LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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	2.190	7	9	10	rVB2	199602	157550	4.93%	0.424%
2	2.247	10	14	17	rBV3	28889	95315	2.98%	0.257%
3	2.293	17	18	21	rVB2	49011	57200	1.79%	0.154%
4	2.350	21	23	24	rBV	33070	59072	1.85%	0.159%
5	2.384	24	26	27	rBV2	135735	218265	6.83%	0.588%
6	2.407	27	28	32	rVB4	136224	247060	7.73%	0.665%
7	2.464	32	33	35	rVB	32344	33615	1.05%	0.091%
8	2.533	35	39	40	rBV2	187717	427707	13.38%	1.152%
9	2.567	40	42	44	rBV3	67599	85844	2.69%	0.231%
10	2.681	49	52	55	rVB5	124795	243044	7.61%	0.654%
11	2.727	55	56	58	rBV2	117765	170962	5.35%	0.460%
12	2.796	60	62	63	rBV2	195448	311390	9.74%	0.838%
13	2.818	63	64	69	rVB4	200050	253789	7.94%	0.683%
14	2.887	69	70	71	rBV	178713	220568	6.90%	0.594%
15	2.921	71	73	76	rVB4	139220	275850	8.63%	0.743%
16	2.990	76	79	82	rBV5	145410	463299	14.50%	1.247%
17	3.036	82	83	84	rVB	148023	101544	3.18%	0.273%
18	3.093	84	88	90	rVB4	191457	395937	12.39%	1.066%
19	3.127	90	91	94	rBV3	154167	403974	12.64%	1.088%
20	3.276	103	104	108	rVB4	176005	403582	12.63%	1.087%
21	3.344	108	110	111	rBV	241021	390397	12.22%	1.051%
22	3.367	111	112	114	rVB	236243	308174	9.64%	0.830%
23	3.413	114	116	118	rBV2	168851	329940	10.32%	0.888%
24	3.459	118	120	121	rVV2	251256	447215	13.99%	1.204%
25	3.516	124	125	128	rVV3	265913	562312	17.60%	1.514%
26	3.584	128	131	135	rVV6	266871	931918	29.16%	2.509%
27	3.664	135	138	139	rVV3	216858	457490	14.32%	1.232%
28	3.699	139	141	142	rVV2	210882	333953	10.45%	0.899%
29	3.733	142	144	149	rVB4	207663	489042	15.30%	1.317%
30	4.156	177	181	182	rBV3	139897	259992	8.14%	0.700%
31	4.190	182	184	186	rVB2	128440	145464	4.55%	0.392%
32	4.499	210	211	214	rBV2	176489	293749	9.19%	0.791%
33	4.613	217	221	223	rVB	219819	379135	11.86%	1.021%
34	4.910	244	247	250	rBV	92697	162749	5.09%	0.438%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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	4.967	250	252	253	rVV	126037	162180	5.07%	0.437%
36	5.013	253	256	258	rVV3	212403	343369	10.74%	0.925%
37	5.070	258	261	269	rVB4	17583	32775	1.03%	0.088%
38	5.333	281	284	286	rBV	2209293	3009145	94.16%	8.102%
39	5.413	289	291	294	rVV4	25670	57480	1.80%	0.155%
40	5.470	294	296	297	rVV2	46278	58012	1.82%	0.156%
41	5.493	297	298	300	rVB	54446	38852	1.22%	0.105%
42	6.385	373	376	378	rBV	2439346	3116861	97.53%	8.392%
43	6.499	383	386	388	rBV	2922786	2899866	90.74%	7.808%
44	6.727	404	406	411	rVB	820628	737578	23.08%	1.986%
45	6.887	417	420	422	rBV	2003092	2472197	77.36%	6.656%
46	7.299	453	456	458	rBV	1852486	1883739	58.94%	5.072%
47	8.008	516	518	521	rBV	761978	894598	27.99%	2.409%
48	9.093	610	613	615	rBV	3095825	3195835	100.00%	8.605%
49	9.482	645	647	650	rBV	270615	335361	10.49%	0.903%
50	9.699	664	666	668	rBV	82026	66603	2.08%	0.179%
51	9.768	669	672	674	rVB	733145	893214	27.95%	2.405%
52	9.928	683	686	690	rBV2	14083	33575	1.05%	0.090%
53	10.202	706	710	711	rBV	88408	107835	3.37%	0.290%
54	10.419	726	729	732	rBV	34530	64018	2.00%	0.172%
55	10.556	738	741	743	rBV	1693124	1687782	52.81%	4.544%
56	10.671	749	751	757	rVB	116449	144761	4.53%	0.390%
57	11.116	788	790	791	rBV	64703	57075	1.79%	0.154%
58	11.242	799	801	804	rBV	870393	791766	24.77%	2.132%
59	11.779	846	848	854	rBV	27027	33983	1.06%	0.091%
60	12.831	937	940	942	rBV	2187452	2185389	68.38%	5.884%
61	13.311	977	982	984	rBV	25529	34483	1.08%	0.093%
62	13.494	997	998	1003	rBV3	44313	77378	2.42%	0.208%
63	13.745	1016	1020	1027	rBV	37630	92569	2.90%	0.249%
64	13.882	1029	1032	1034	rBV	675572	683767	21.40%	1.841%
65	14.763	1106	1109	1112	rBV2	178916	190378	5.96%	0.513%
66	14.808	1112	1113	1115	rVB2	99196	103175	3.23%	0.278%
67	15.277	1151	1154	1157	rBV	439928	537480	16.82%	1.447%

Sum of corrected areas: 37140176

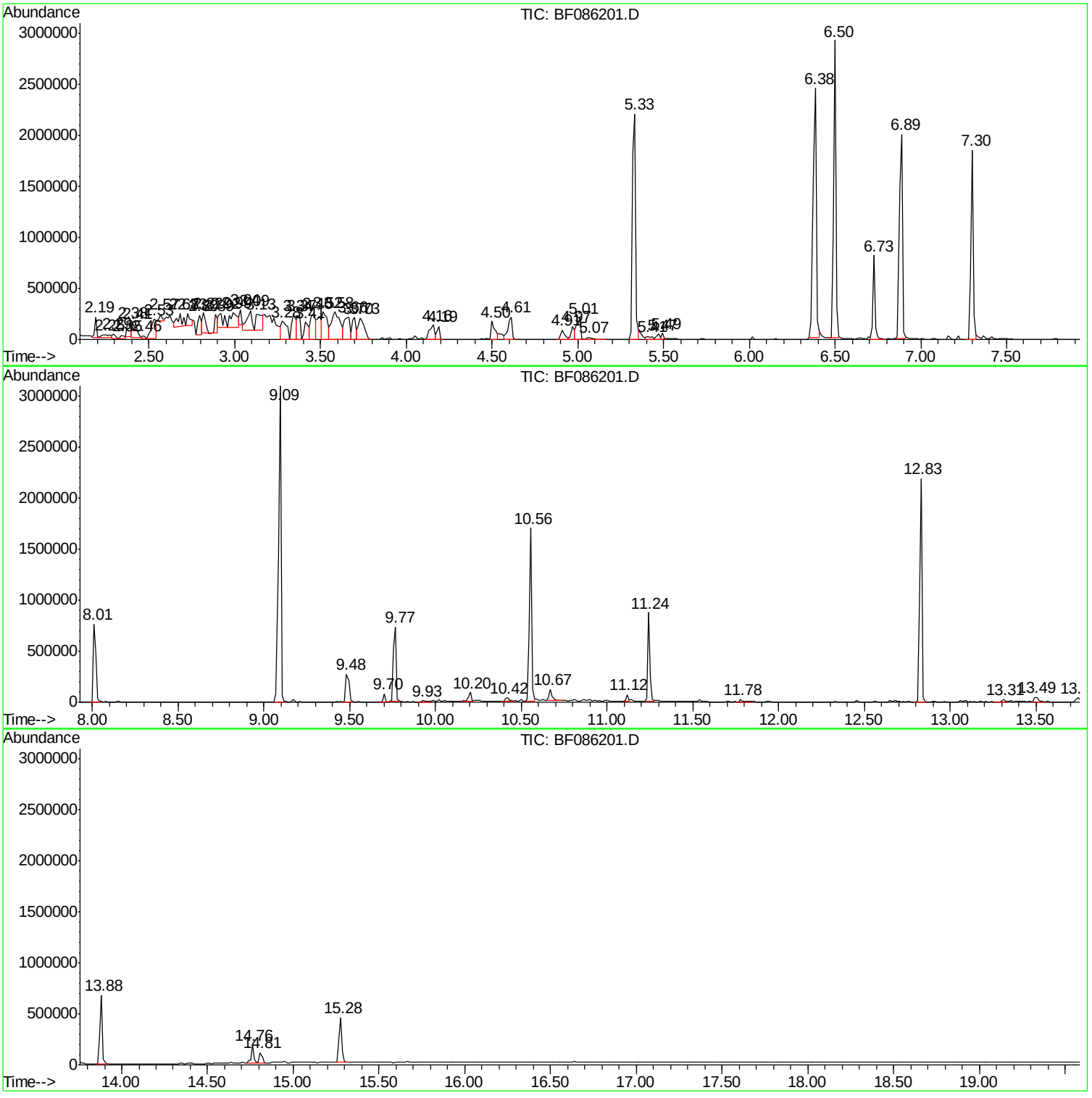
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AMBOY-SB-02(0.5-20.0)

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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

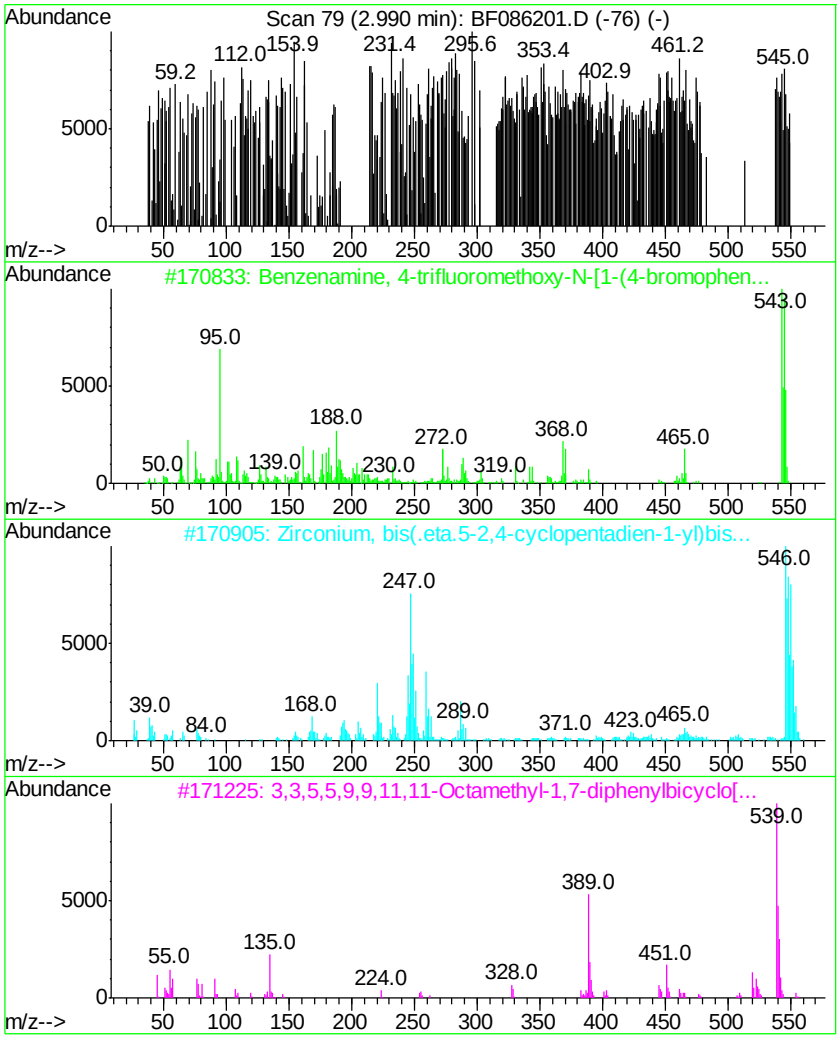
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

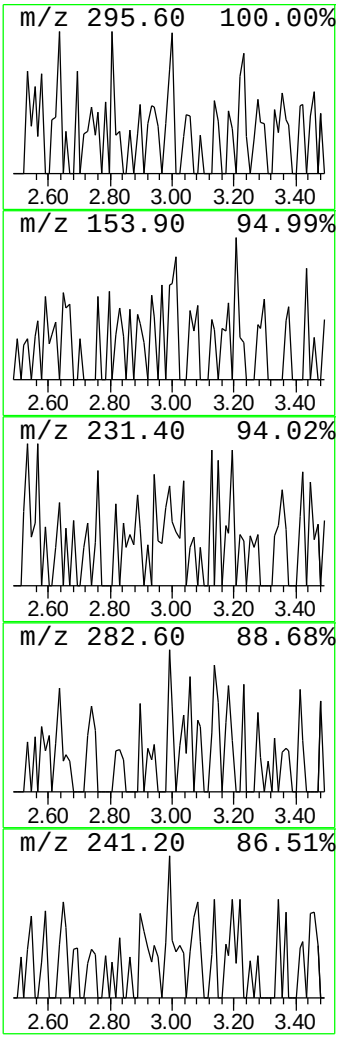
****

Peak Number 3 unknown2.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	12.56 ng	463299	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 4-trifluoromethoxy-...	544	C23H15BrF6N2O2	284495-96-1	42
2	Zirconium, bis(.eta.5-2,4-cyclop...	546	C28H30Zr2	119144-91-1	10
3	3,3,5,5,9,9,11,11-Octamethyl-1,7...	554	C20H34O7Si6	049538-51-4	10
4	Nickel, bis[1,2-diphenyl-1,2-eth...	542	C28H20NiS4	028984-20-5	9
5	Copper, [2,8,12,18-tetraethyl-3,...	539	C32H36CuN4	014055-18-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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

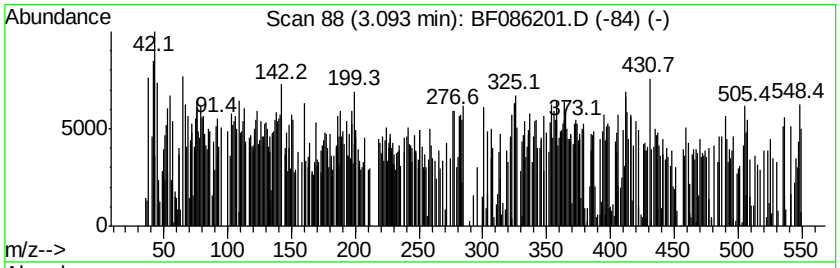
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

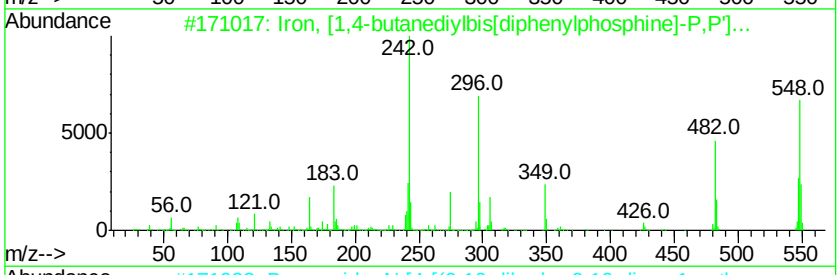
****

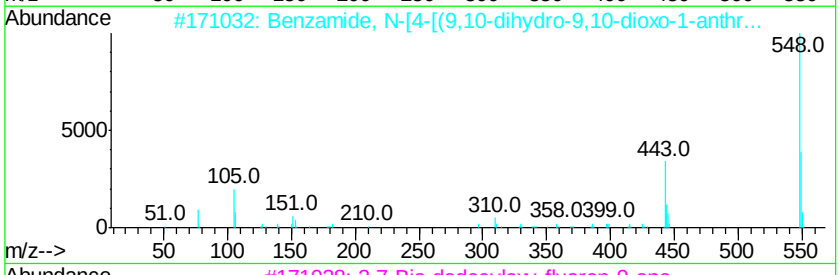
Peak Number 4 unknown3.09 Concentration Rank 12

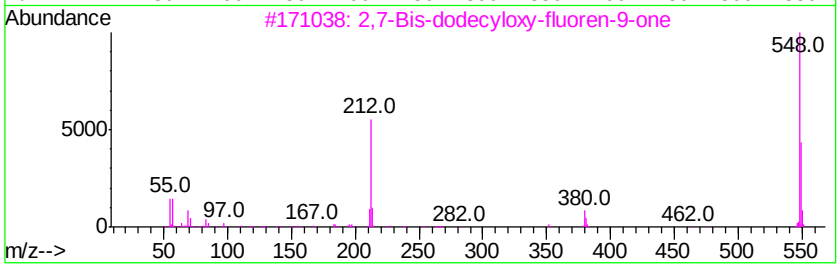
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.09	10.74 ng	395937	1,4-Dichlorobenzene-d4	6.73

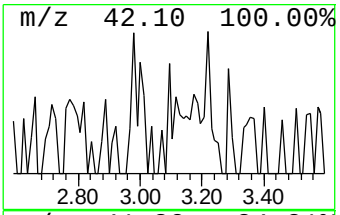
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Iron, [1,4-butanediylbis[diphenv...	548	C33H34FeP2	097959-87-0	25
2	Benzamide, N-[4-[(9,10-dihydro-9...	548	C35H20N2O5	075083-42-0	11
3	2,7-Bis-dodecyloxy-fluoren-9-one	548	C37H56O3	303736-14-3	10
4	1,10-Phenanthroline, 2,9-bis(dip...	548	C36H26N2P2	122768-46-1	7
5	1,2,4,5-Benzenetetracarboxylic 1...	548	C36H24N2O4	031663-80-6	7

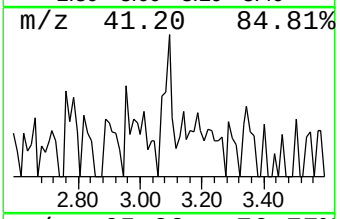


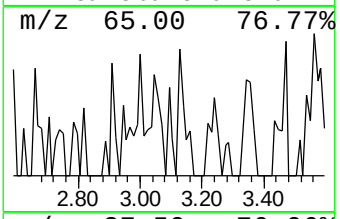


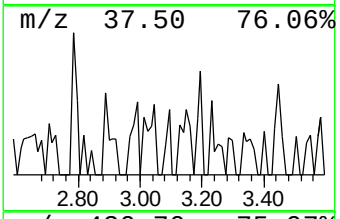


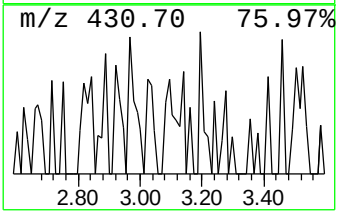












Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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

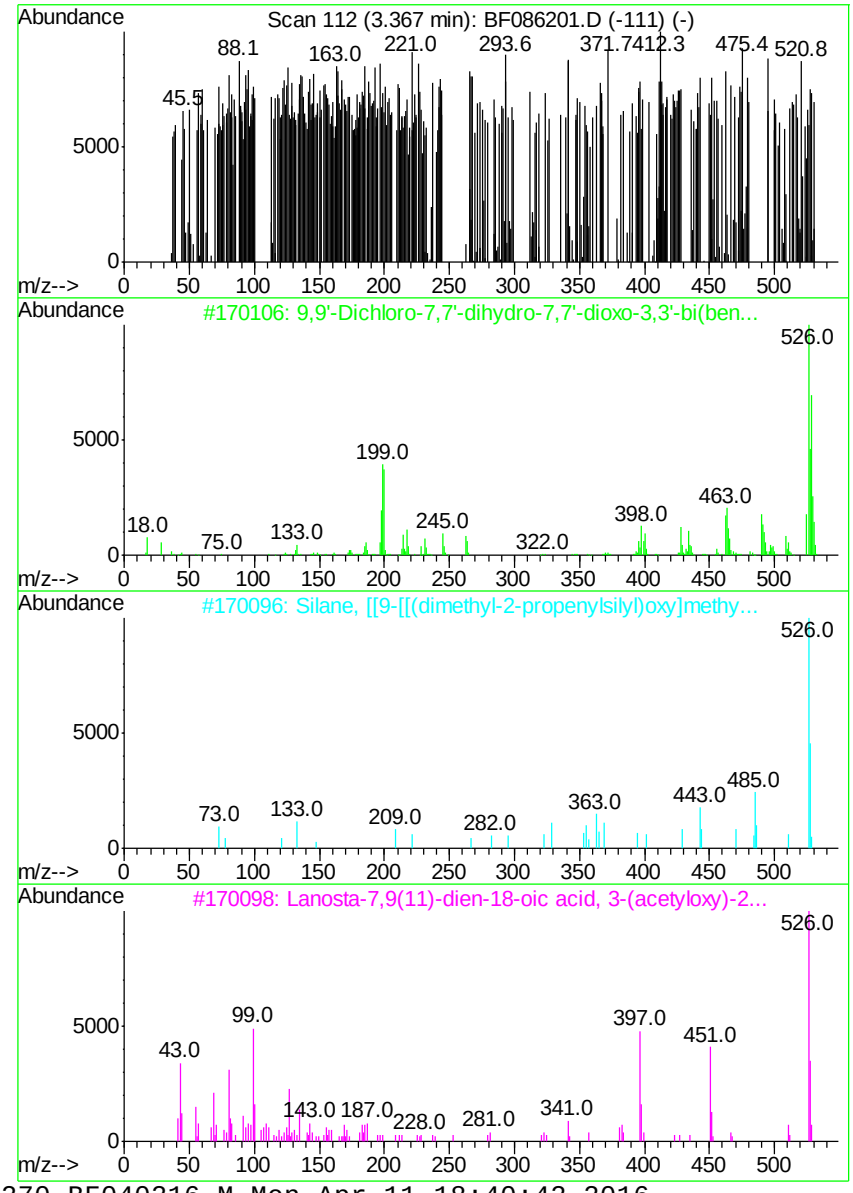
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

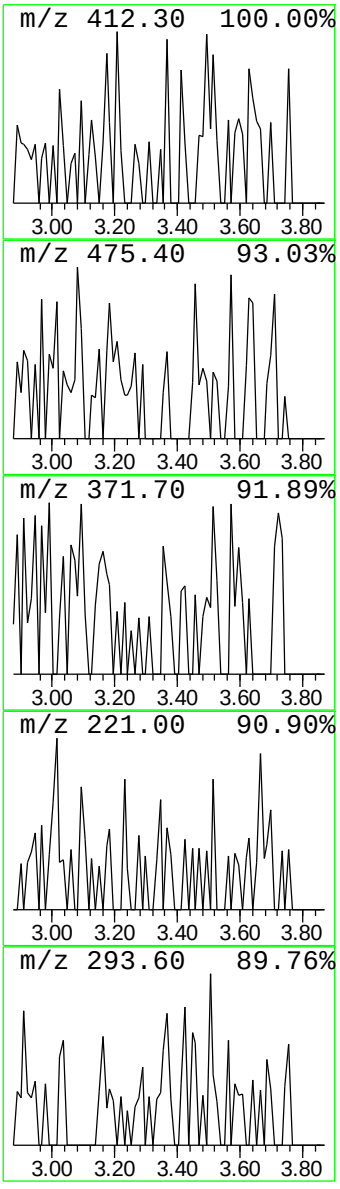
****

Peak Number 8 unknown3.37 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	8.36 ng	308174	1,4-Dichlorobenzene-d4	6.73

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	9,9'-Dichloro-7,7'-dihydro-7,7'-...	526	C34H16Cl2O2	024092-43-1	25
2	Silane, [[9-[[(dimethyl-2-propen...	526	C31H50O3Si2	065598-56-3	9
3	Lanosta-7,9(11)-dien-18-oic acid...	526	C32H46O6	056143-26-1	3





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

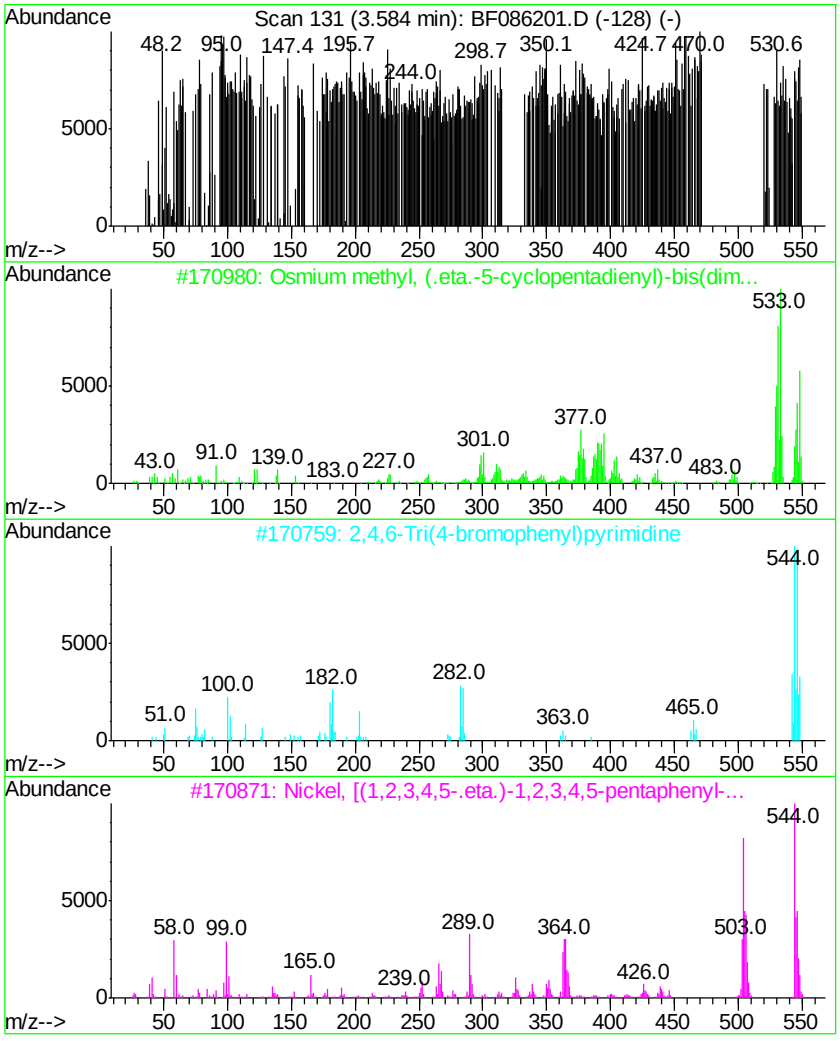
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

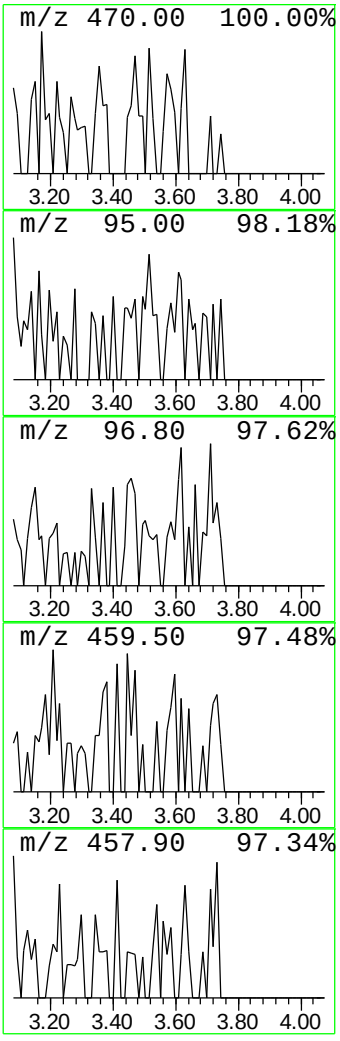
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Osmium methyl, (.eta.-5-cyc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.58	25.27 ng	931918	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Osmium methyl, (.eta.-5-cyclopen...	548	C22H30OsP2	1000158-92-4	55
2	2,4,6-Tri(4-bromophenyl)pyrimidine	542	C22H13Br3N2	1000070-62-6	30
3	Nickel, [(1,2,3,4,5-.eta.)-1,2,3...	544	C38H30Ni	129447-18-3	25
4	2-Butenal, 2-methyl-4-[3a,4,5,7-...	544	C33H36O7	001183-12-6	11
5	trans-Zearalen-.beta.-ol, tri-TMS	536	C27H48O5Si3	1000105-55-4	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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

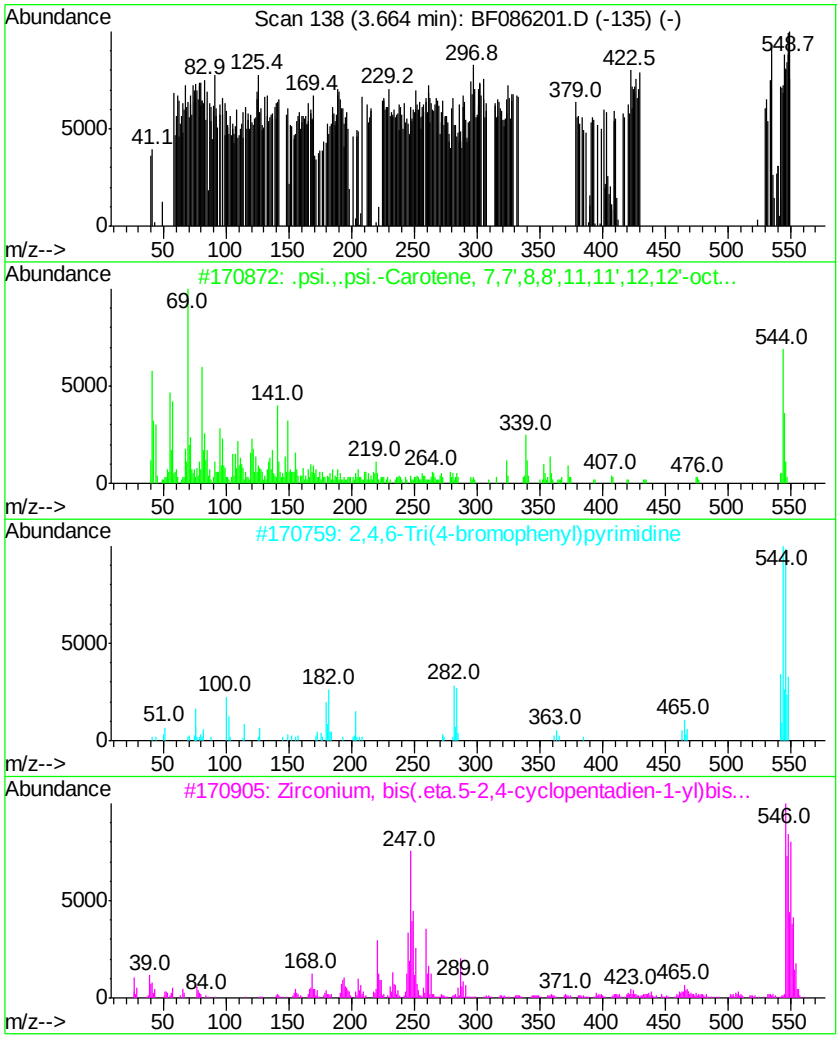
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

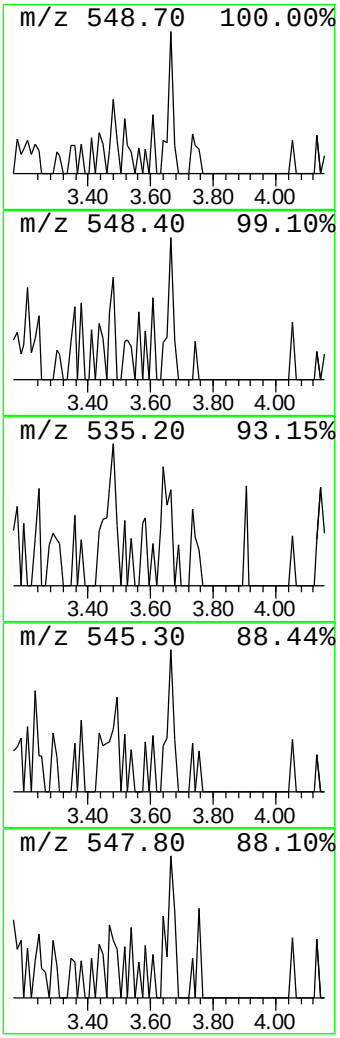
****

Peak Number 13 unknown3.66 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.66	12.41 ng	457490	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.psi.,.psi.-Carotene, 7,7',8,8',...	545	C40H64	000540-04-5	25
2	2,4,6-Tri(4-bromophenyl)pyrimidine	542	C22H13Br3N2	1000070-62-6	22
3	Zirconium, bis(.eta.5-2,4-cyclop...	546	C28H30Zr2	119144-91-1	18
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	10
5	Benzenamine, 4-trifluoromethoxy-...	544	C23H15BrF6N2O2	284495-96-1	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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

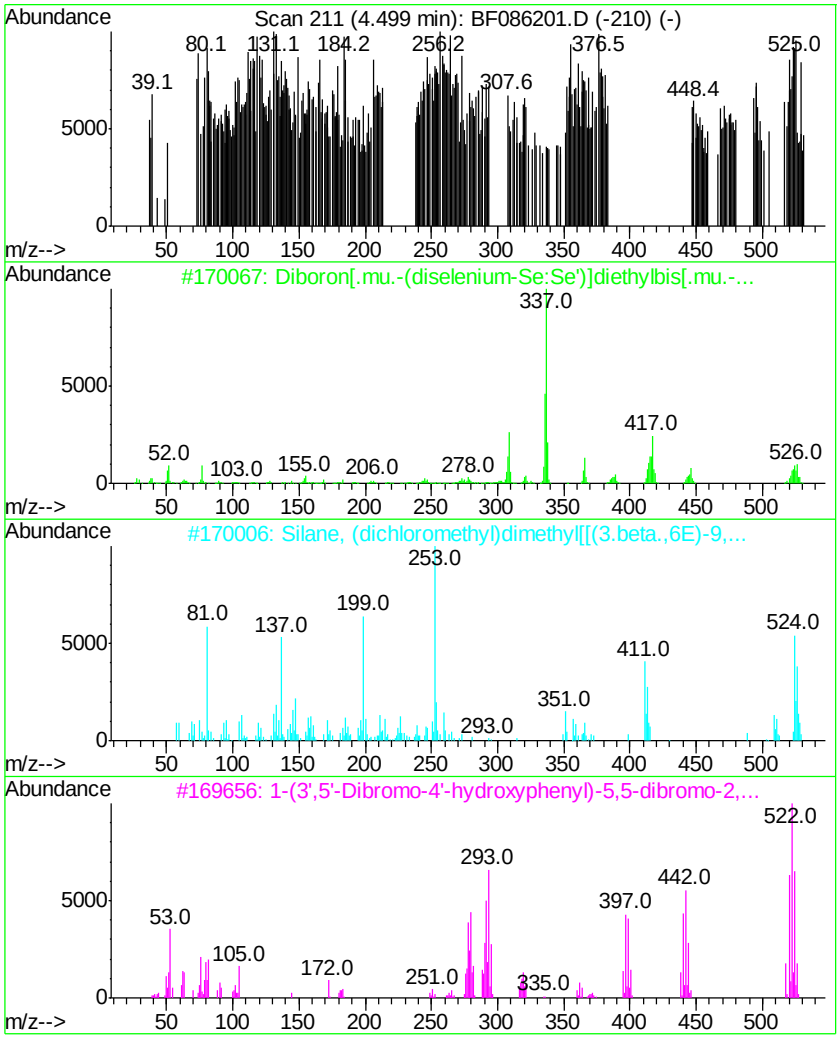
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

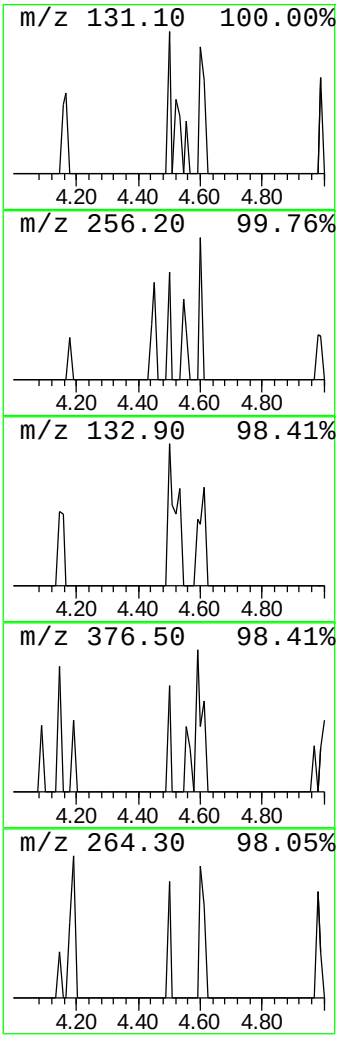
****

Peak Number 16 unknown4.50 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	7.97 ng	293749	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diboron[.mu.-(diselenium-Se:Se')...	526	C22H24B2N4Se2	1000158-10-7	40
2	Silane, (dichloromethyl)dimethyl...	524	C30H50Cl2OSi	069688-11-5	11
3	1-(3',5'-Dibromo-4'-hydroxyphenyl...	518	C10H6Br4N2O3	083809-80-7	10
4	3ALPHA-METHOXY-3BETA-(METHANESUL...	521	C30H51NO4S	1000241-18-6	10
5	Butyric acid, 2-{(2-butyryloxy-e...	521	C26H30F3N3O5	115011-30-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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

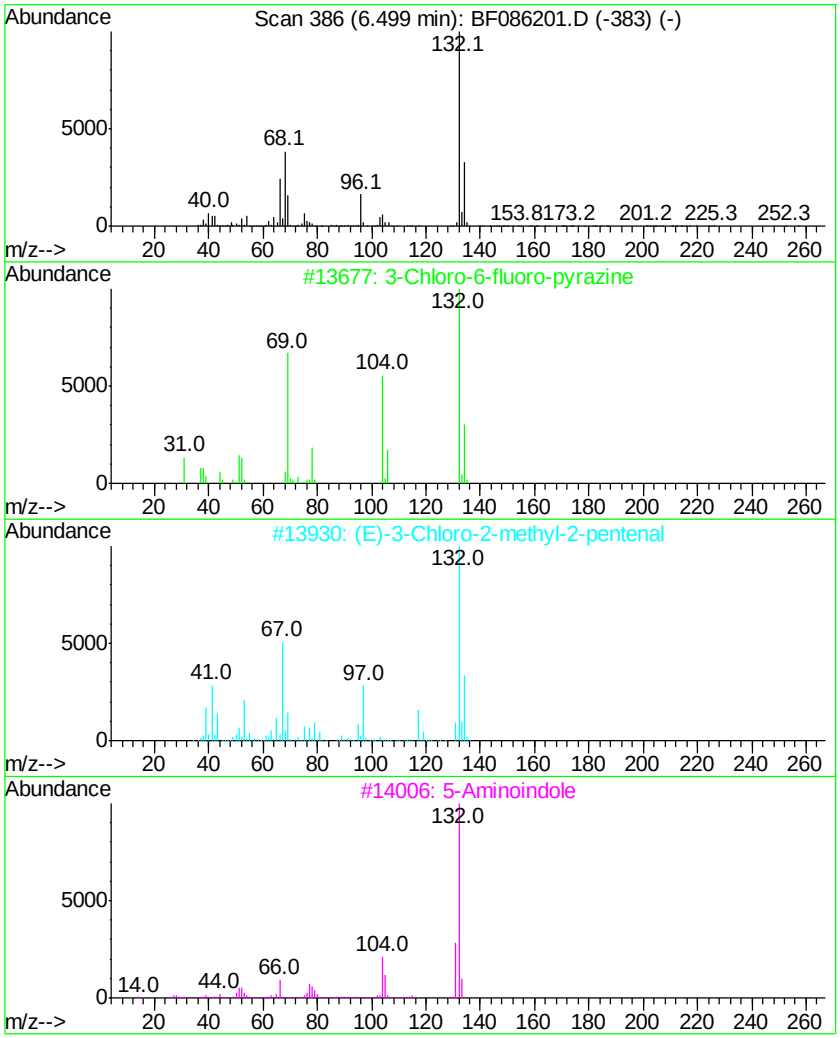
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

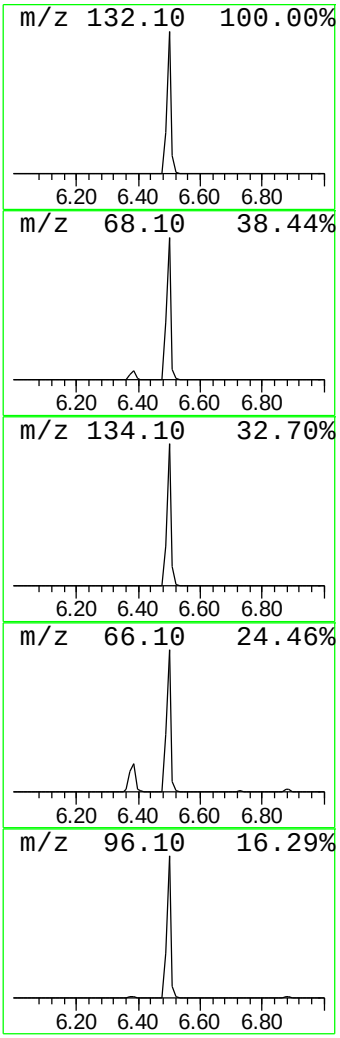
****

Peak Number 19 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	78.63 ng	2899870	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086201.D
Acq On : 9 Apr 2016 6:42
Operator : UM/SJ
Sample : H2373-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AMBOY-SB-02(0.5-20.0)

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
unknown2.99	2.99	12.6	ng	463299	1	6.73	737578	20.0
unknown3.09	3.09	10.7	ng	395937	1	6.73	737578	20.0
unknown3.37	3.37	8.4	ng	308174	1	6.73	737578	20.0
Osmium methyl, (....	3.58	25.3	ng	931918	1	6.73	737578	20.0
unknown3.66	3.66	12.4	ng	457490	1	6.73	737578	20.0
unknown4.50	4.50	8.0	ng	293749	1	6.73	737578	20.0
unknown6.50	6.50	78.6	ng	2899870	1	6.73	737578	20.0