LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

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-BF090115.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	1.463	8	11	16	rBV	49738	142247	7.13%	0.910%
2	1.543	16	18	58	rVB	573770	1995606	100.00%	12.761%
3	4.514	274	278	295	rBV	238567	632254	31.68%	4.043%
4	5.383	351	354	370	rBV	534770	1056701	52.95%	6.757%
5	7.646	549	552	558	rBV	568655	1126253	56.44%	7.202%
6	7.749	558	561	567	rVB	683272	1118804	56.06%	7.154%
7	8.229	600	603	607	rBV	232068	363596	18.22%	2.325%
8	8.560	628	632	635	rBV	485640	800094	40.09%	5.116%
9	9.532	712	717	720	rBV	390285	716345	35.90%	4.581%
10	11.132	853	857	860	rBV	300016	470445	23.57%	3.008%
11	13.772	1084	1088	1091	rBV	638782	1141177	57.18%	7.297%
12	14.824	1177	1180	1184	rBV	124887	218848	10.97%	1.399%
13	15.270	1215	1219	1223	rBV	281304	469647	23.53%	3.003%
14	17.167	1381	1385	1391	rBB	382967	633399	31.74%	4.050%
15	17.807	1438	1441	1447	rBB	10323	24091	1.21%	0.154%
16	18.779	1522	1526	1528	rBV	245997	431214	21.61%	2.757%
17	18.824	1528	1530	1534	rVV	155285	236339	11.84%	1.511%
18	18.950	1538	1541	1545	rVB	31133	52826	2.65%	0.338%
19	19.430	1580	1583	1587	rBB	11662	21154	1.06%	0.135%
20	20.002	1630	1633	1636	rBV	15639	26072	1.31%	0.167%
21	20.059	1636	1638	1642	rVB	17901	32244	1.62%	0.206%
22	20.219	1650	1652	1657	rVV2	15131	43472	2.18%	0.278%
23	20.527	1676	1679	1687	rBV2	29120	67971	3.41%	0.435%
24	20.756	1695	1699	1702	rVV2	15289	36542	1.83%	0.234%
25	21.213	1736	1739	1741	rBV	13190	21119	1.06%	0.135%
26	21.442	1756	1759	1762	rVV	315268	366679	18.37%	2.345%
27	21.785	1786	1789	1793	rBV	246320	377208	18.90%	2.412%
28	21.910	1798	1800	1803	rBV3	14400	27604	1.38%	0.177%
29	22.036	1807	1811	1816	rVB2	21216	46743	2.34%	0.299%
30	22.116	1816	1818	1820	rBV	547220	708644	35.51%	4.531%
31	22.162	1820	1822	1825	rVB2	15241	25626	1.28%	0.164%
32	22.310	1828	1835	1837	rBV2	21323	59528	2.98%	0.381%
33	22.436	1844	1846	1848	rBV	20243	26501	1.33%	0.169%
34	22.550	1854	1856	1858	rVV	21229	20213	1.01%	0.129%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.973	1889	1893	1894	rBV2	30919	52410	2.63%	0.335%
36	23.088	1901	1903	1905	rBV2	21838	34165	1.71%	0.218%
37	23.133	1905	1907	1910	rVB2	22913	41600	2.08%	0.266%
38	23.225	1913	1915	1917	rVB	39932	38589	1.93%	0.247%
39	23.396	1925	1930	1931	rBV2	333546	586404	29.38%	3.750%
40	23.419	1931	1932	1934	rVB	171177	169110	8.47%	1.081%
41	23.499	1938	1939	1941	rBV	24918	27849	1.40%	0.178%
42	23.682	1953	1955	1957	rBV3	18477	27322	1.37%	0.175%
43	23.842	1967	1969	1971	rVB	33425	37617	1.88%	0.241%
44	24.356	2011	2014	2017	rBV2	18174	40548	2.03%	0.259%
45	24.413	2017	2019	2021	rBV2	15300	31854	1.60%	0.204%
46	24.494	2023	2026	2030	rBV	178846	313538	15.71%	2.005%
47	24.585	2032	2034	2036	rVB	21126	28861	1.45%	0.185%
48	24.734	2045	2047	2049	rBV	100934	100592	5.04%	0.643%
49	24.779	2049	2051	2053	rVB	129162	125875	6.31%	0.805%
50	24.825	2053	2055	2063	rBV2	161816	291546	14.61%	1.864%
51	25.888	2145	2148	2151	rBV	44983	82478	4.13%	0.527%
52	26.185	2172	2174	2178	rBV	42968	70626	3.54%	0.452%

Sum of corrected areas: 15638190

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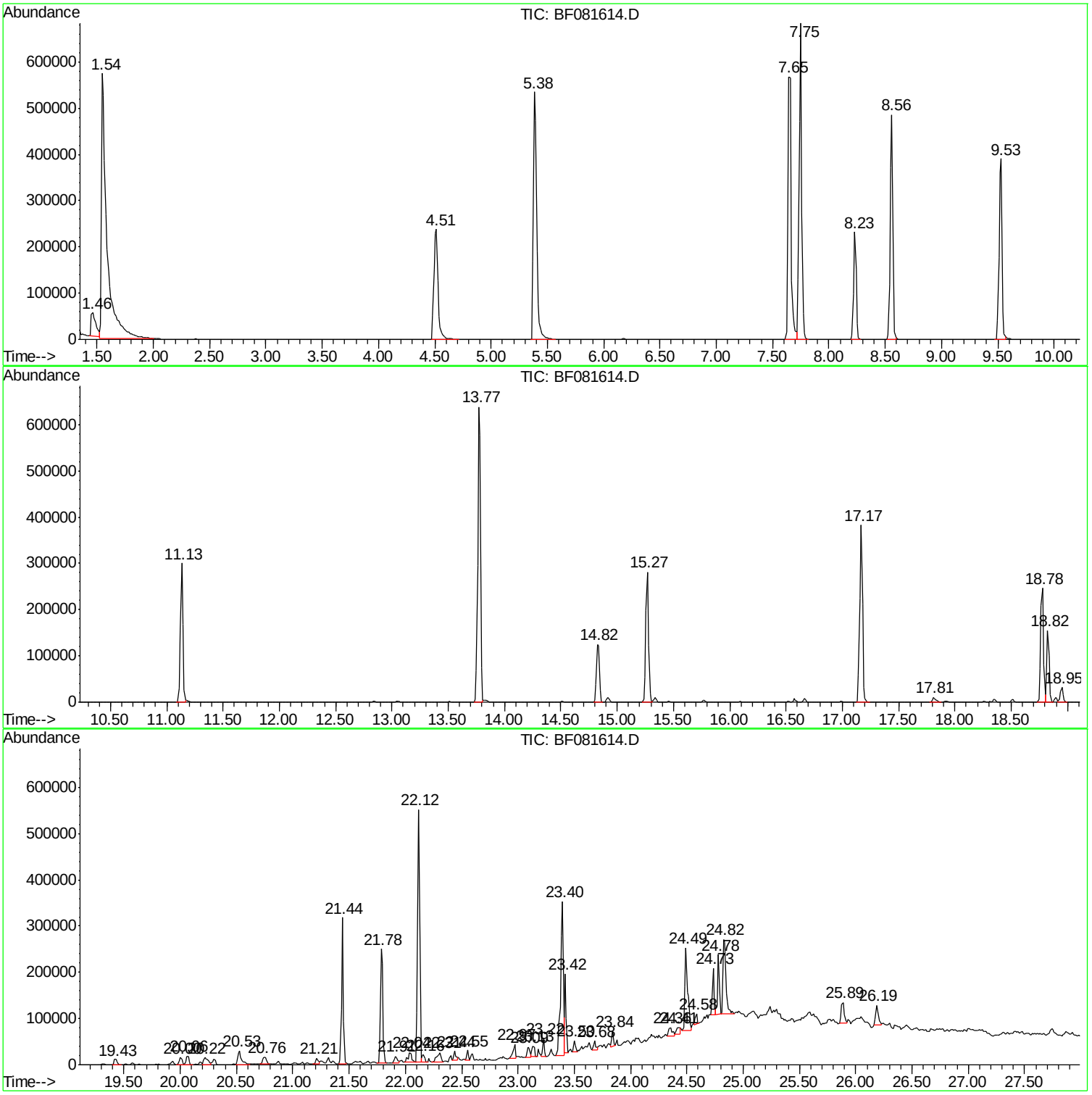
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF091415\
Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

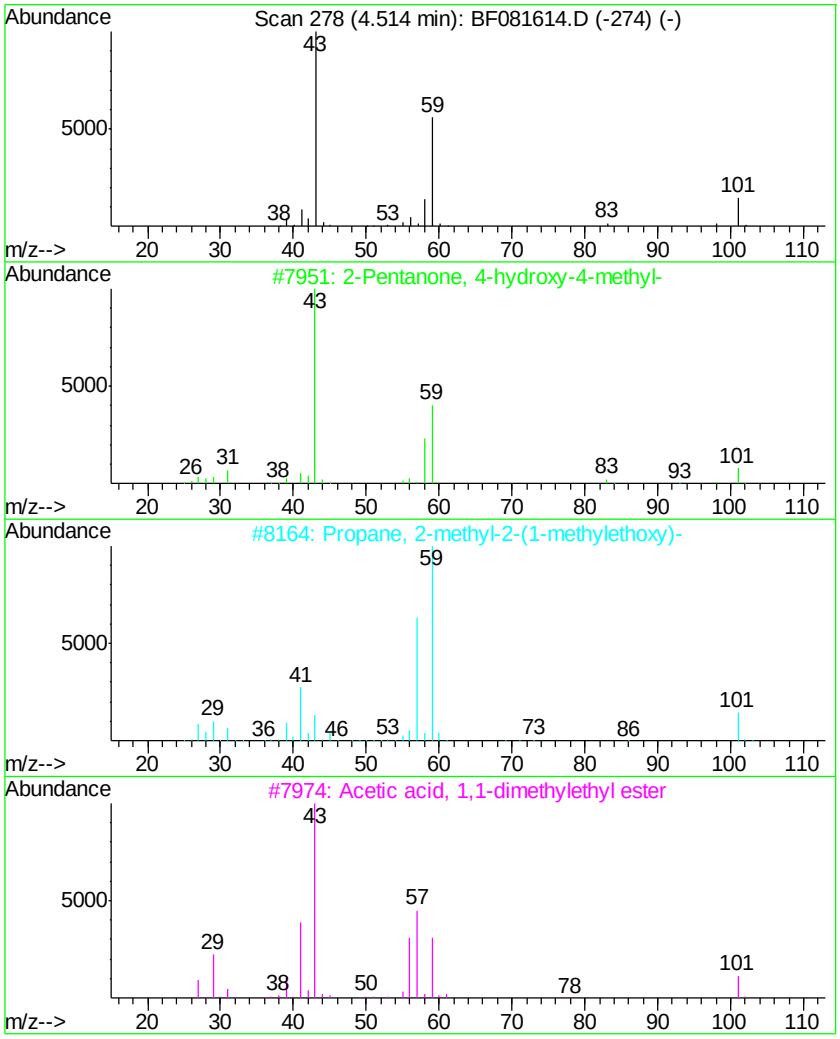
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

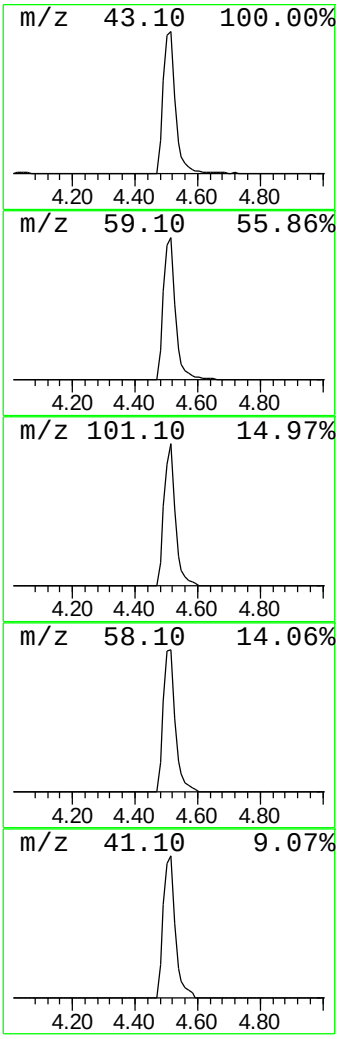
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.51	34.78 ng	632254	1,4-Dichlorobenzene-d4	8.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





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Data File : BF081614.D
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Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

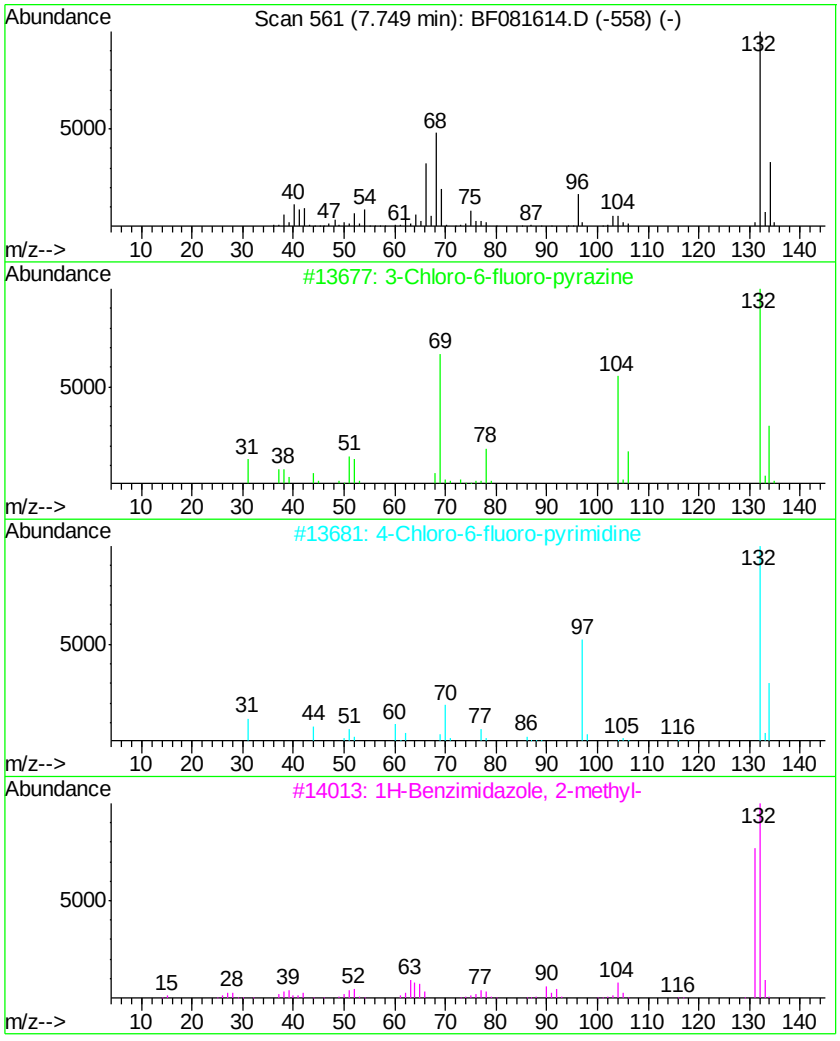
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

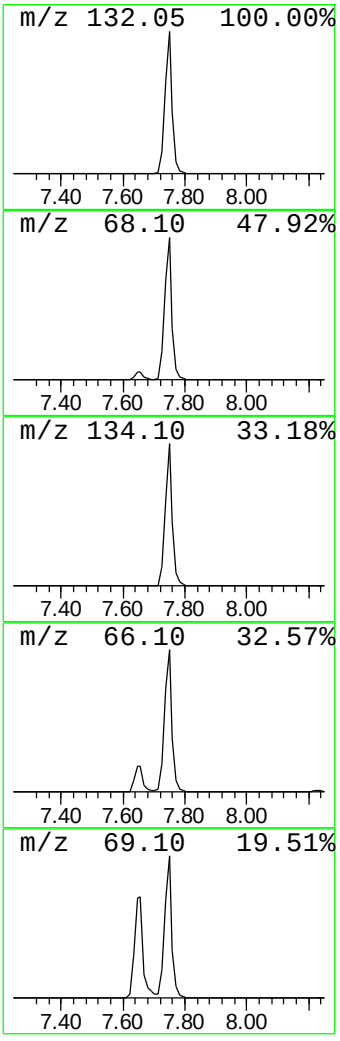
****

Peak Number 4 unknown7.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	61.54 ng	1118800	1,4-Dichlorobenzene-d4	8.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

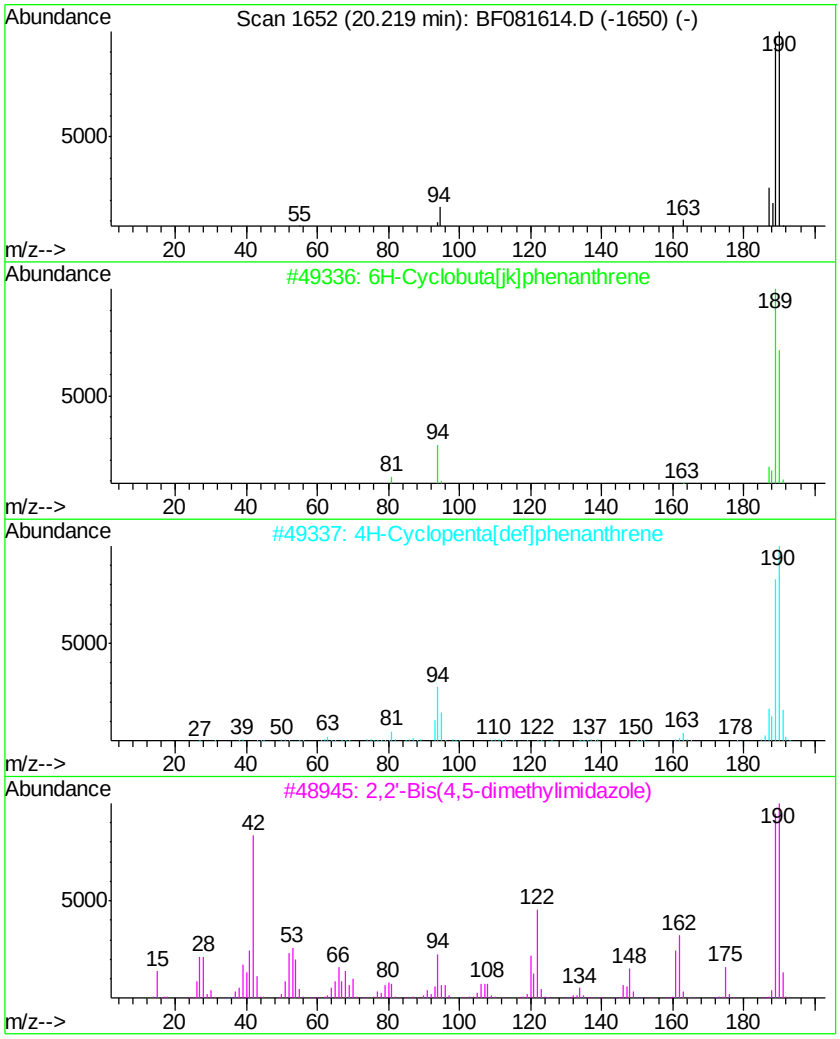
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

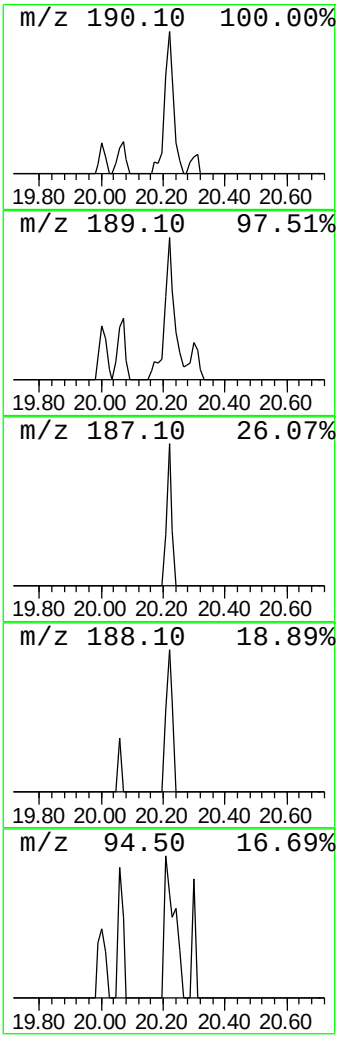
****

Peak Number 6 6H-Cyclobuta[jk]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	2.02 ng	43472	Phenanthrene-d10	18.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	78
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	74
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	9
5	Benzaldehyde, 4-(trifluoromethoxy)-	190	C8H5F3O2	000659-28-9	9





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Sample : G3597-08 2X
Misc :
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Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

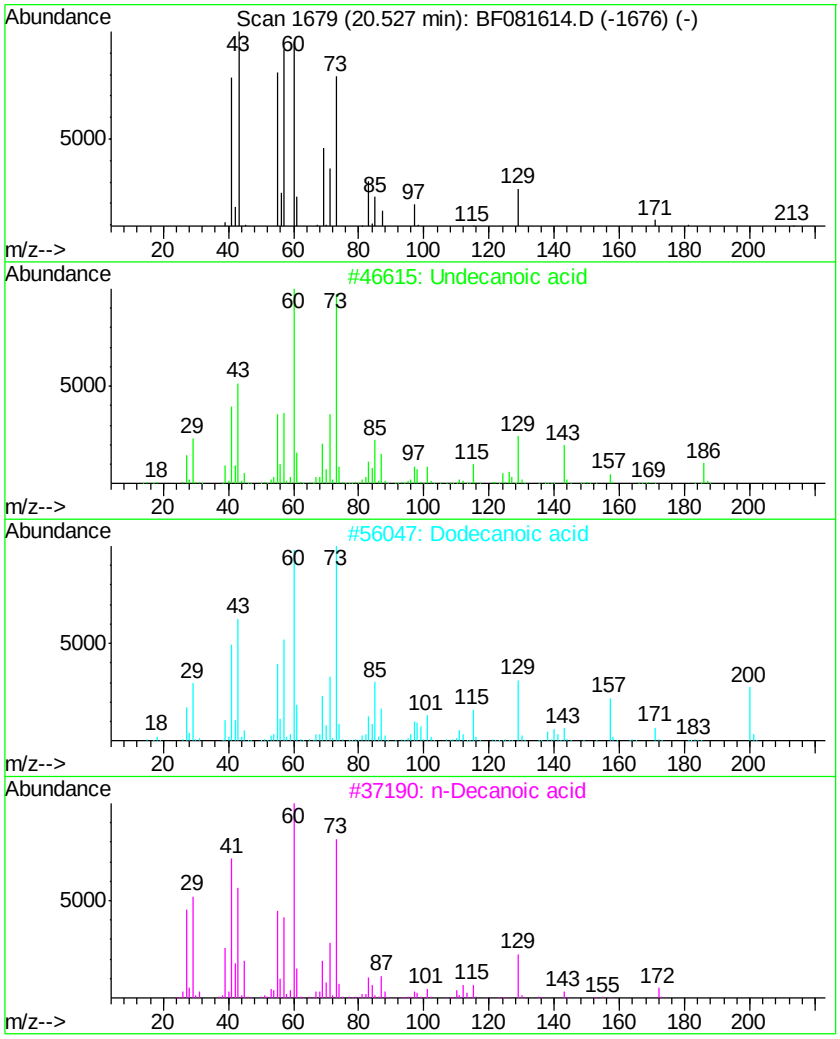
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

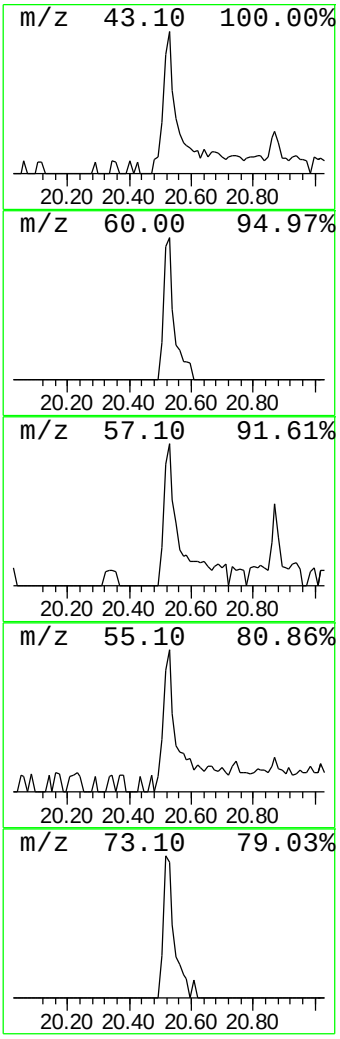
****

Peak Number 7 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.53	3.15 ng	67971	Phenanthrene-d10	18.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	Dodecanoic acid	200	C12H24O2	000143-07-7	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	43
5	(1R,3R,4R,5R)-(-)-Quinic acid	192	C7H12O6	000077-95-2	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

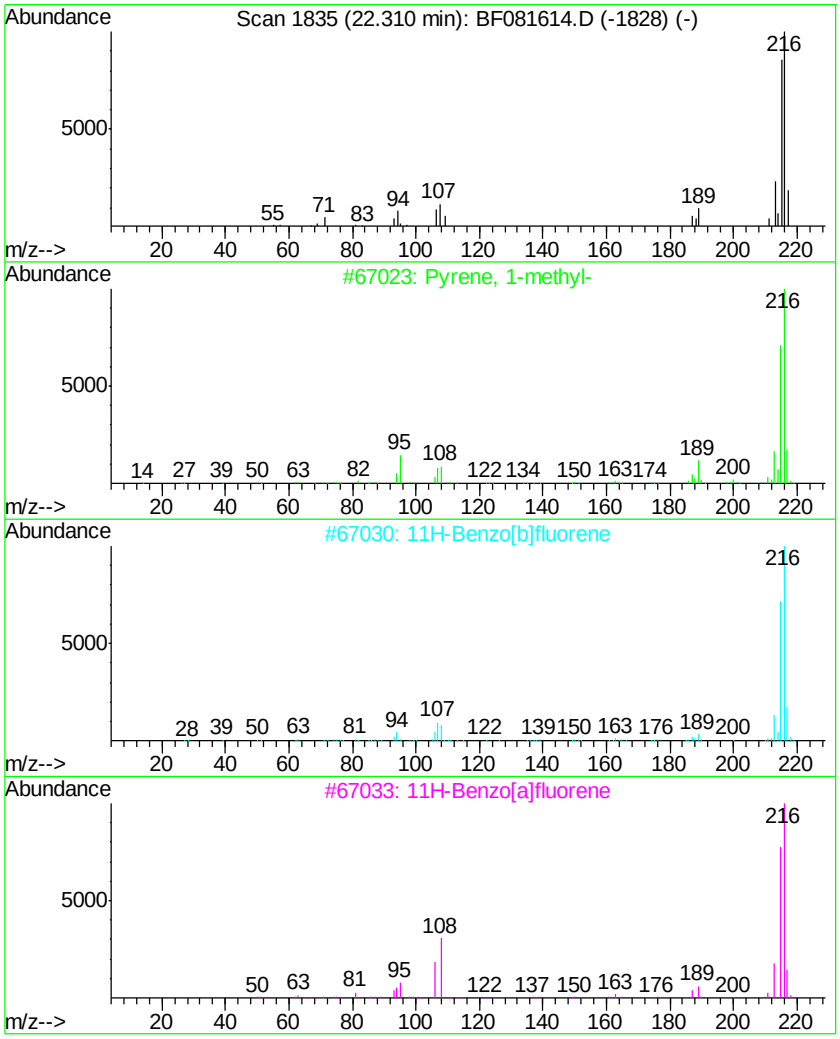
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

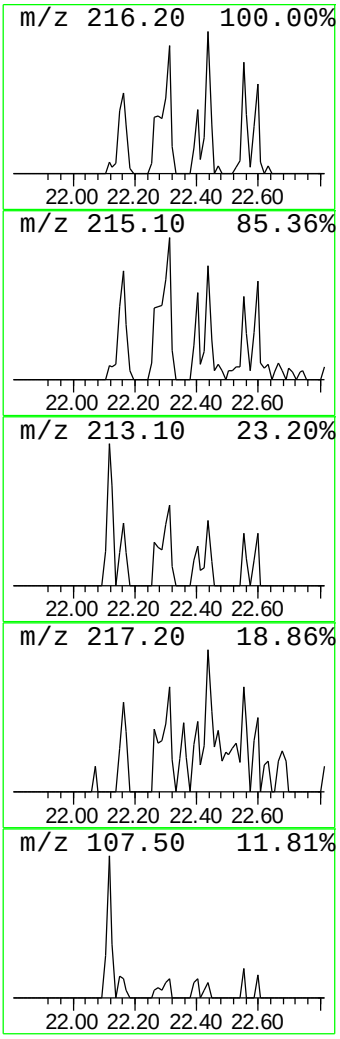
****

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.31	2.03 ng	59528	Chrysene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	80





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Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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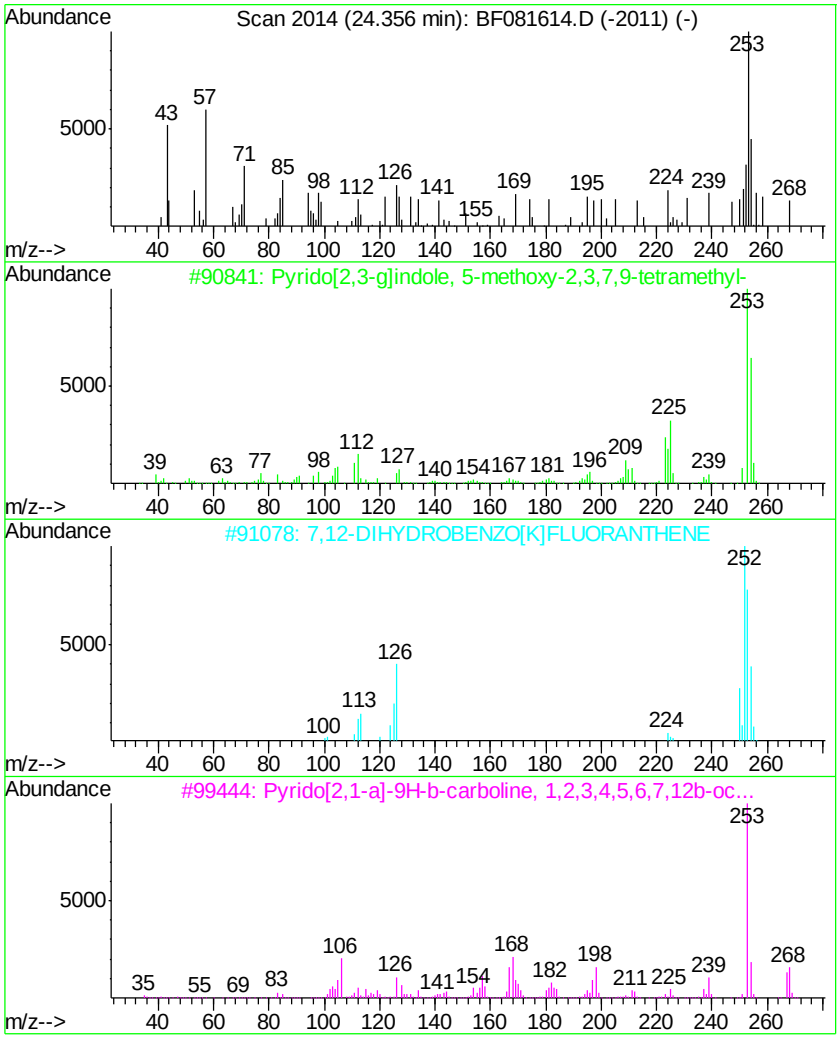
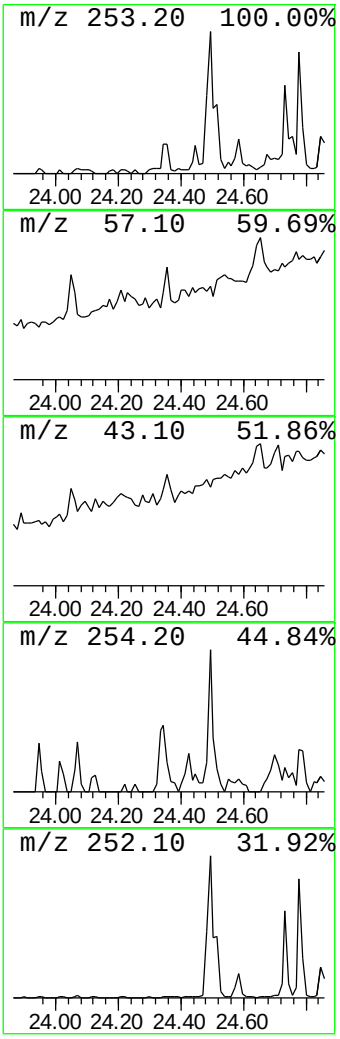
Peak Number 9 unknown24.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.36	2.78 ng	40548	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[2,3-g]indole, 5-methoxy-2...	254	C16H18N2O	201991-45-9	43
2	7,12-DIHYDROBENZO[K]FLUORANTHENE	254	C20H14	1000080-17-7	40
3	Pyrido[2,1-a]-9H-b-carboline, 1,...	268	C18H24N2	082605-35-4	35
4	3,6-Bis(N-formamido)carbazole	253	C14H11N3O2	098805-10-8	27
5	2,5-Cyclohexadien-1-one, 2,5-dim...	253	C17H19NO	054245-93-1	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081614.D
Acq On : 14 Sep 2015 18:50
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.51	34.8	ng	632254	1	8.23	363596	20.0
unknown7.75	7.75	61.5	ng	1118800	1	8.23	363596	20.0
6H-Cyclobuta[jk]p...	20.22	2.0	ng	43472	4	18.78	431214	20.0
Undecanoic acid	20.53	3.1	ng	67971	4	18.78	431214	20.0
Pyrene, 1-methyl-	22.31	2.0	ng	59528	5	23.40	586404	20.0
unknown24.36	24.36	2.8	ng	40548	6	24.84	291546	20.0