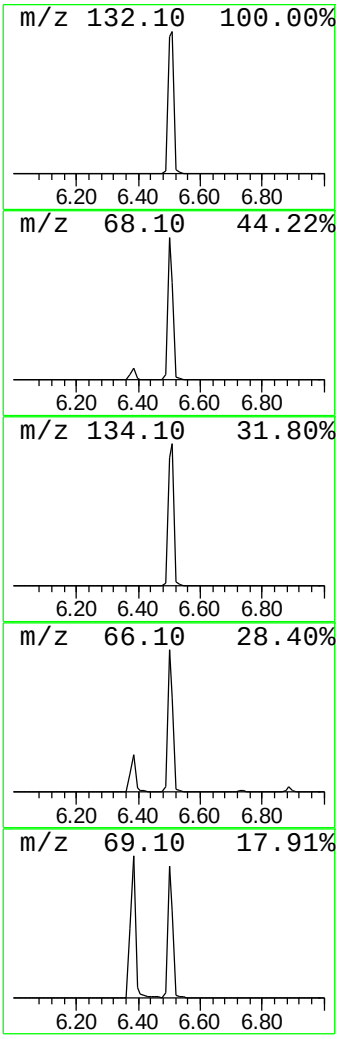
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	75.48 ng	2490430	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

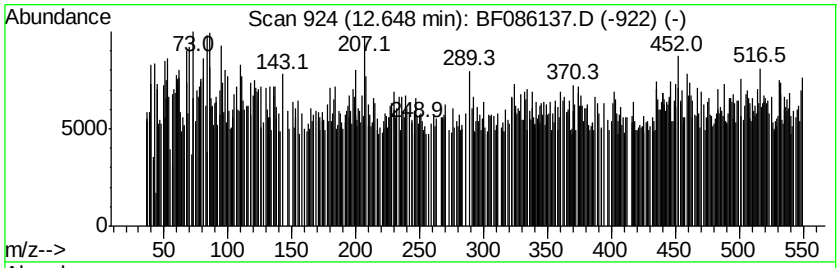
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

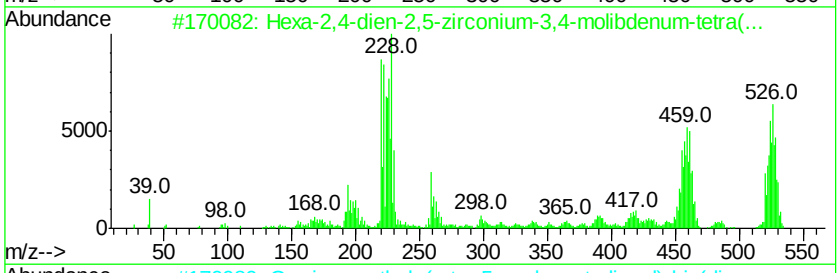
****

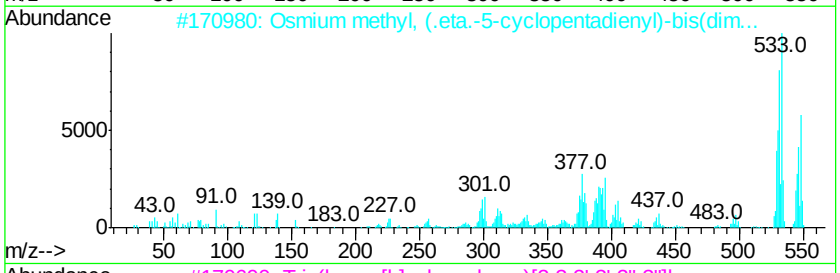
Peak Number 6 Hexa-2,4-dien-2,5-zirconium... Concentration Rank 17

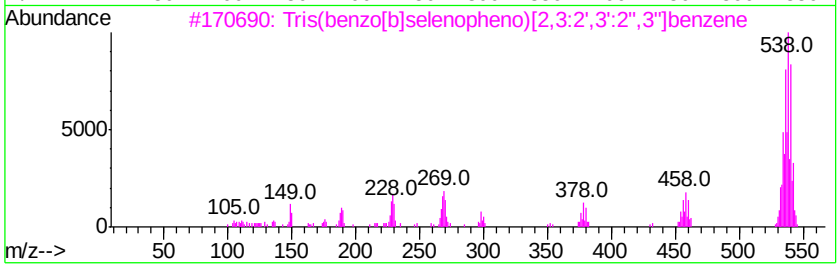
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	9.57 ng	460177	Chrysene-d12	13.89

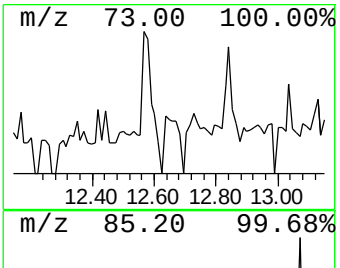
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexa-2,4-dien-2,5-zirconium-3,4-...	526	C26H26MoZr	1000154-45-6	55
2	Osmium methyl, (.eta.-5-cyclopen...	548	C22H30OsP2	1000158-92-4	25
3	Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	20
4	Phenol, 4,4'-(1-methylethylidene...	540	C15H12Br4O2	000079-94-7	14
5	N,5-Bis[3,4-dichlorophenyl]-3,5-...	540	C27H20Cl4N4	333399-40-9	10

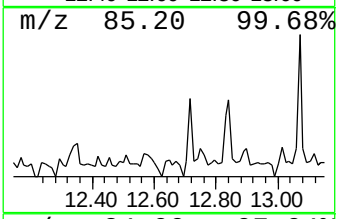


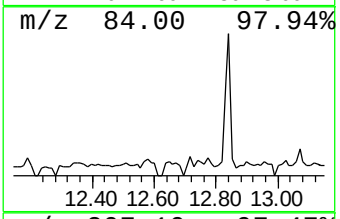


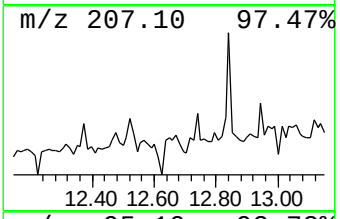


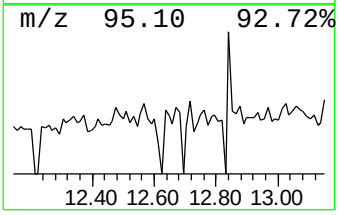












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040716\
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Acq On : 7 Apr 2016 18:38
Operator : UM/SJ
Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

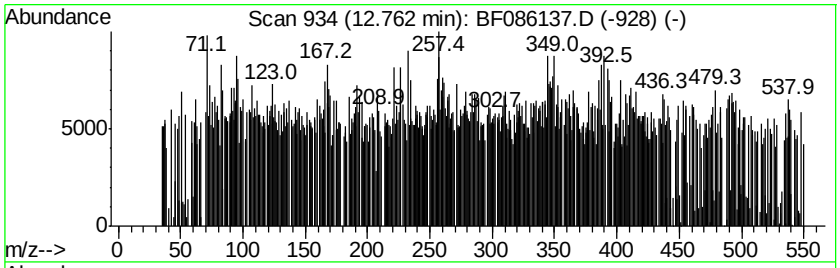
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

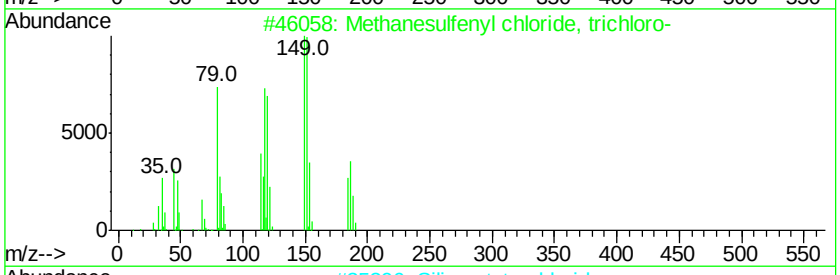
****

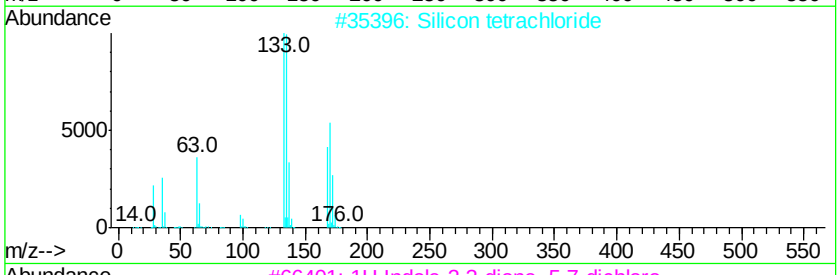
Peak Number 7 unknown12.76 Concentration Rank 7

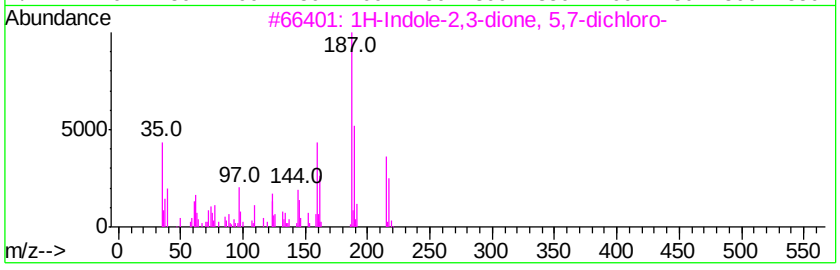
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	18.57 ng	893287	Chrysene-d12	13.89

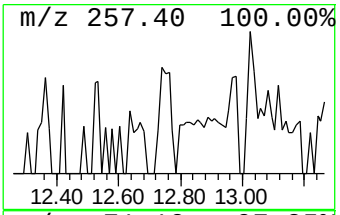
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanesulfenyl chloride, trichl...	184	CCl4S	000594-42-3	25
2	Silicon tetrachloride	168	Cl4Si	010026-04-7	25
3	1H-Indole-2,3-dione, 5,7-dichloro-	215	C8H3Cl2NO2	006374-92-1	10
4	1,3,5-Triazine, 2,4,6-trichloro-	183	C3Cl3N3	000108-77-0	10
5	2-Propenoyl chloride, 2,3,3-tric...	192	C3Cl4O	000815-58-7	10

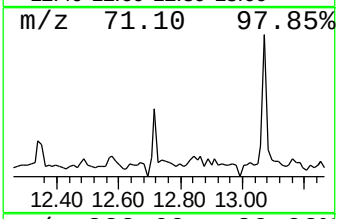


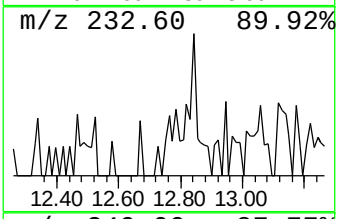


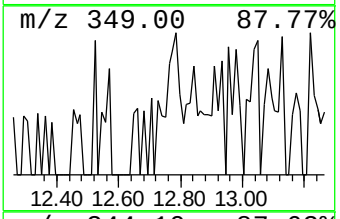


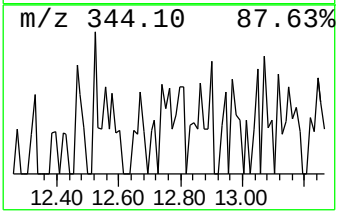












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Acq On : 7 Apr 2016 18:38
Operator : UM/SJ
Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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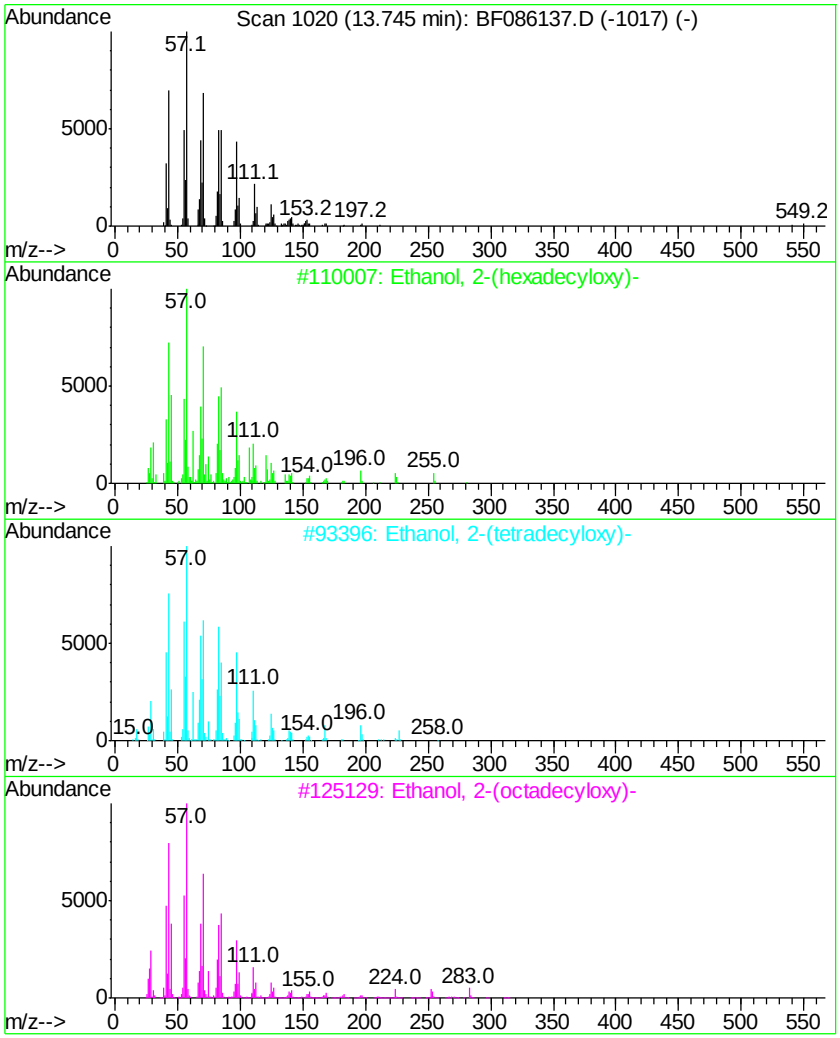
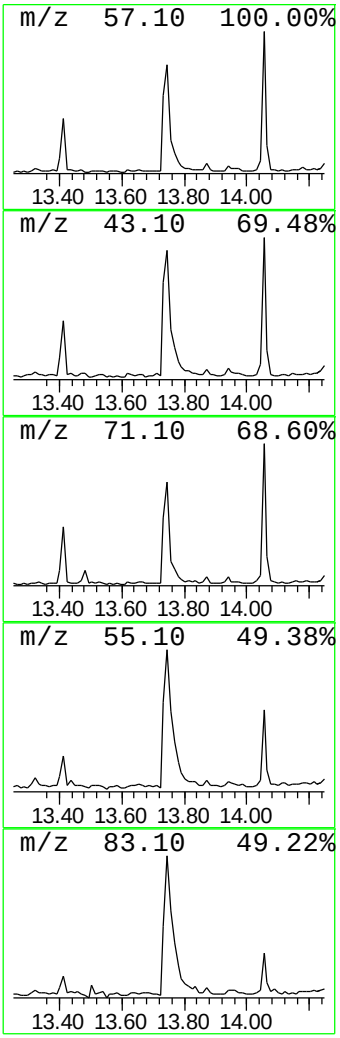
Peak Number 13 Ethanol, 2-(hexadecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	13.30 ng	639568	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74
3	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	72
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	64
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	62





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Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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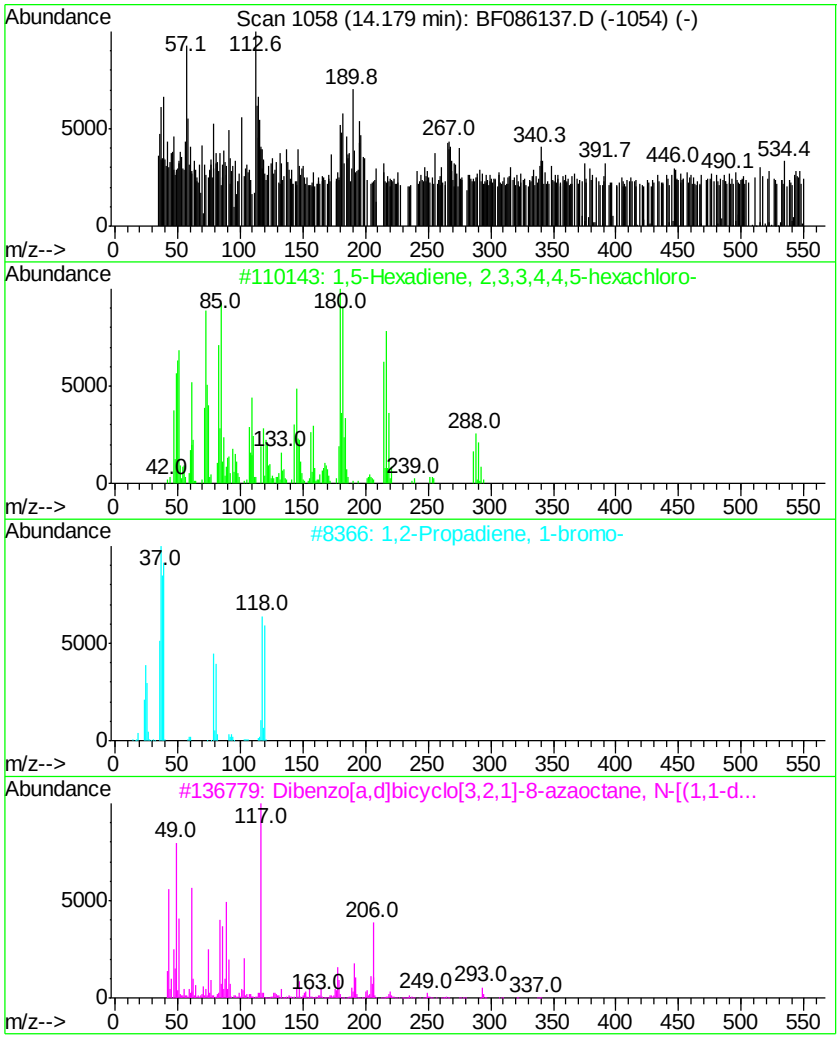
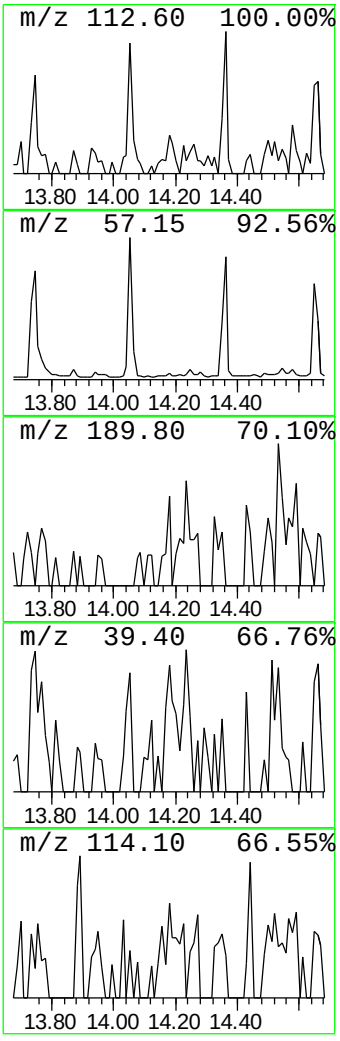
Peak Number 14 unknown14.18 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	11.69 ng	562403	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Hexadiene, 2,3,3,4,4,5-hexac...	286	C6H4Cl6	108562-66-9	30
2	1,2-Propadiene, 1-bromo-	118	C3H3Br	010024-18-7	27
3	Dibenzo[a,d]bicyclo[3,2,1]-8-aza...	339	C21H25NO3	1000128-43-4	27
4	Chloroacetic acid, 3-chloropropy...	170	C5H8Cl2O2	062116-55-6	16
5	Dihydroepinatalensine	303	C17H21NO4	098843-28-8	16





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Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

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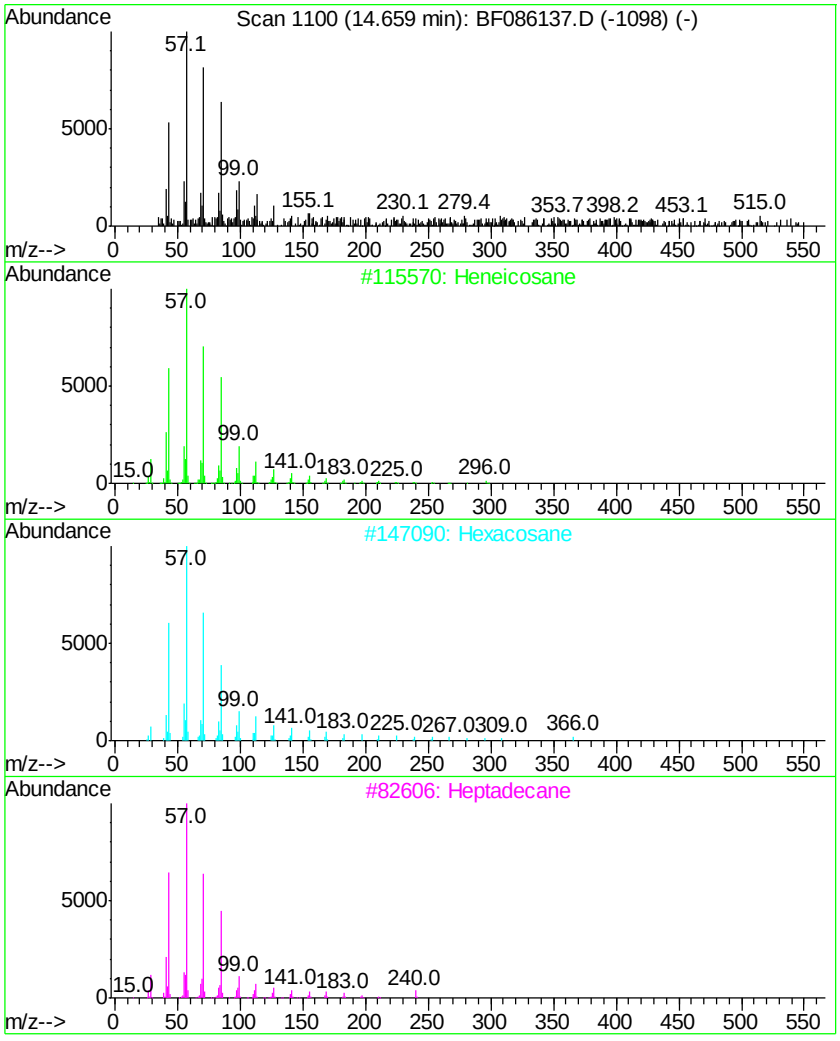
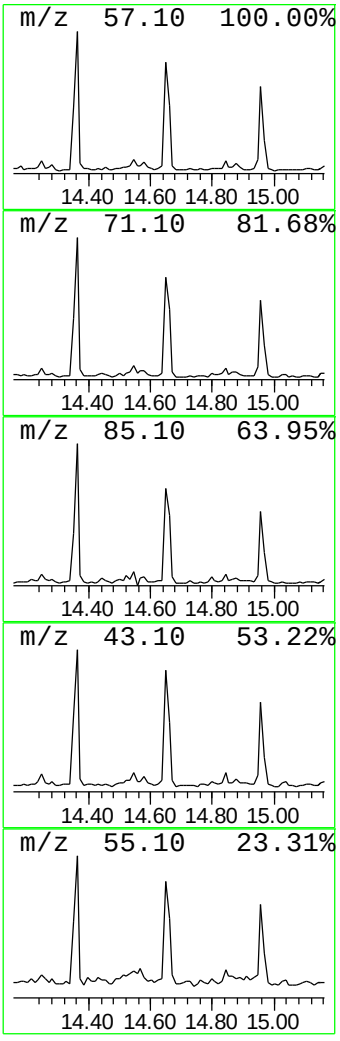
Peak Number 17 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	23.53 ng	836145	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Hexacosane	366	C26H54	000630-01-3	97
3	Heptadecane	240	C17H36	000629-78-7	95
4	Triacontane	422	C30H62	000638-68-6	93
5	Docosane	310	C22H46	000629-97-0	93





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Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

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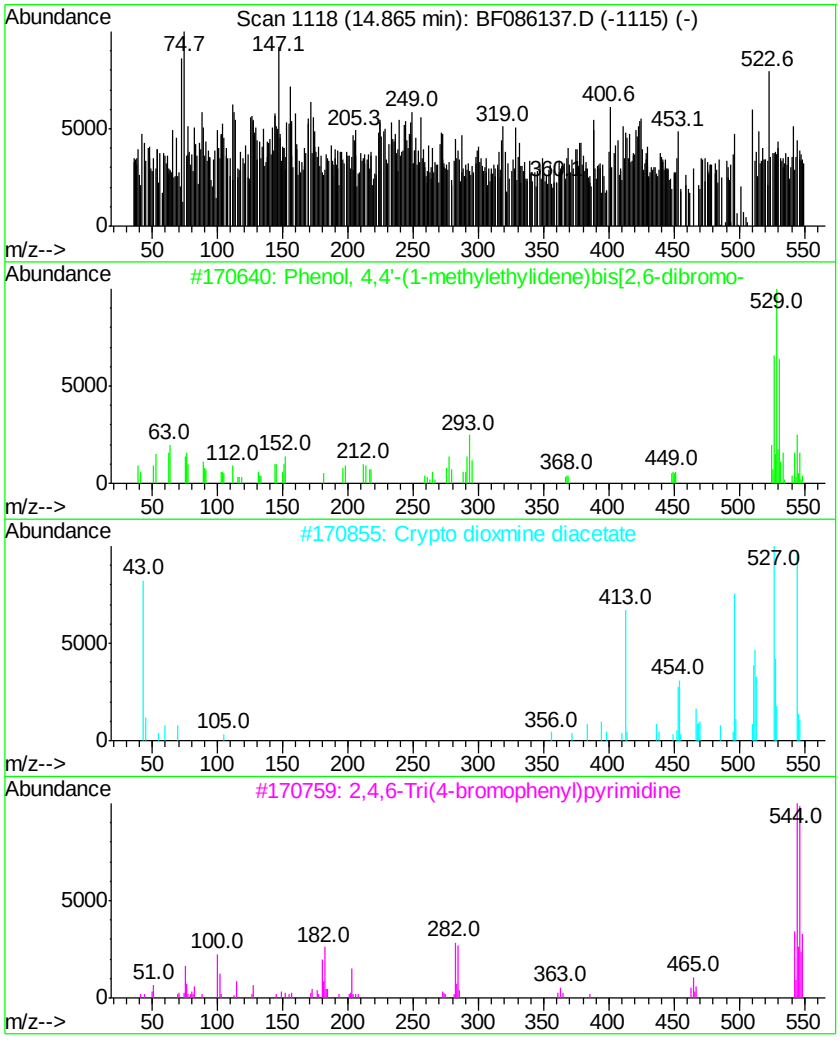
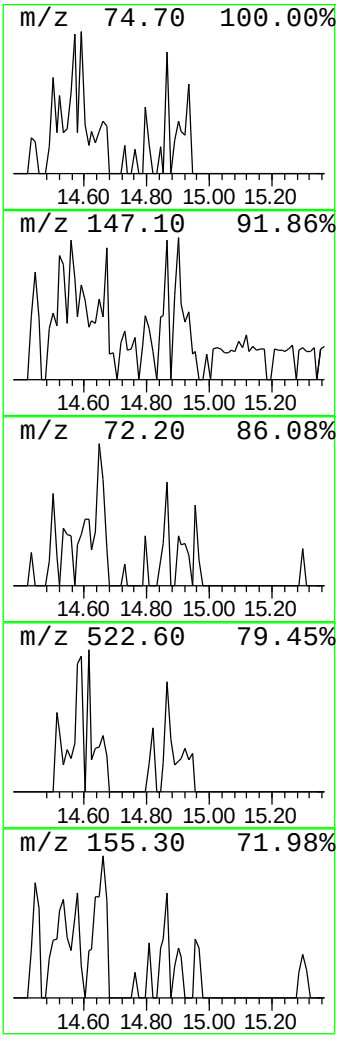
Peak Number 19 unknown14.87 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	17.95 ng	637741	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	540	C15H12Br4O2	000079-94-7	30
2	Crypto dioxmine diacetate	544	C31H48N2O6	1000128-11-7	18
3	2,4,6-Tri(4-bromophenyl)pyrimidine	542	C22H13Br3N2	1000070-62-6	11
4	Ferrocene, 1,1'-bis[(pentafluoro...	546	C24H12F10Fe	055494-16-1	10
5	5,5',6,6',7,7',8,8'-Octahydro-9,...	542	C32H30O8	099968-11-3	9





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Acq On : 7 Apr 2016 18:38
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Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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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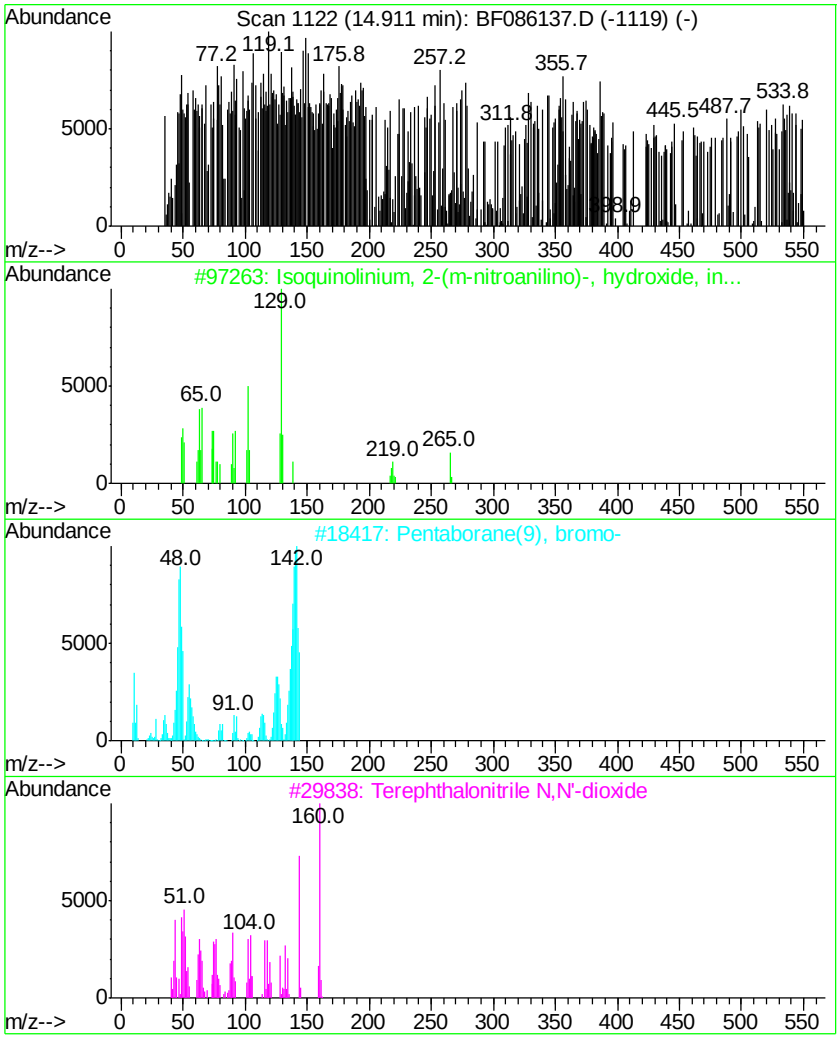
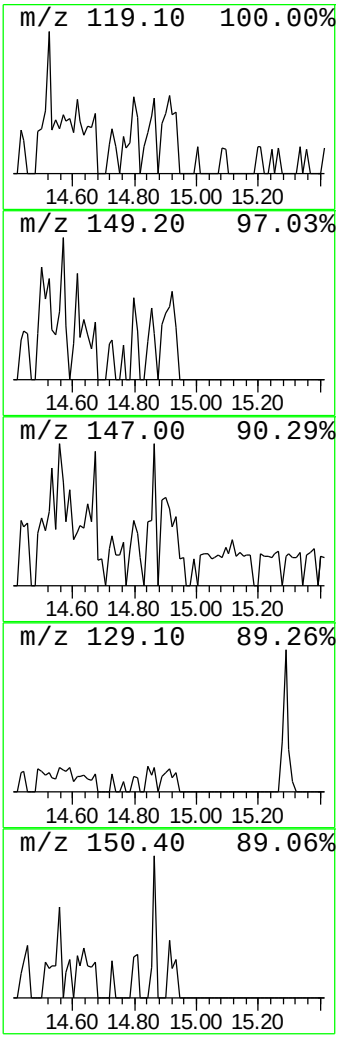
Peak Number 20 Isoquinolinium, 2-(m-nitroa... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	34.40 ng	1222070	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinolinium, 2-(m-nitroanilin...	265	C15H11N3O2	031383-03-6	81
2	Pentaborane(9), bromo-	142	B5BrH8	066794-48-7	60
3	Terephthalonitrile N,N'-dioxide	160	C8H4N2O2	003729-34-8	59
4	Acetanilide, 2-chloro-4'-nitro-	214	C8H7ClN2O3	017329-87-2	43
5	Methane, bromochloro-	128	CH2BrCl	000074-97-5	35





Tentatively Identified Compound (LSC) summary

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Data File : BF086137.D
Acq On : 7 Apr 2016 18:38
Operator : UM/SJ
Sample : H2345-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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...	4.90	11.8	ng	387768	1	6.74	659884	20.0
unknown6.50	6.50	75.5	ng	2490430	1	6.74	659884	20.0
Hexa-2,4-dien-2,5...	12.65	9.6	ng	460177	5	13.89	961915	20.0
unknown12.76	12.76	18.6	ng	893287	5	13.89	961915	20.0
Ethanol, 2-(hexad...	13.75	13.3	ng	639568	5	13.89	961915	20.0
unknown14.18	14.18	11.7	ng	562403	5	13.89	961915	20.0
Heneicosane	14.66	23.5	ng	836145	6	15.29	710603	20.0
unknown14.87	14.87	17.9	ng	637741	6	15.29	710603	20.0
Isoquinolinium, 2...	14.91	34.4	ng	1222070	6	15.29	710603	20.0