LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
Data File : BF107488.D
Acq On : 18 Jul 2018 20:00
Operator : JU/SJ
Sample : J4035-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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	5.225	487	491	499	rVB	315521	372871	11.03%	1.205%
2	5.613	552	557	560	rBV	3056067	2839078	83.96%	9.174%
3	6.613	721	727	730	rBV	2868192	3056256	90.39%	9.876%
4	6.754	746	751	754	rBV	3273759	3089008	91.35%	9.982%
5	6.801	754	759	766	rVB	44161	46499	1.38%	0.150%
6	6.984	786	790	793	rBV	1301358	1055373	31.21%	3.410%
7	7.142	812	817	820	rBV	2626829	2363125	69.89%	7.636%
8	7.548	880	886	889	rBV	2027708	1949884	57.67%	6.301%
9	8.266	1004	1008	1012	rBV	1459906	1238648	36.63%	4.003%
10	9.342	1185	1191	1194	rBV	3796464	3381355	100.00%	10.927%
11	9.730	1252	1257	1261	rBV	665383	547787	16.20%	1.770%
12	10.030	1303	1308	1312	rBV	1449998	1331233	39.37%	4.302%
13	10.819	1438	1442	1445	rBV	1921786	1715773	50.74%	5.545%
14	10.919	1455	1459	1465	rBV3	63710	84261	2.49%	0.272%
15	11.019	1473	1476	1480	rBV4	45894	55037	1.63%	0.178%
16	11.054	1480	1482	1485	rBV3	47598	43425	1.28%	0.140%
17	11.160	1498	1500	1505	rVB4	37084	48643	1.44%	0.157%
18	11.207	1505	1508	1510	rBV	38356	37596	1.11%	0.121%
19	11.519	1557	1561	1564	rBV	1273575	1213514	35.89%	3.921%
20	11.542	1564	1565	1569	rVV	161079	107103	3.17%	0.346%
21	11.595	1569	1574	1577	rVV3	32206	38221	1.13%	0.124%
22	12.018	1642	1646	1649	rBV4	36460	51853	1.53%	0.168%
23	12.130	1662	1665	1668	rBV4	38908	46104	1.36%	0.149%
24	12.571	1734	1740	1742	rBV5	34648	56981	1.69%	0.184%
25	12.736	1764	1768	1770	rBV	197670	163826	4.84%	0.529%
26	12.965	1800	1807	1809	rBV	203624	219874	6.50%	0.711%
27	13.107	1826	1831	1834	rBV	2721710	2455828	72.63%	7.936%
28	13.177	1841	1843	1849	rBV7	31577	51647	1.53%	0.167%
29	13.295	1860	1863	1865	rVB3	46492	43065	1.27%	0.139%
30	13.318	1865	1867	1870	rVB4	53740	42748	1.26%	0.138%
31	13.360	1870	1874	1876	rVB5	31468	37793	1.12%	0.122%
32	13.660	1922	1925	1928	rBV3	76702	82423	2.44%	0.266%
33	13.918	1964	1969	1972	rBV4	31579	54966	1.63%	0.178%
34	13.989	1975	1981	1984	rBV4	183291	220612	6.52%	0.713%

LSC Area Percent Report

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Sample : J4035-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.089	1995	1998	2001	rBV5	27192	45029	1.33%	0.146%
36	14.171	2007	2012	2014	rBV	1025587	1107266	32.75%	3.578%
37	14.195	2014	2016	2020	rVB3	91406	82607	2.44%	0.267%
38	14.307	2033	2035	2039	rBV5	93780	90902	2.69%	0.294%
39	14.618	2085	2088	2092	rVB4	127834	143453	4.24%	0.464%
40	14.942	2141	2143	2147	rVB4	75914	53487	1.58%	0.173%
41	15.054	2160	2162	2165	rBV4	33908	39195	1.16%	0.127%
42	15.248	2192	2195	2198	rBV4	61089	96495	2.85%	0.312%
43	15.301	2202	2204	2210	rVB7	94718	105505	3.12%	0.341%
44	15.636	2256	2261	2265	rBV5	59680	106602	3.15%	0.344%
45	15.712	2268	2274	2281	rVV	671725	932520	27.58%	3.013%

Sum of corrected areas: 30945471

LSC Report - Integrated Chromatogram

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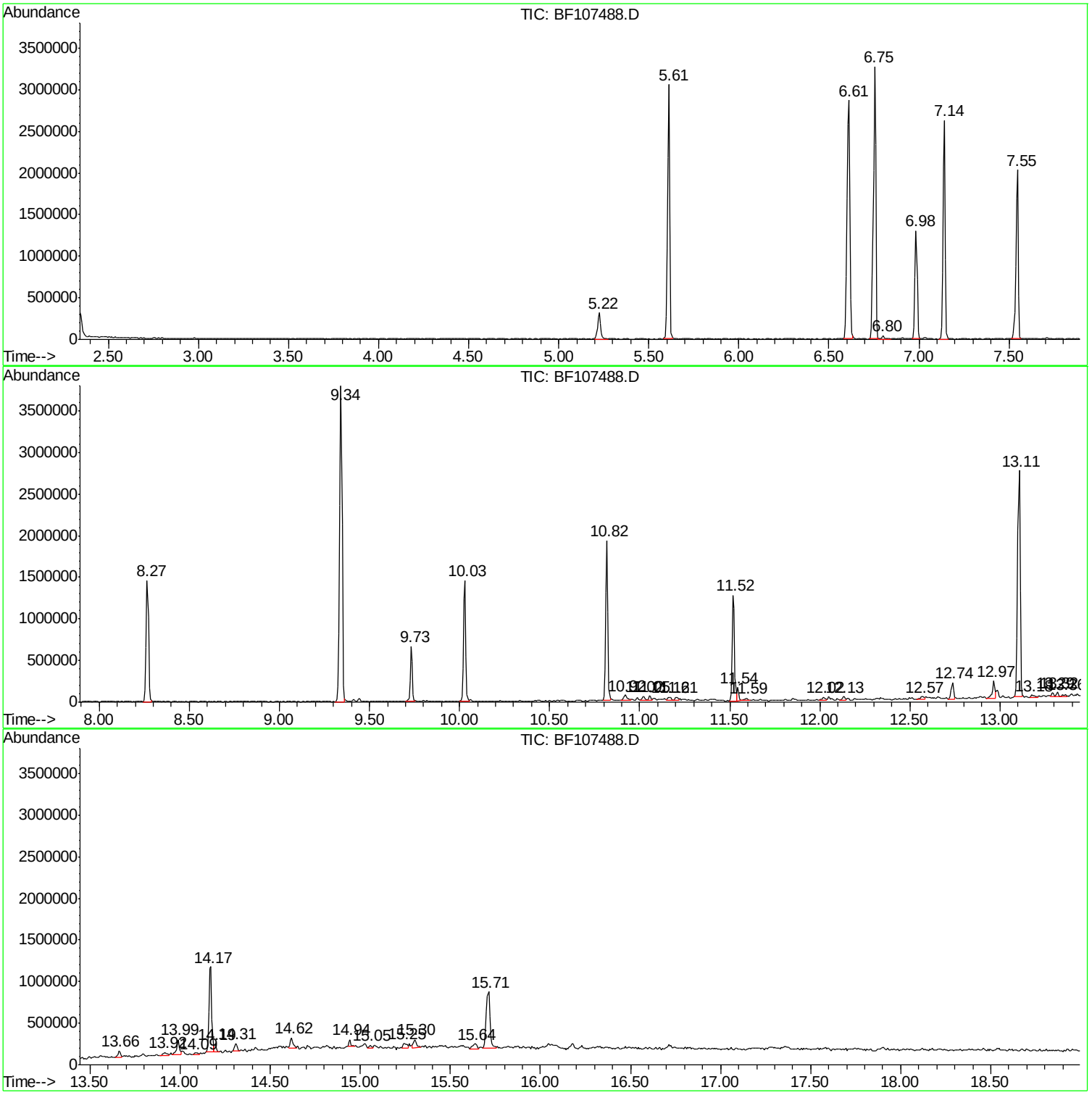
Operator : JU/SJ
Sample : J4035-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
Data File : BF107488.D
Acq On : 18 Jul 2018 20:00
Operator : JU/SJ
Sample : J4035-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

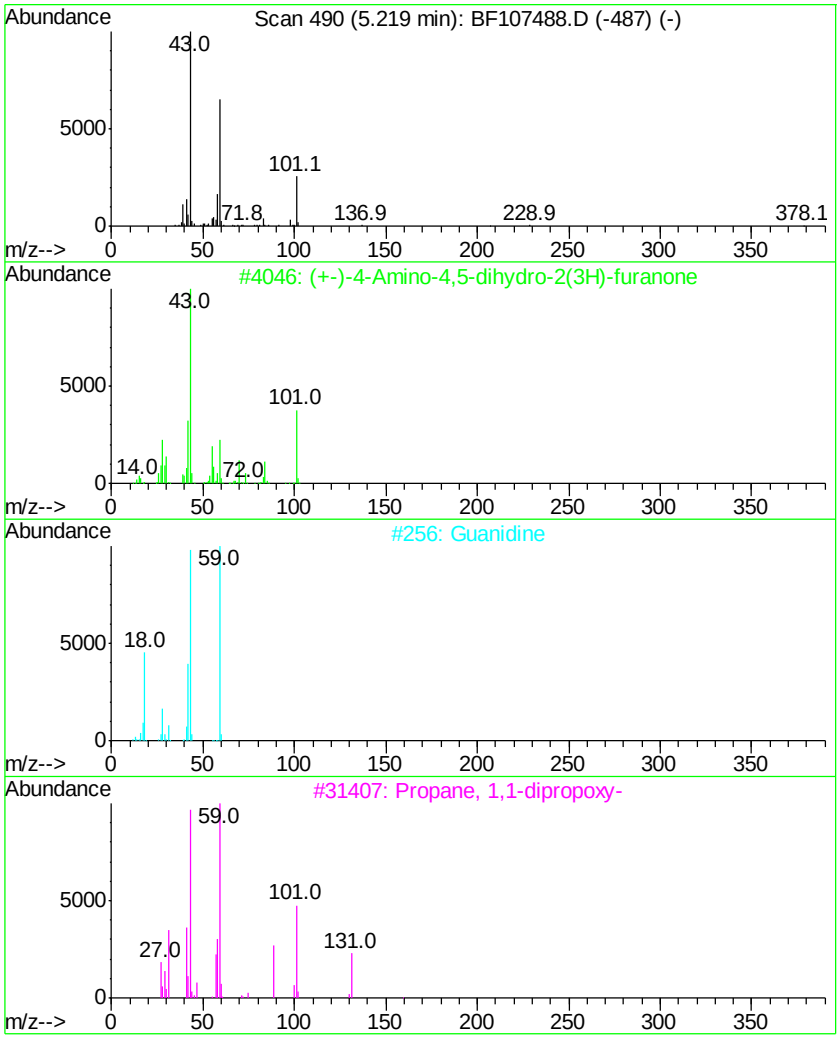
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

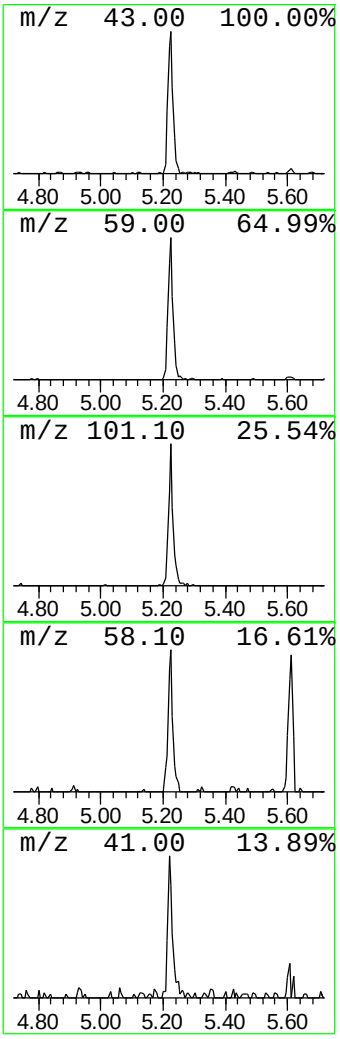
****

Peak Number 1 (+-)-4-Amino-4,5-dihydro-2(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	7.07 ng	372871	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	32
5	Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	28





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Data File : BF107488.D
Acq On : 18 Jul 2018 20:00
Operator : JU/SJ
Sample : J4035-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

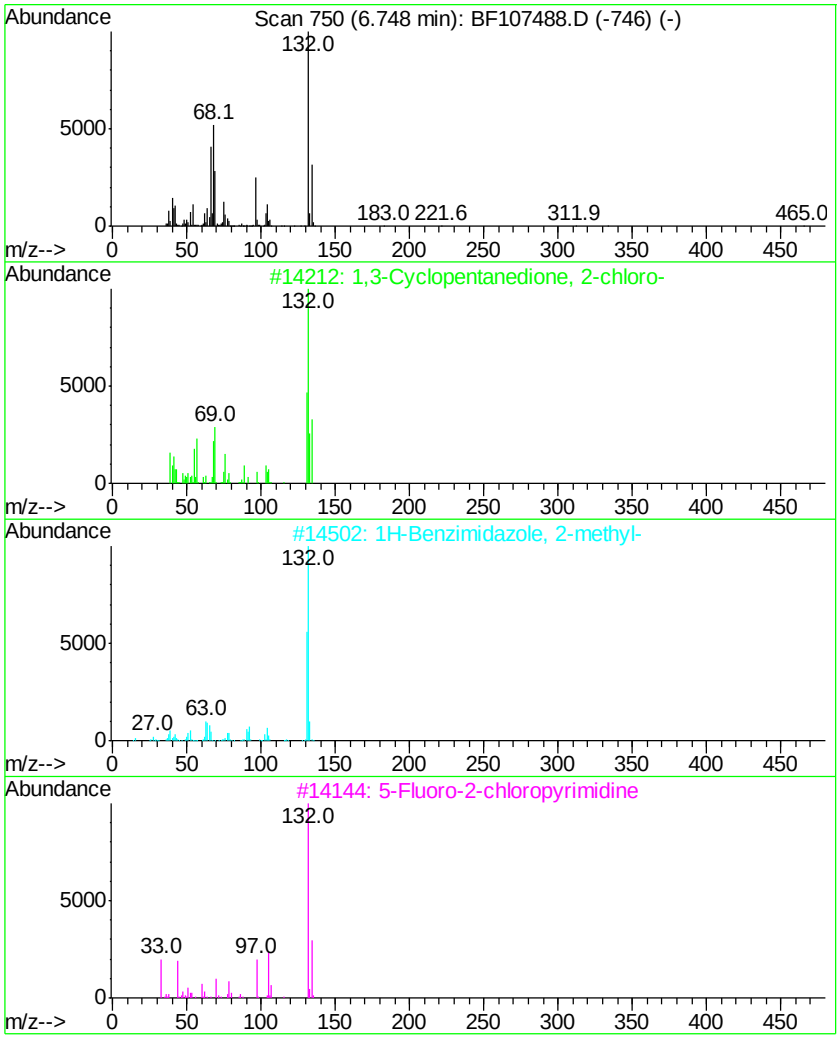
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

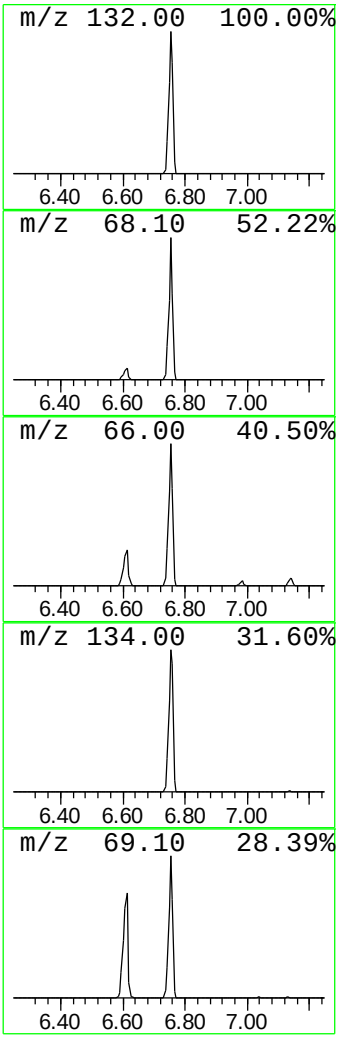
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	58.54 ng	3089010	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
Data File : BF107488.D
Acq On : 18 Jul 2018 20:00
Operator : JU/SJ
Sample : J4035-07
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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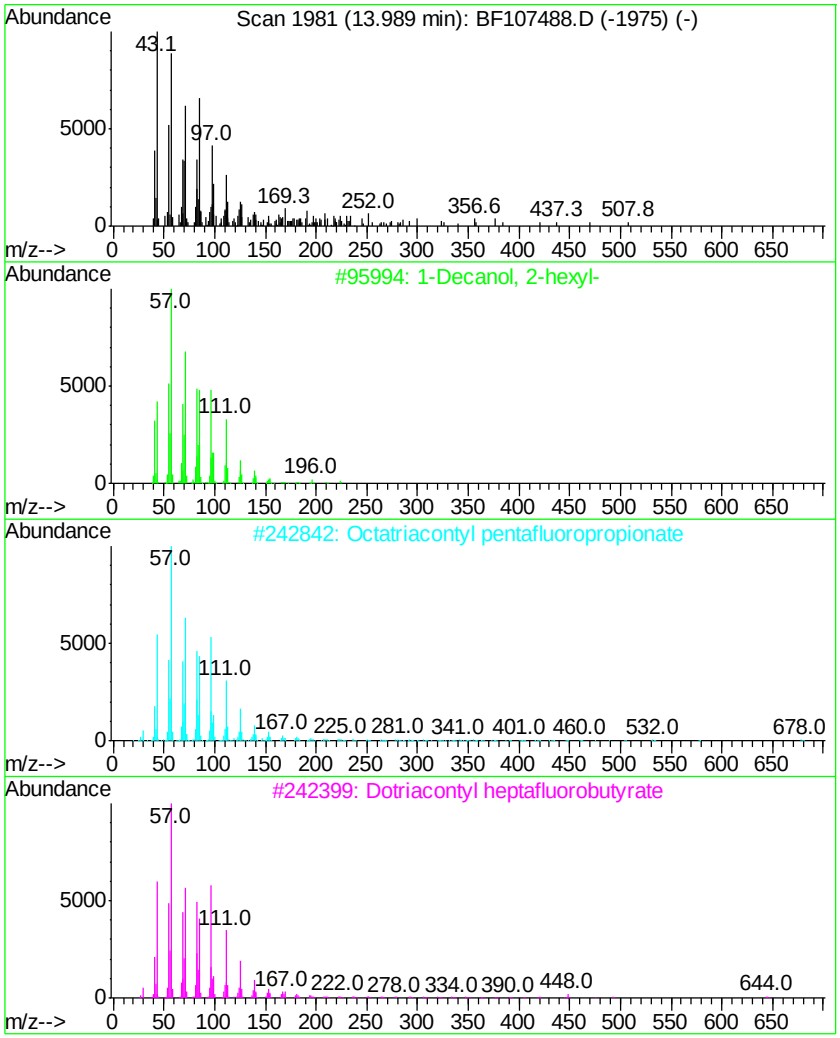
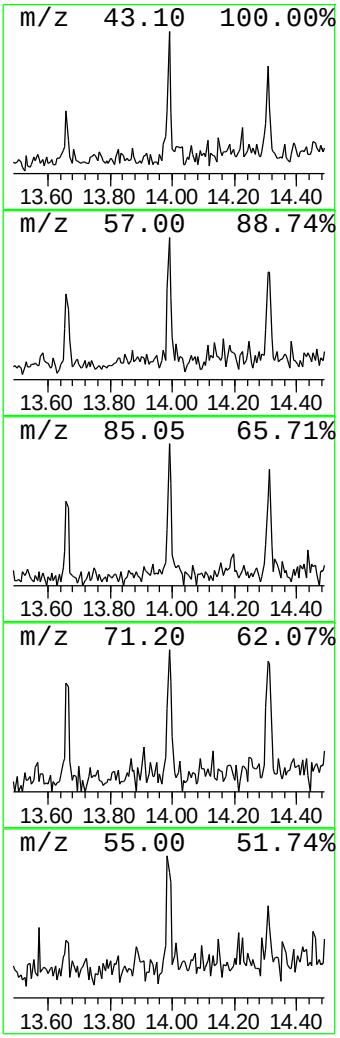
Peak Number 4 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	3.98 ng	220612	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	58
3	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	49
4	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	49
5	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071818\
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Sample : J4035-07
Misc :
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Instrument : BNA_F
ClientSampleId : MH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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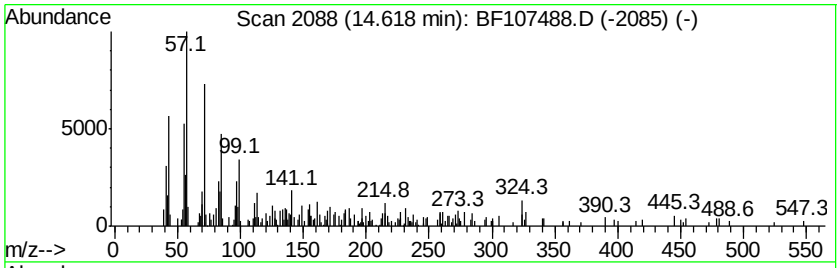
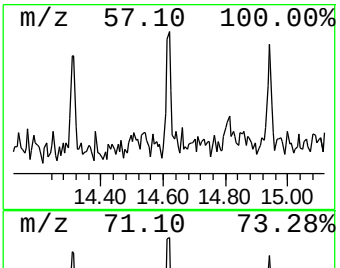
Peak Number 5 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.59 ng	143453	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	81
2	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	76
3	Pentadecane	212	C15H32	000629-62-9	76
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	76
5	Tridecane	184	C13H28	000629-50-5	68





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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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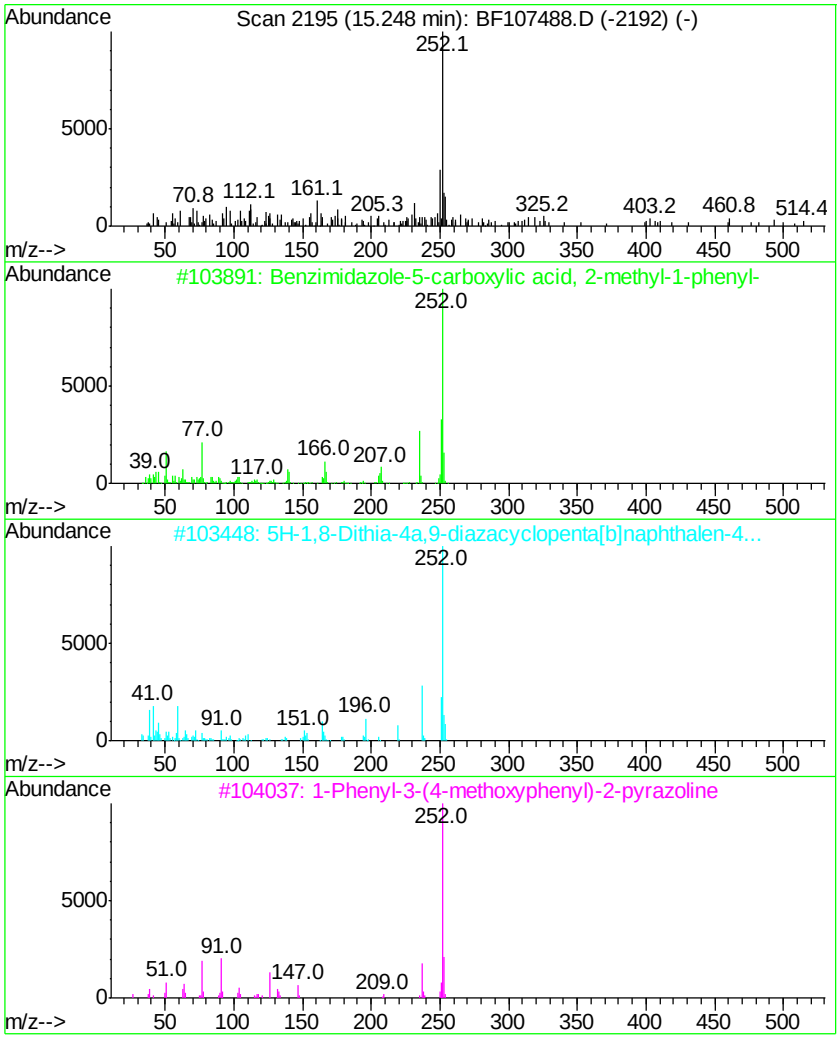
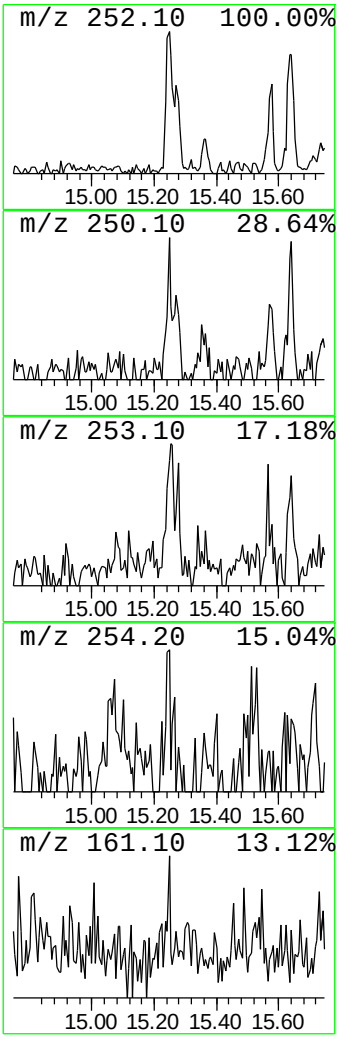
Peak Number 6 Benzimidazole-5-carboxylic ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.07 ng	96495	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzimidazole-5-carboxylic acid,...	252	C15H12N2O2	092437-43-9	50
2	5H-1,8-Dithia-4a,9-diazacyclopen...	252	C11H12N2OS2	1000315-96-2	50
3	1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	49
4	3,5,6-Trimethyl-p-quinone, 2-(2,...	280	C13H12O5S	126848-01-9	49
5	3,5-Pyridinedicarboxylic acid, 1...	267	C14H21NO4	000632-93-9	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

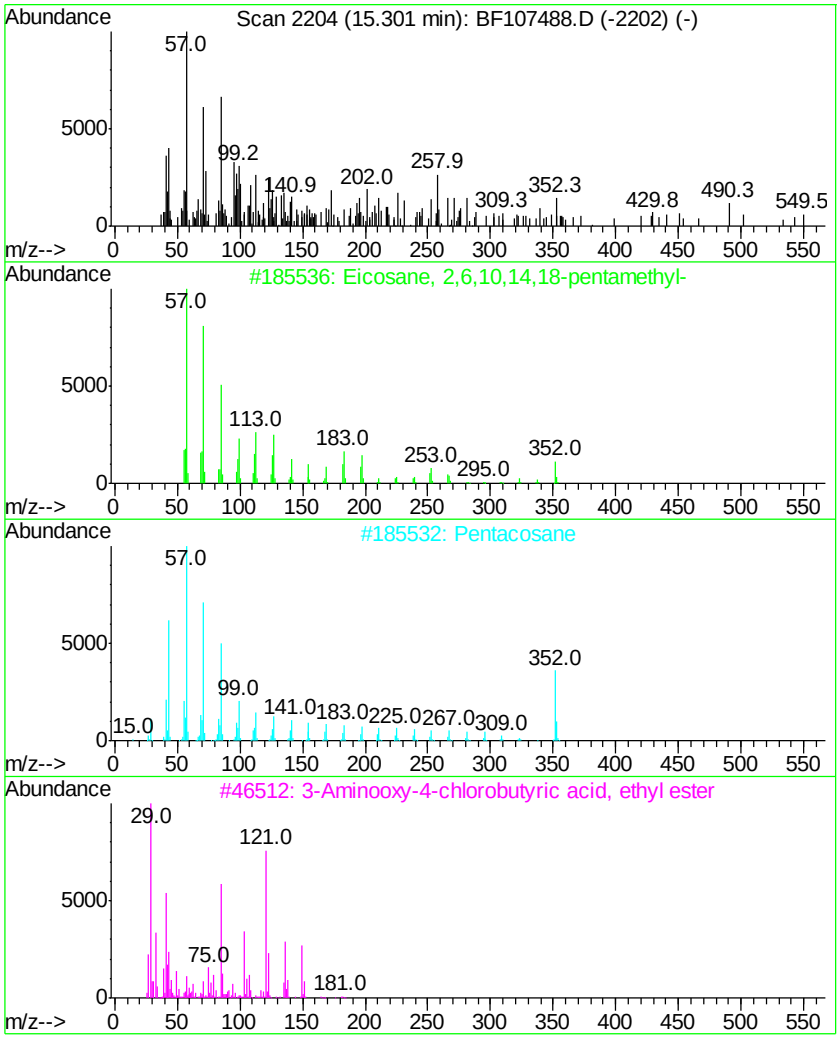
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

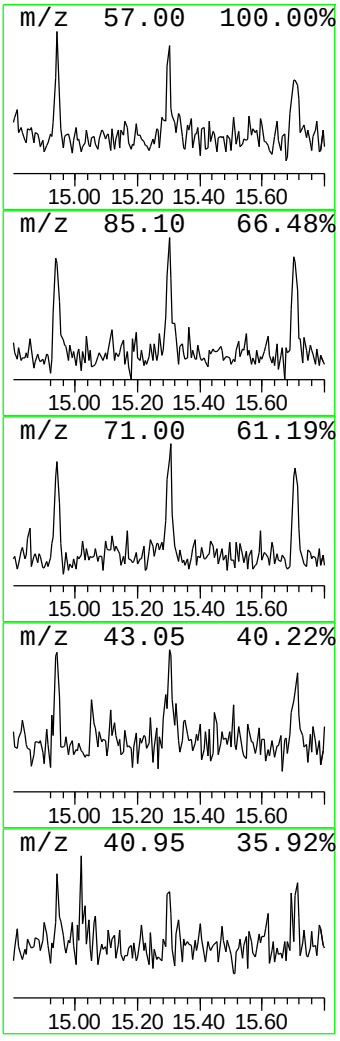
****

Peak Number 7 unknown15.30 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.26 ng	105505	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 2,6,10,14,18-pentamethyl-	352	C25H52	051794-16-2	27
2	Pentacosane	352	C25H52	000629-99-2	16
3	3-Aminooxy-4-chlorobutyric acid,...	181	C6H12ClNO3	1000186-78-9	9
4	Fumaric acid, 3,3-dimethylbut-2-...	452	C28H52O4	1000348-71-7	8
5	Cholestan-3-one, 4,4-dimethyl-, ...	429	C29H51NO	014732-99-1	4





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(+-)-4-Amino-4,5-...	5.22	7.1	ng	372871	1	6.98	1055370	20.0
unknown6.75	6.75	58.5	ng	3089010	1	6.98	1055370	20.0
1-Decanol, 2-hexyl-	13.99	4.0	ng	220612	5	14.17	1107270	20.0
Tricosane	14.62	2.6	ng	143453	5	14.17	1107270	20.0
Benzimidazole-5-c...	15.25	2.1	ng	96495	6	15.71	932520	20.0
unknown15.30	15.30	2.3	ng	105505	6	15.71	932520	20.0