LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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-BF011415.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	1.384	23	26	31	rBV	5392	14169	1.43%	0.136%
2	1.453	31	32	42	rVV	35274	77021	7.79%	0.740%
3	4.104	261	264	280	rVB	119180	266295	26.93%	2.558%
4	5.042	342	346	361	rVB	456360	858391	86.80%	8.245%
5	7.373	547	550	555	rBV	468835	856350	86.59%	8.226%
6	7.465	555	558	565	rVB	528581	944934	95.55%	9.077%
7	7.979	600	603	607	rBV	140431	235918	23.86%	2.266%
8	8.299	627	631	634	rBV	427797	676352	68.39%	6.497%
9	9.271	712	716	719	rBV	373111	545102	55.12%	5.236%
10	10.882	853	857	860	rBV	214056	323958	32.76%	3.112%
11	12.357	983	986	989	rBV	26206	45232	4.57%	0.434%
12	13.534	1085	1089	1092	rBV	659021	988939	100.00%	9.499%
13	14.597	1179	1182	1185	rBV	62363	87551	8.85%	0.841%
14	15.008	1215	1218	1222	rVB	210377	353281	35.72%	3.393%
15	16.243	1323	1326	1330	rVB	19851	27570	2.79%	0.265%
16	16.631	1357	1360	1362	rBV	144836	185341	18.74%	1.780%
17	16.688	1362	1365	1368	rBV	403513	630803	63.79%	6.059%
18	17.774	1458	1460	1462	rBV	269249	353606	35.76%	3.397%
19	17.809	1462	1463	1466	rVV	28261	40841	4.13%	0.392%
20	17.889	1469	1470	1473	rVB	10003	11081	1.12%	0.106%
21	18.769	1544	1547	1551	rBV	40762	61042	6.17%	0.586%
22	18.963	1561	1564	1569	rBV4	7064	17467	1.77%	0.168%
23	19.454	1605	1607	1609	rBV	74690	80091	8.10%	0.769%
24	19.740	1629	1632	1634	rBV	78455	82616	8.35%	0.794%
25	19.786	1634	1636	1639	rVV3	10530	18328	1.85%	0.176%
26	19.900	1641	1646	1650	rBV2	39537	54828	5.54%	0.527%
27	20.003	1653	1655	1658	rVB	750102	905424	91.56%	8.697%
28	20.186	1669	1671	1677	rVB5	6253	12946	1.31%	0.124%
29	20.426	1689	1692	1693	rVB2	10507	15883	1.61%	0.153%
30	20.792	1722	1724	1726	rBV	33171	40573	4.10%	0.390%
31	20.963	1734	1739	1740	rBV4	9005	20406	2.06%	0.196%
32	21.009	1740	1743	1745	rVB3	8549	13198	1.33%	0.127%
33	21.169	1755	1757	1759	rBV3	6830	12738	1.29%	0.122%
34	21.272	1761	1766	1768	rBV	327945	516318	52.21%	4.959%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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-BF011415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.397	1775	1777	1779	rBV2	9315	14741	1.49%	0.142%
36	21.477	1781	1784	1786	rVB4	9900	20125	2.04%	0.193%
37	21.546	1786	1790	1791	rBV4	8319	23984	2.43%	0.230%
38	21.580	1791	1793	1796	rBV4	6345	11253	1.14%	0.108%
39	21.660	1797	1800	1801	rBV2	12620	16830	1.70%	0.162%
40	22.049	1831	1834	1835	rVB2	15546	23065	2.33%	0.222%
41	22.483	1869	1872	1873	rBV2	16727	29686	3.00%	0.285%
42	22.518	1873	1875	1882	rVB	51372	103502	10.47%	0.994%
43	22.815	1899	1901	1903	rVB	28767	35450	3.58%	0.341%
44	22.872	1904	1906	1908	rVB	36332	37277	3.77%	0.358%
45	22.929	1908	1911	1914	rBV	267750	359549	36.36%	3.454%
46	23.546	1960	1965	1967	rBV5	34400	103261	10.44%	0.992%
47	24.049	2007	2009	2012	rBV	23204	29634	3.00%	0.285%
48	24.346	2032	2035	2037	rVB	28868	41387	4.18%	0.398%
49	24.506	2046	2049	2053	rVB5	19994	43799	4.43%	0.421%
50	24.724	2063	2068	2072	rBV3	33972	125871	12.73%	1.209%
51	25.569	2140	2142	2144	rBV3	9447	16760	1.69%	0.161%

Sum of corrected areas: 10410767

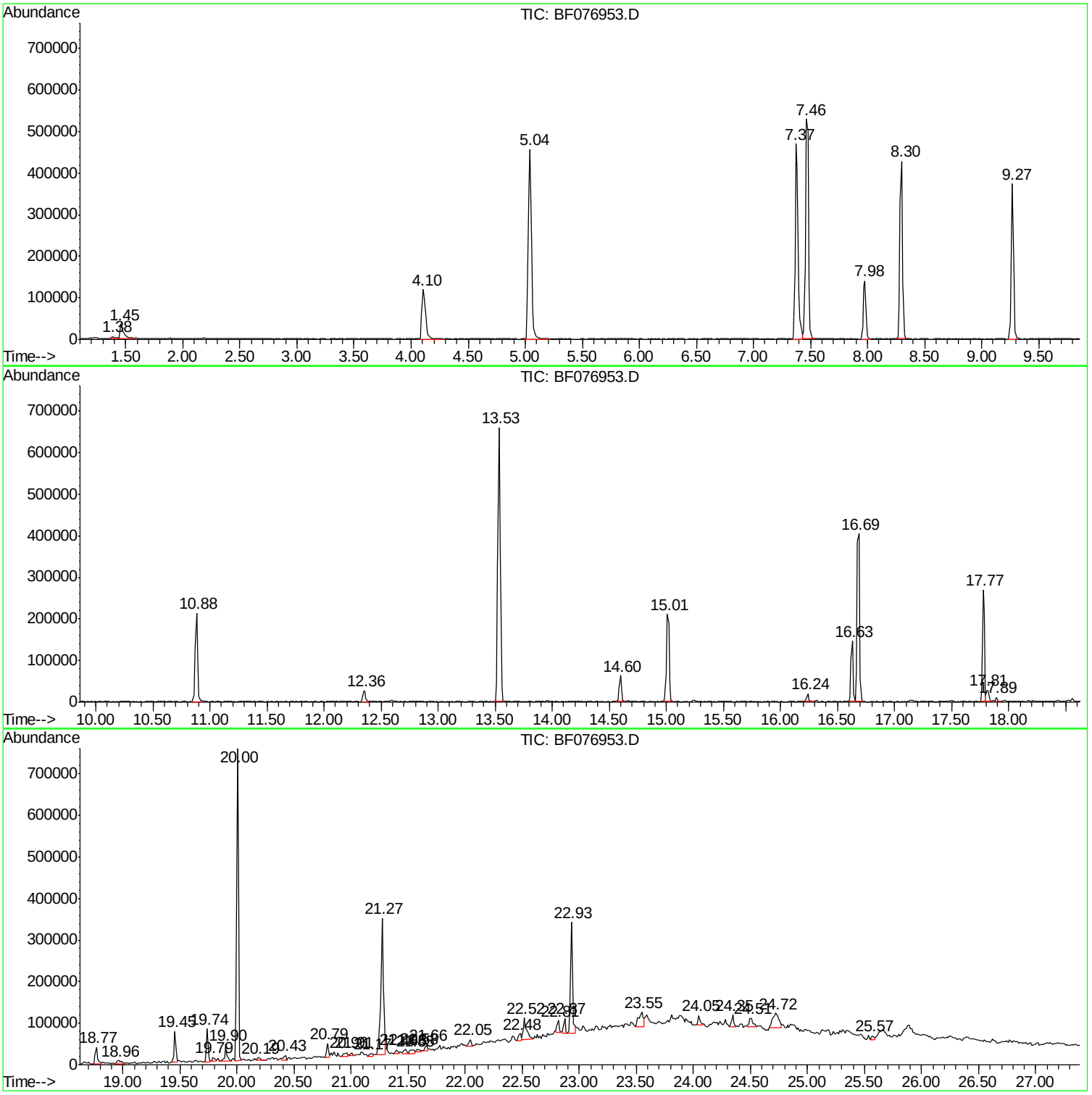
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

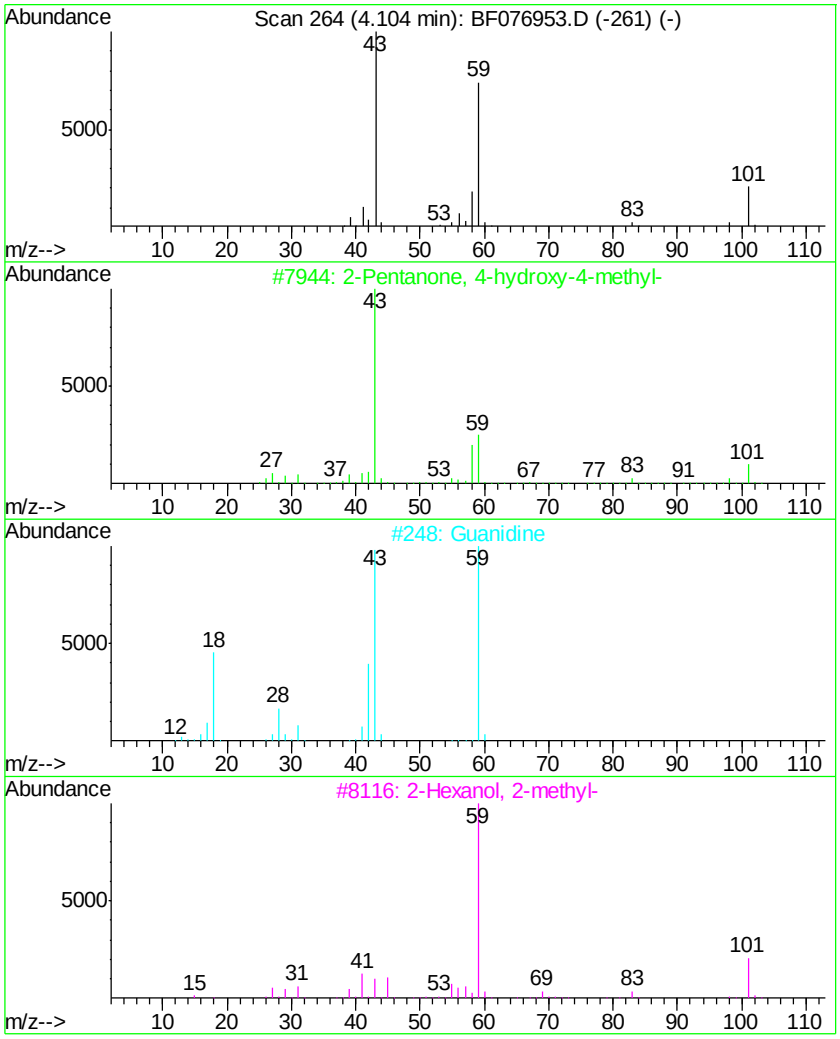
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

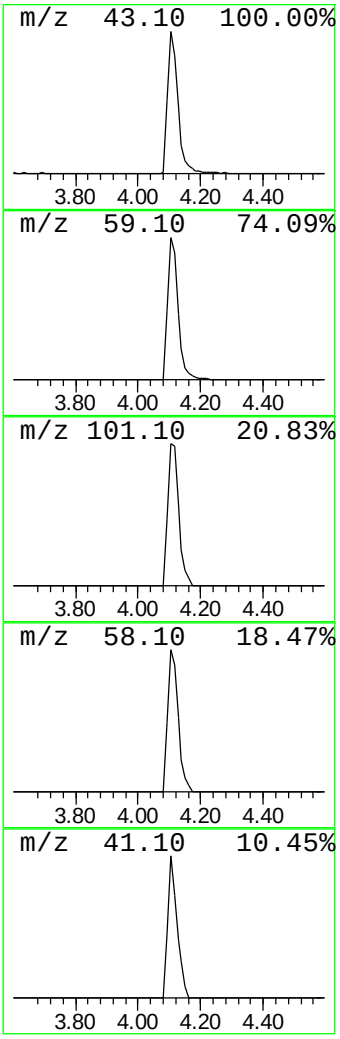
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	22.58 ng	266295	1,4-Dichlorobenzene-d4	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	50
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4	3-Octanol	130	C8H18O	000589-98-0	38
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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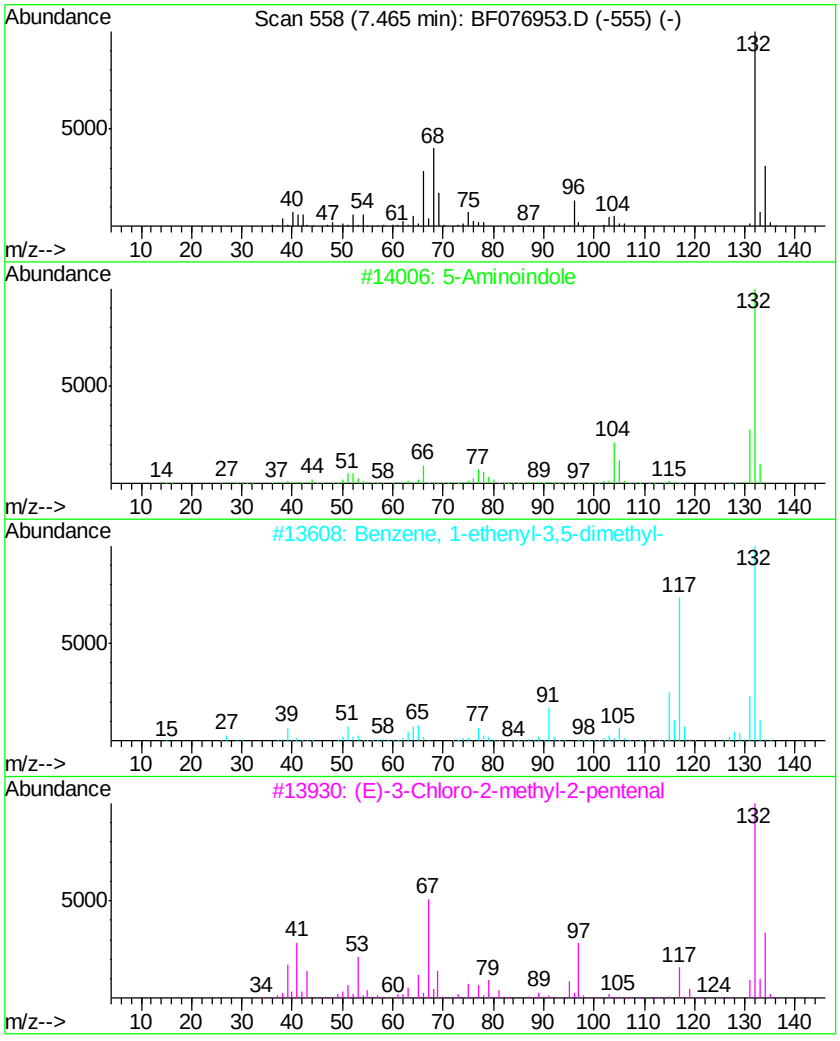
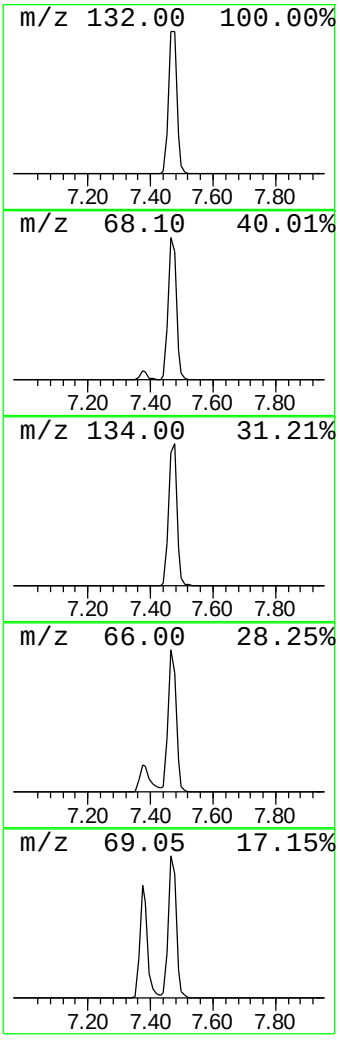
Peak Number 3 unknown7.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	80.11 ng	944934	1,4-Dichlorobenzene-d4	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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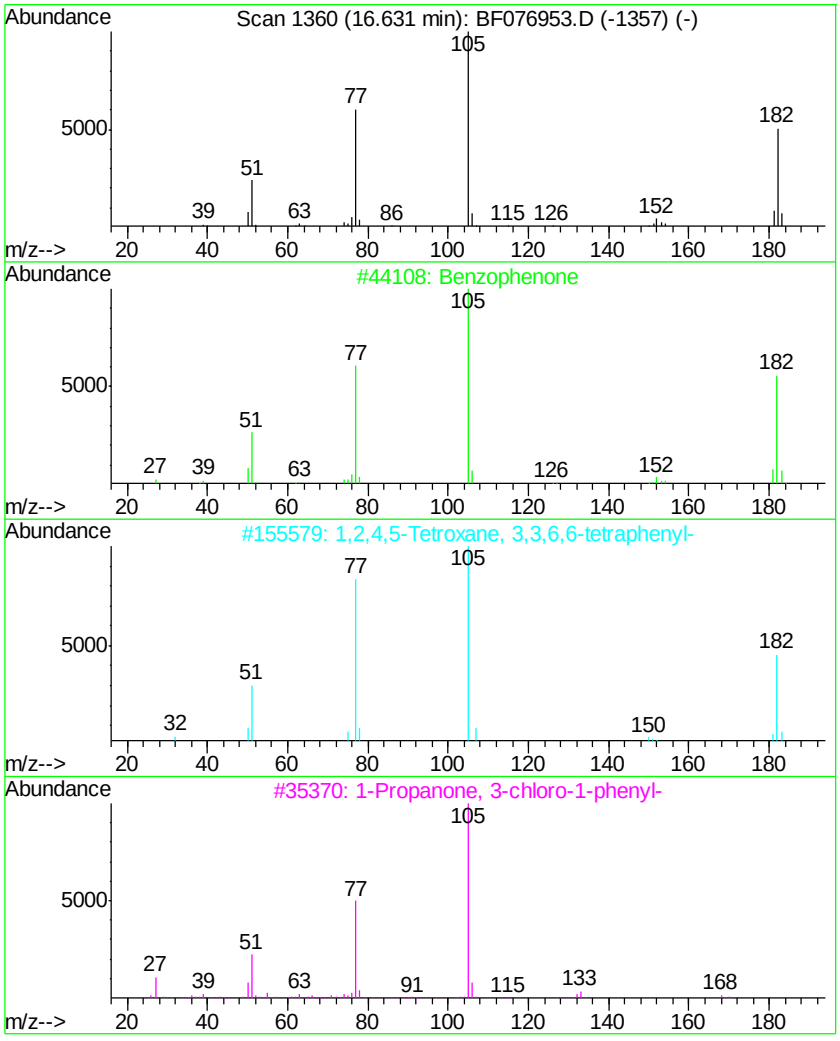
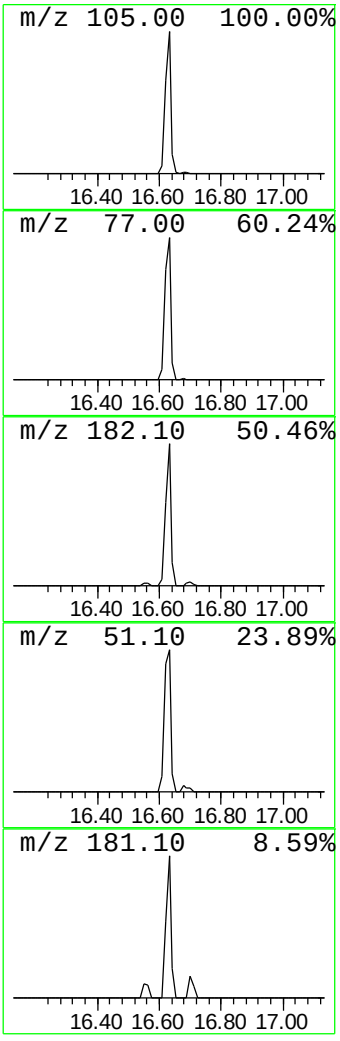
Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	10.48 ng	185341	Phenanthrene-d10	17.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	Phenacylidene diacetate	236	C12H12O5	005062-30-6	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

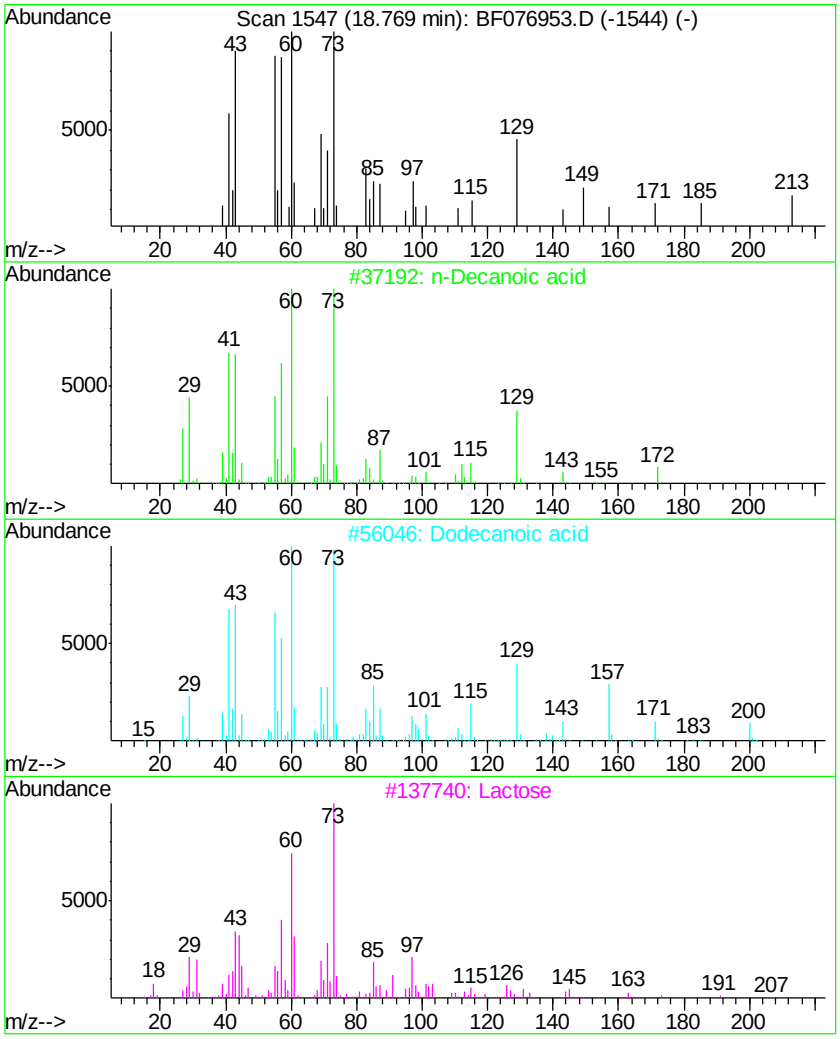
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

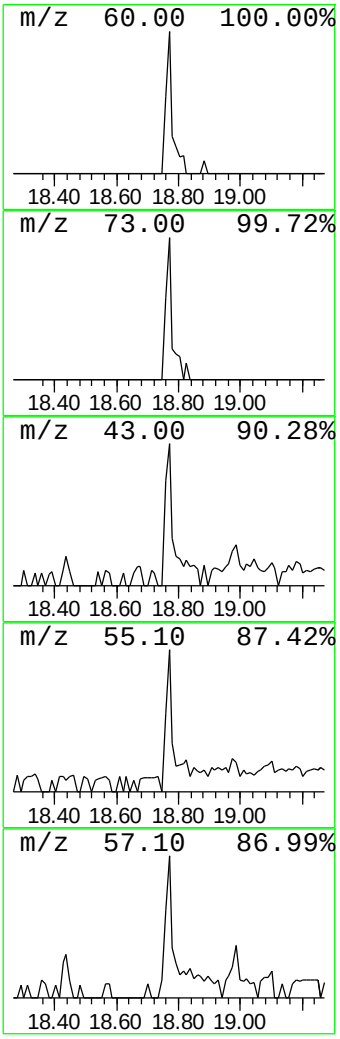
****

Peak Number 7 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	3.45 ng	61042	Phenanthrene-d10	17.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	59
2	Dodecanoic acid	200	C12H24O2	000143-07-7	53
3	Lactose	342	C12H22O11	000063-42-3	47
4	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	10





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Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
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Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

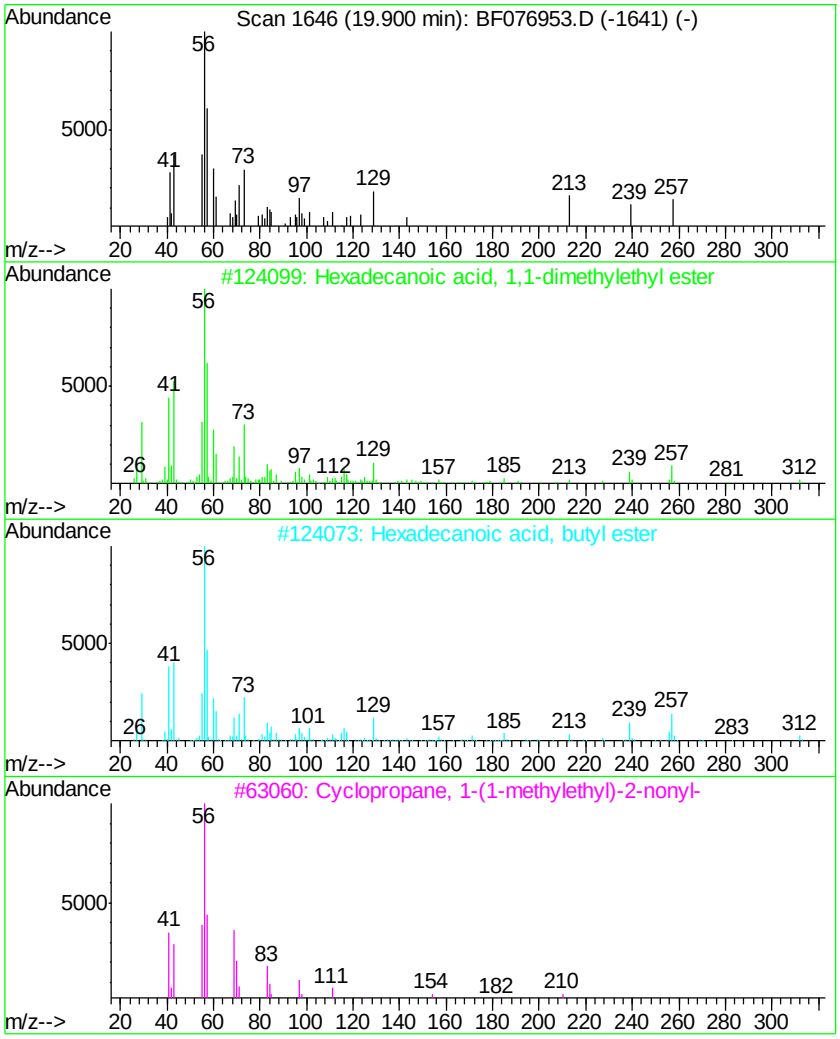
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

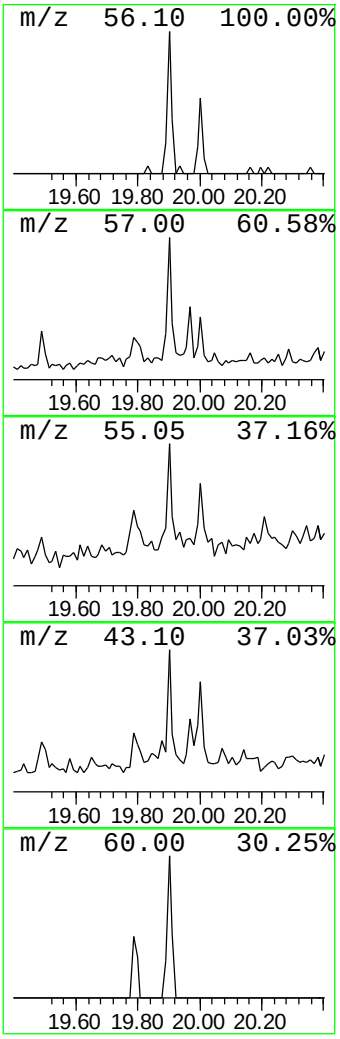
****

Peak Number 8 Hexadecanoic acid, 1,1-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	2.12 ng	54828	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	80
3	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	32





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Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

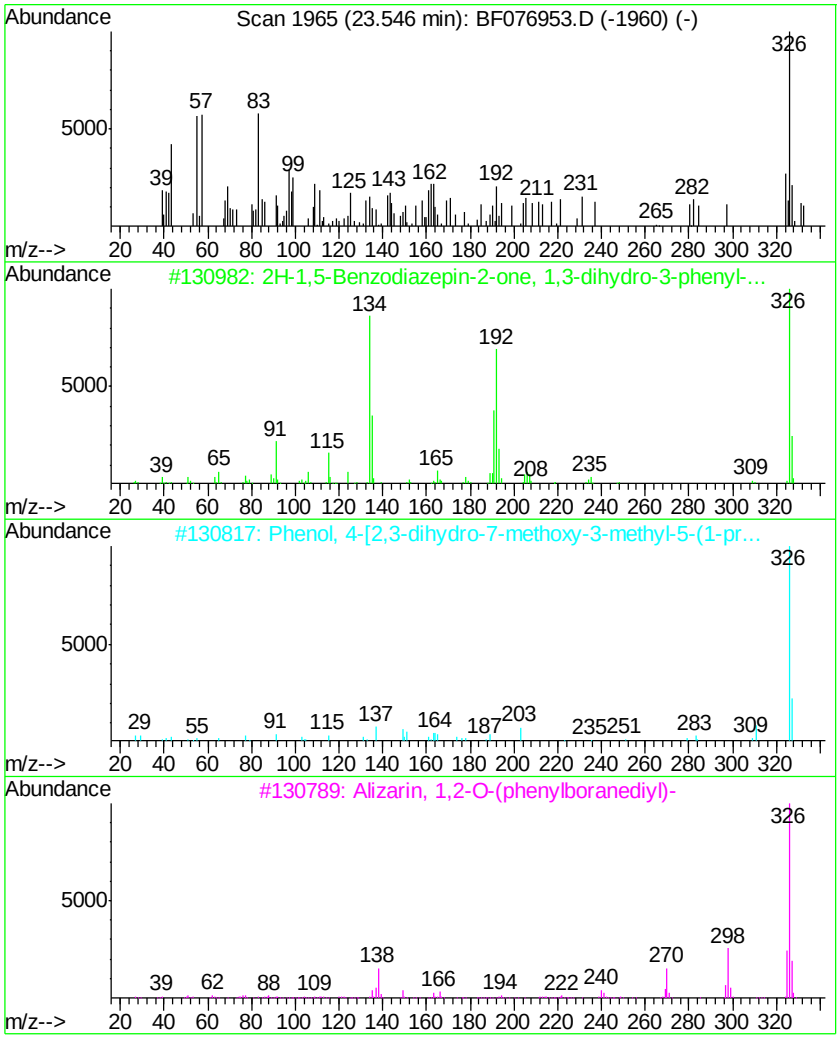
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

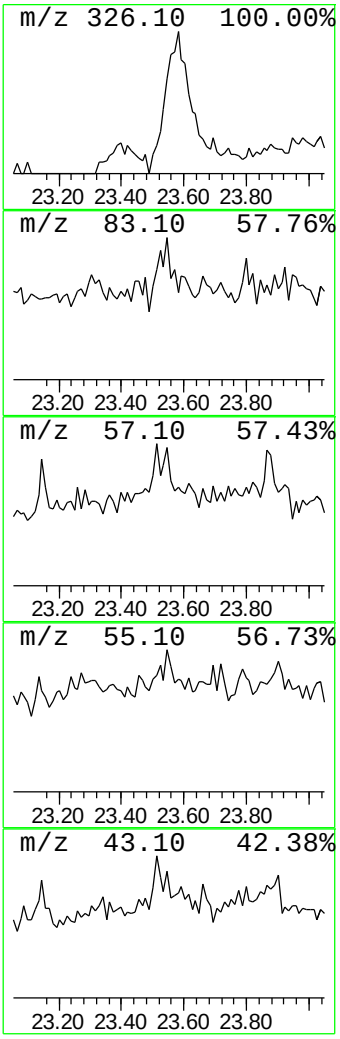
****

Peak Number 10 unknown23.55 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.55	5.74 ng	103261	Perylene-d12	22.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,5-Benzodiazepin-2-one, 1,3-...	326	C22H18N2O	056771-67-6	47
2	Phenol, 4-[2,3-dihydro-7-methoxy...	326	C20H22O4	002680-81-1	43
3	Alizarin, 1,2-O-(phenylboranediyl)-	326	C20H11BO4	1000161-74-3	43
4	Triphenylphosphonium cyclopentad...	326	C23H19P	029473-30-1	43
5	3-(4-Amino-6-piperidin-1-yl-[1,3...	326	C16H18N6O2	1000275-96-8	40





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Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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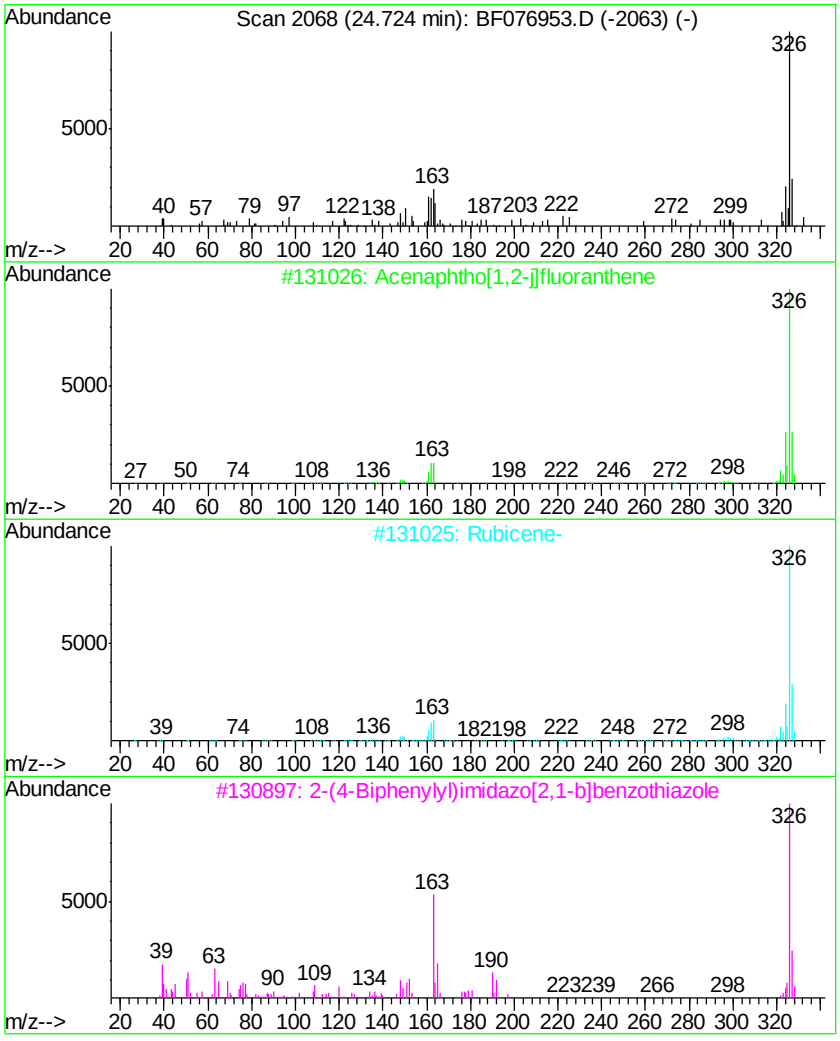
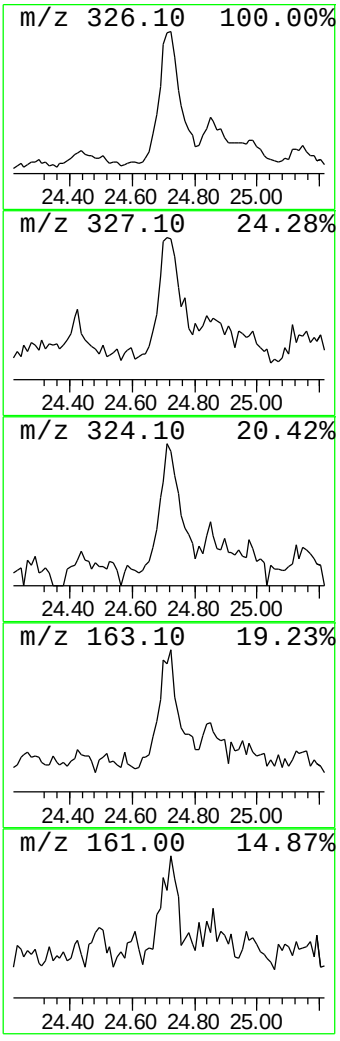
Peak Number 12 Acenaphtho[1,2-j]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.72	7.00 ng	125871	Perylene-d12	22.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphtho[1,2-j]fluoranthene	326	C26H14	000193-21-5	62
2	Rubicene-	326	C26H14	000197-61-5	62
3	2-(4-Biphenylyl)imidazo[2,1-b]be...	326	C21H14N2S	038956-29-5	59
4	Bis(pentamethylcyclopentadienyl)...	326	C20H30Fe	012126-50-0	58
5	Benzene, 1,3-bis(4-phenyl-1,3-bu...	326	C26H14	037902-13-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076953.D
Acq On : 20 Jan 2015 6:53
Operator : IZ / TP
Sample : G1076-03
Misc : W
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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...	4.10	22.6	ng	266295	1	7.98	235918	20.0
unknown7.46	7.46	80.1	ng	944934	1	7.98	235918	20.0
Benzophenone	16.63	10.5	ng	185341	4	17.77	353606	20.0
n-Decanoic acid	18.77	3.5	ng	61042	4	17.77	353606	20.0
Hexadecanoic acid...	19.90	2.1	ng	54828	5	21.27	516318	20.0
unknown23.55	23.55	5.7	ng	103261	6	22.93	359549	20.0
Acenaphtho[1,2-j]...	24.72	7.0	ng	125871	6	22.93	359549	20.0