LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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	6593	19022	1.81%	0.133%
2	1.543	16	18	40	rVB	108138	361592	34.44%	2.520%
3	4.480	271	275	292	rBV	234858	586023	55.82%	4.083%
4	5.360	349	352	371	rBB	525805	981359	93.47%	6.838%
5	7.623	547	550	555	rBV	582631	997290	94.99%	6.949%
6	7.726	555	559	565	rVB	599416	1049874	100.00%	7.316%
7	8.206	598	601	607	rBB	214203	336684	32.07%	2.346%
8	8.538	626	630	633	rBV	421700	734423	69.95%	5.118%
9	9.498	710	714	728	rBB	343595	667629	63.59%	4.652%
10	11.109	851	855	858	rBV	273661	423060	40.30%	2.948%
11	13.750	1082	1086	1089	rBV	607386	1048386	99.86%	7.305%
12	14.813	1175	1179	1182	rBV	112863	196685	18.73%	1.371%
13	14.893	1184	1186	1191	rVB	9770	15076	1.44%	0.105%
14	15.247	1213	1217	1221	rBV	251757	442571	42.15%	3.084%
15	15.315	1221	1223	1226	rVB	8890	12799	1.22%	0.089%
16	16.550	1329	1331	1334	rBB	7149	10513	1.00%	0.073%
17	16.641	1337	1339	1342	rBB	7114	11007	1.05%	0.077%
18	17.144	1379	1383	1391	rBB	372743	628425	59.86%	4.379%
19	17.784	1436	1439	1445	rBV	9815	25288	2.41%	0.176%
20	18.321	1484	1486	1490	rBB	7786	12349	1.18%	0.086%
21	18.493	1496	1501	1504	rBB	5591	10832	1.03%	0.075%
22	18.744	1519	1523	1526	rBV	239052	441726	42.07%	3.078%
23	18.802	1526	1528	1531	rVV	160304	241320	22.99%	1.682%
24	18.870	1531	1534	1536	rVV2	10925	19172	1.83%	0.134%
25	18.927	1536	1539	1543	rVB	30694	53634	5.11%	0.374%
26	19.407	1578	1581	1585	rVB	12494	21653	2.06%	0.151%
27	19.910	1619	1625	1628	rBB	7884	16477	1.57%	0.115%
28	19.979	1628	1631	1634	rBV	17813	28588	2.72%	0.199%
29	20.036	1634	1636	1640	rVB	18552	33919	3.23%	0.236%
30	20.150	1644	1646	1648	rVV	6149	12878	1.23%	0.090%
31	20.196	1648	1650	1654	rVV2	16151	43894	4.18%	0.306%
32	20.276	1654	1657	1661	rVB	12181	23209	2.21%	0.162%
33	20.505	1674	1677	1685	rBV	37291	74509	7.10%	0.519%
34	20.733	1693	1697	1700	rVB2	16943	39374	3.75%	0.274%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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	21.190	1734	1737	1739	rBV	15477	24067	2.29%	0.168%
36	21.236	1739	1741	1744	rVV3	7424	16679	1.59%	0.116%
37	21.293	1744	1746	1748	rVV2	12826	21850	2.08%	0.152%
38	21.419	1754	1757	1760	rVV	294040	417218	39.74%	2.907%
39	21.545	1763	1768	1770	rBV	7409	16526	1.57%	0.115%
40	21.773	1785	1788	1792	rBV	342200	444944	42.38%	3.100%
41	21.899	1796	1799	1802	rBV2	16047	36848	3.51%	0.257%
42	21.990	1806	1807	1808	rBV	12120	15929	1.52%	0.111%
43	22.025	1808	1810	1814	rVB	31518	47908	4.56%	0.334%
44	22.105	1814	1817	1819	rBV	758656	847795	80.75%	5.908%
45	22.139	1819	1820	1823	rVB	20914	28457	2.71%	0.198%
46	22.196	1823	1825	1828	rBV	8304	12755	1.21%	0.089%
47	22.265	1828	1831	1832	rBV	16602	36616	3.49%	0.255%
48	22.288	1832	1833	1836	rVB	23278	26808	2.55%	0.187%
49	22.379	1839	1841	1843	rBV	13195	20802	1.98%	0.145%
50	22.425	1843	1845	1846	rBV	19709	29007	2.76%	0.202%
51	22.539	1853	1855	1856	rBV2	20800	23773	2.26%	0.166%
52	22.573	1856	1858	1860	rVB	20656	21430	2.04%	0.149%
53	22.836	1876	1881	1882	rBV2	5848	14975	1.43%	0.104%
54	22.951	1888	1891	1893	rBV	38166	58759	5.60%	0.409%
55	23.076	1899	1902	1904	rBV2	24207	37997	3.62%	0.265%
56	23.111	1904	1905	1908	rVB2	28173	47313	4.51%	0.330%
57	23.168	1908	1910	1912	rBV	19953	23019	2.19%	0.160%
58	23.213	1912	1914	1917	rBV	38492	42923	4.09%	0.299%
59	23.282	1917	1920	1922	rBV	17044	19482	1.86%	0.136%
60	23.373	1922	1928	1930	rBV2	368650	656862	62.57%	4.577%
61	23.408	1930	1931	1933	rVB	200242	155702	14.83%	1.085%
62	23.442	1933	1934	1936	rVB2	9401	12068	1.15%	0.084%
63	23.488	1936	1938	1940	rBV	33787	37826	3.60%	0.264%
64	23.556	1941	1944	1945	rBV2	8424	12206	1.16%	0.085%
65	23.613	1948	1949	1952	rVB2	15725	19628	1.87%	0.137%
66	23.671	1952	1954	1955	rBV	16471	23467	2.24%	0.164%
67	23.705	1955	1957	1960	rBV4	10359	19282	1.84%	0.134%
68	23.785	1962	1964	1965	rBV	11532	12320	1.17%	0.086%
69	23.831	1965	1968	1969	rBV	32443	39765	3.79%	0.277%
70	24.036	1984	1986	1990	rVB4	10429	20606	1.96%	0.144%
71	24.174	1996	1998	2001	rBV3	8935	14709	1.40%	0.102%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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

72	24.334	2010	2012	2014	rBV3	18463	37439	3.57%	0.261%
73	24.482	2022	2025	2029	rBV	163402	342891	32.66%	2.389%
74	24.562	2030	2032	2034	rVB2	29281	39977	3.81%	0.279%
75	24.722	2044	2046	2048	rBV	96131	112356	10.70%	0.783%
76	24.768	2048	2050	2052	rVV	157677	154558	14.72%	1.077%
77	24.814	2052	2054	2060	rVB2	277662	352386	33.56%	2.455%
78	25.568	2118	2120	2122	rBV3	14815	23219	2.21%	0.162%
79	25.739	2132	2135	2137	rBV3	15614	37990	3.62%	0.265%
80	25.865	2143	2146	2149	rBV	75193	123045	11.72%	0.857%
81	26.162	2169	2172	2176	rBV	67659	128957	12.28%	0.899%
82	26.425	2193	2195	2199	rVB4	9908	18620	1.77%	0.130%

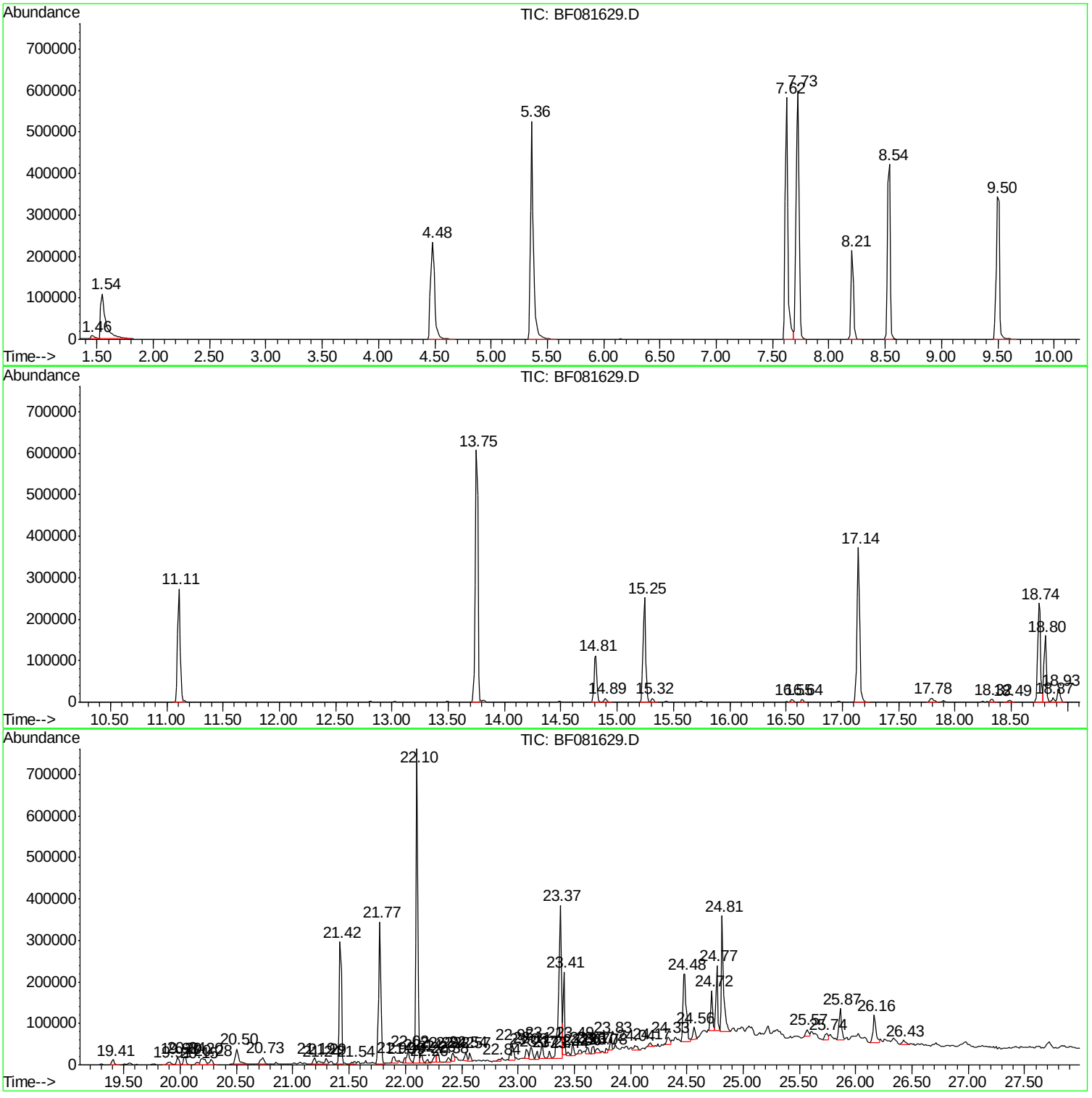
Sum of corrected areas: 14350999

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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

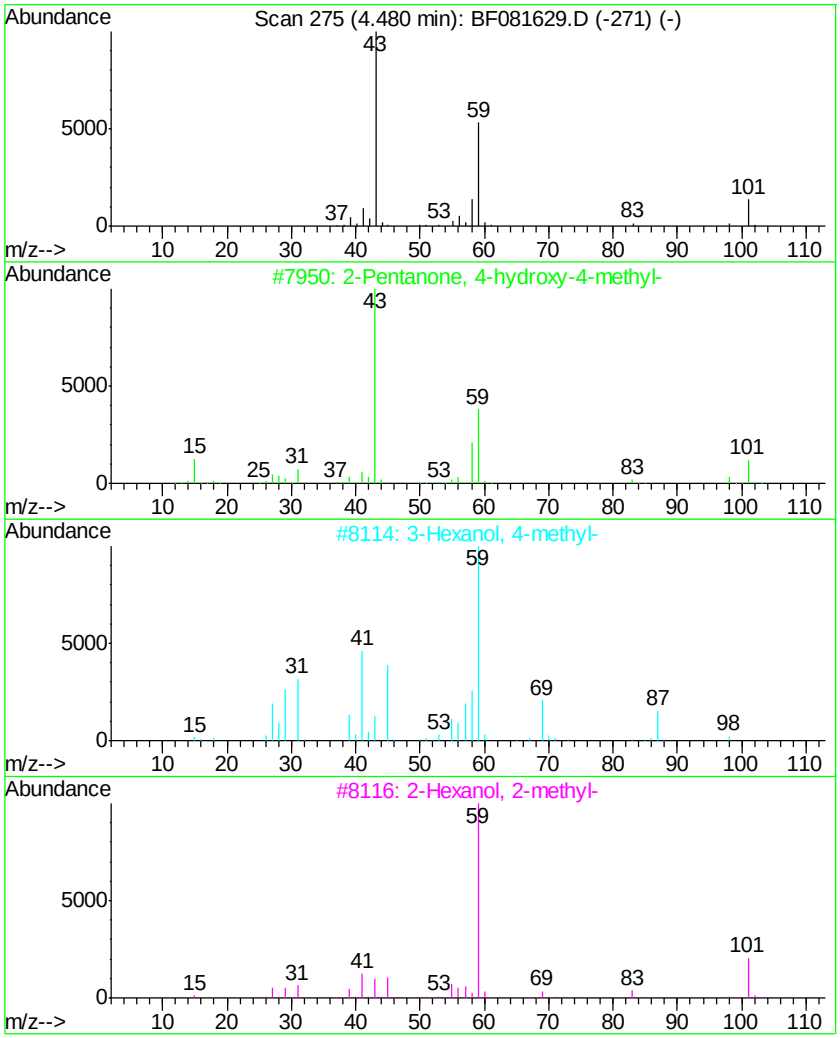
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

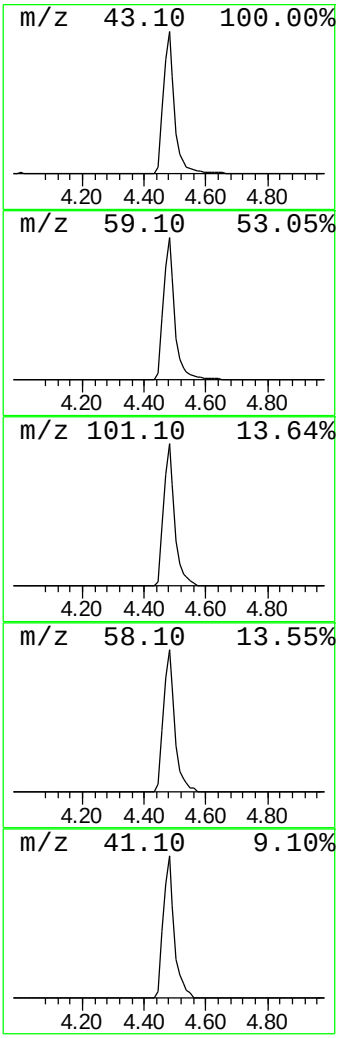
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	34.81 ng	586023	1,4-Dichlorobenzene-d4	8.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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

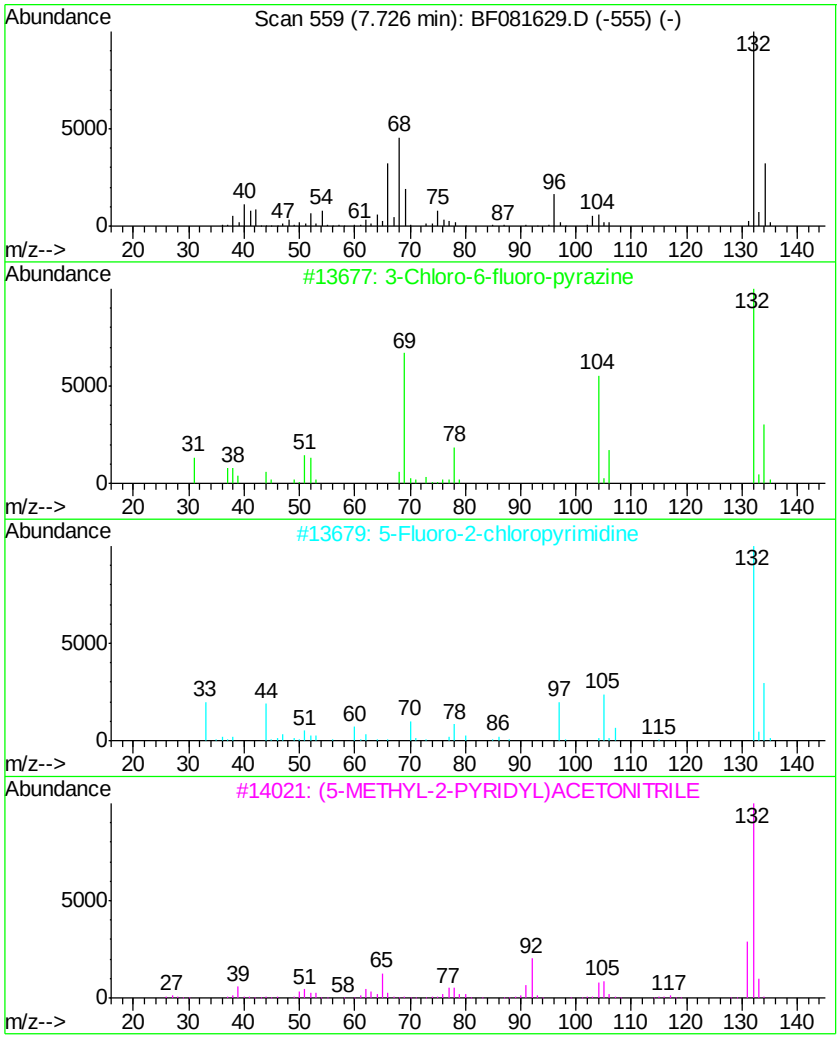
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

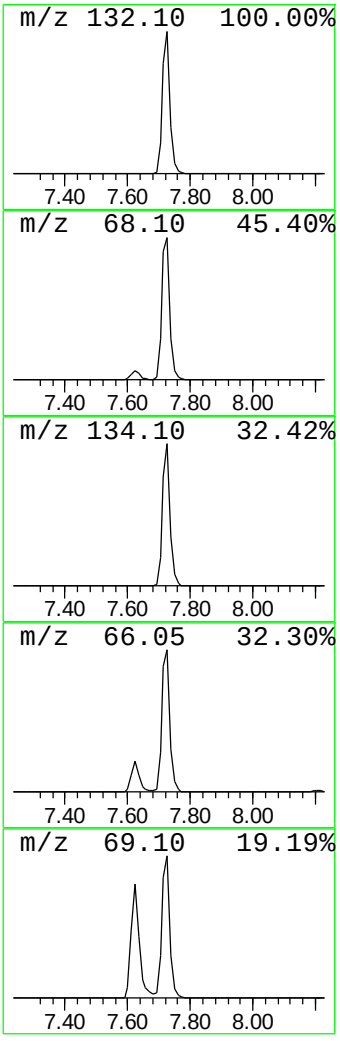
****

Peak Number 3 unknown7.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	62.37 ng	1049870	1,4-Dichlorobenzene-d4	8.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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

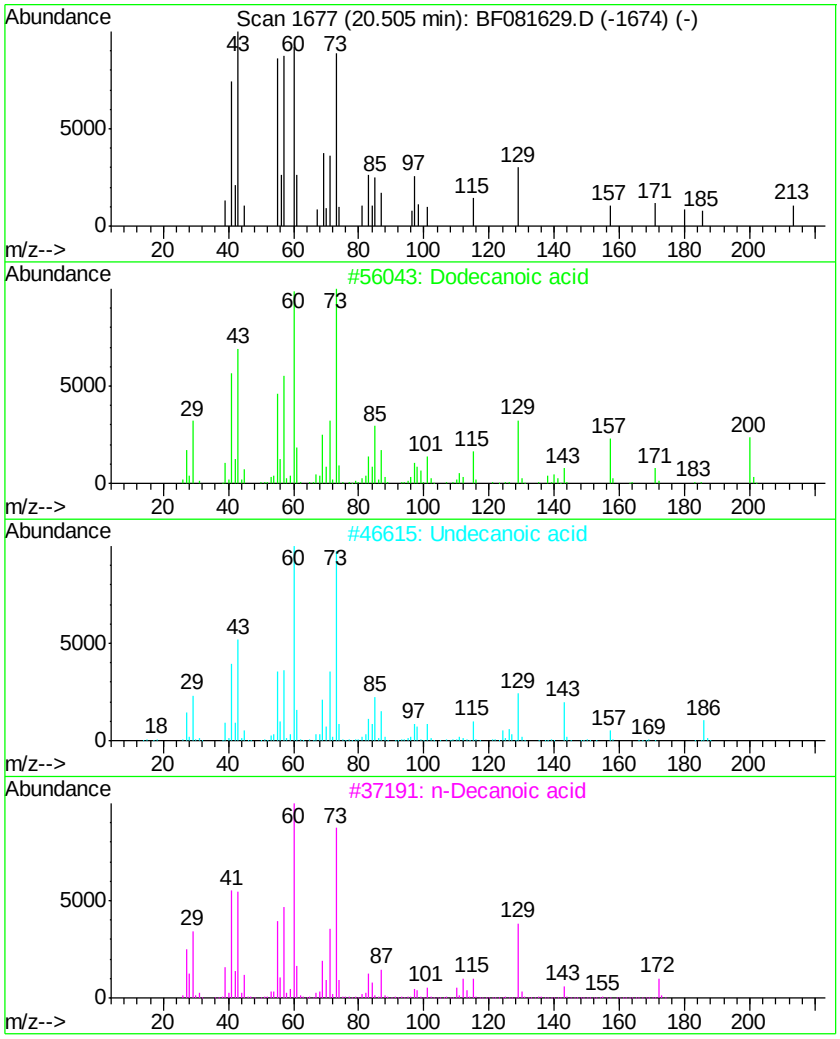
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

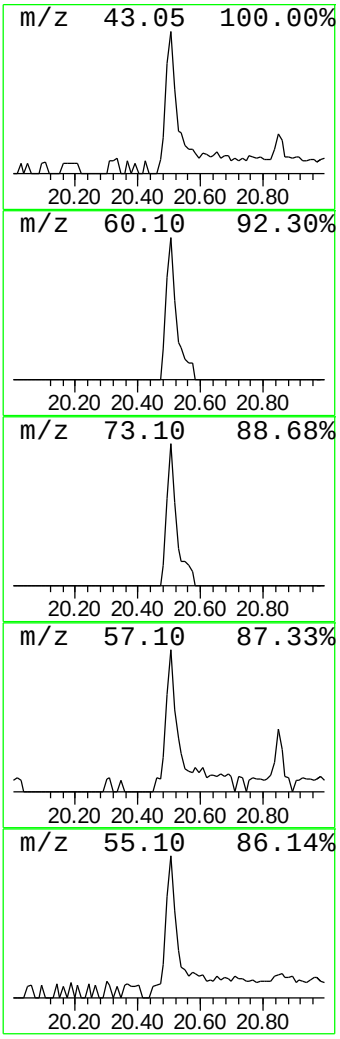
****

Peak Number 5 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.50	3.37 ng	74509	Phenanthrene-d10	18.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	43
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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

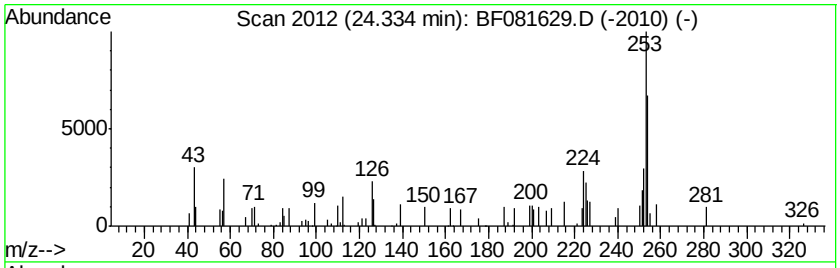
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

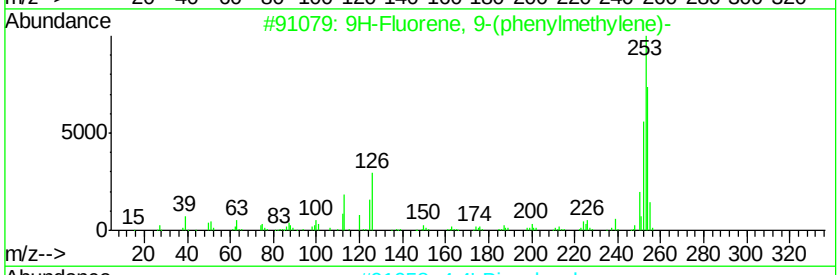
****

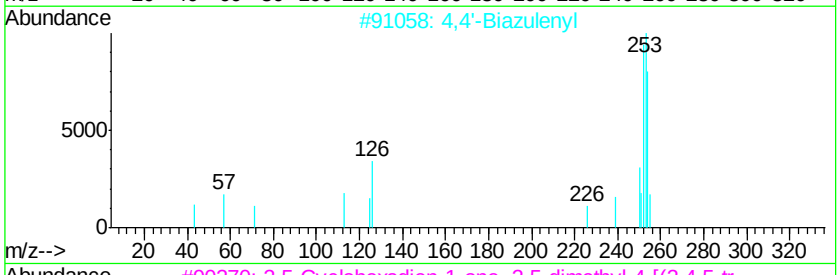
Peak Number 6 unknown24.33 Concentration Rank 8

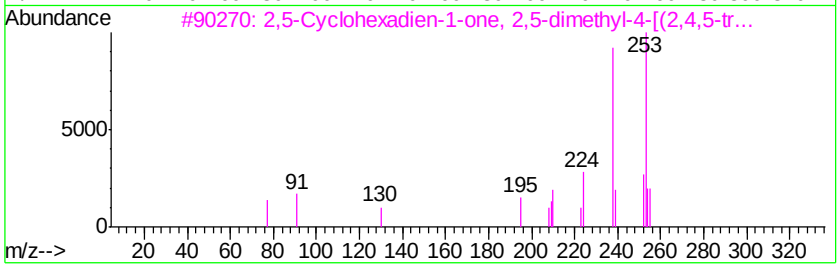
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.33	2.12 ng	37439	Perylene-d12	24.81

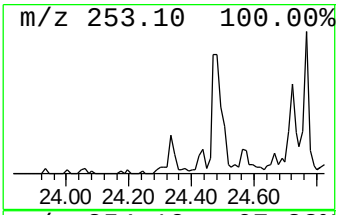
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9-(phenylmethylene)-	254	C20H14	001836-87-9	43
2	4,4'-Biazulenyl	254	C20H14	094053-54-0	43
3	2,5-Cyclohexadien-1-one, 2,5-dim...	253	C17H19NO	054245-93-1	43
4	Pyrido[2,3-g]indole, 5-methoxy-2...	254	C16H18N2O	201991-45-9	40
5	1H-Indene, 1,1'-(1,2-ethanediyli...	254	C20H14	072088-04-1	37

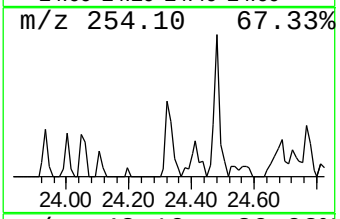


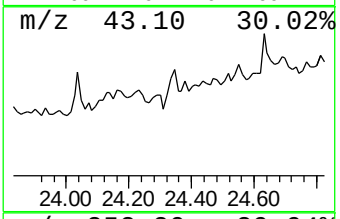


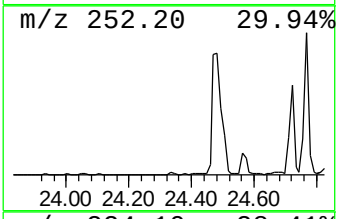


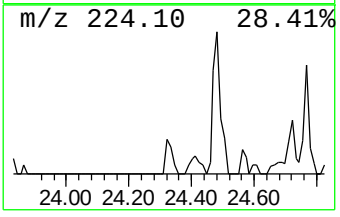












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

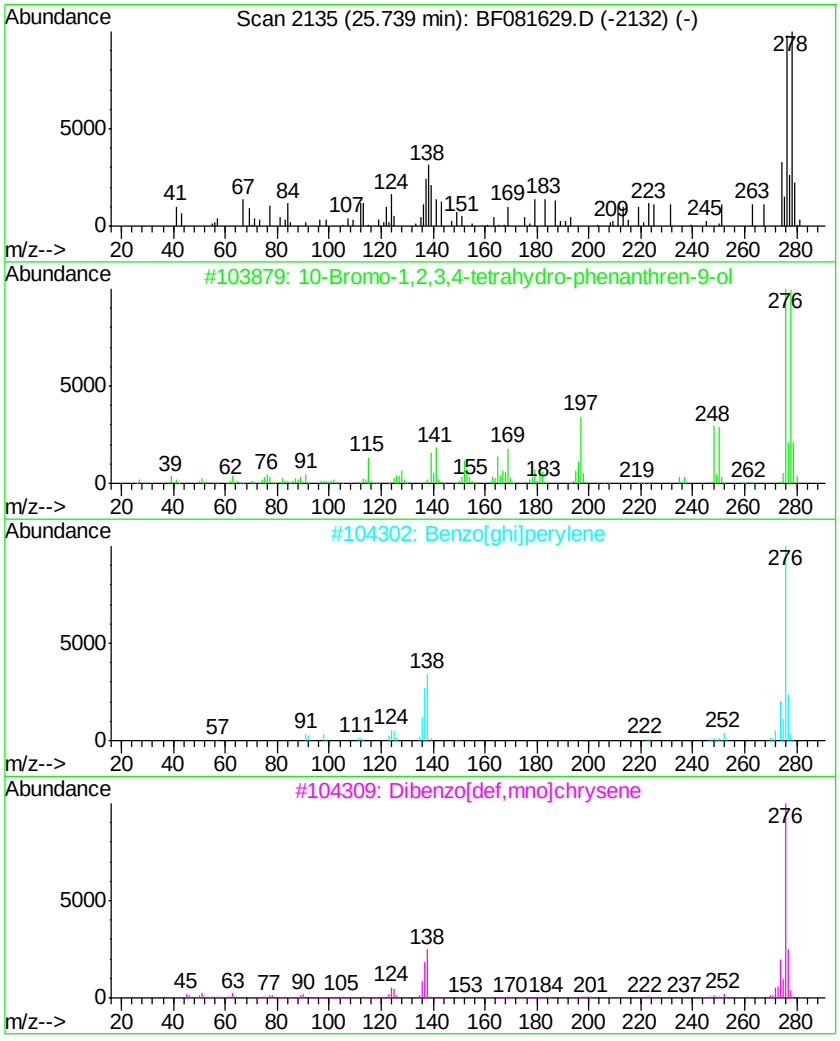
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

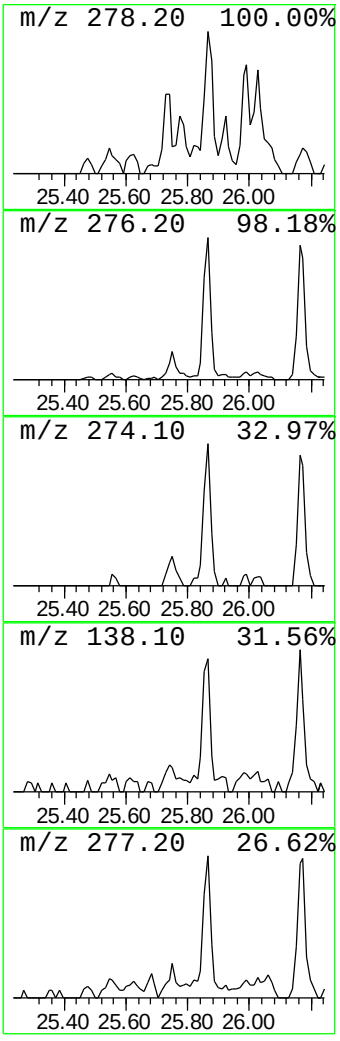
****

Peak Number 8 10-Bromo-1,2,3,4-tetrahydro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.74	2.16 ng	37990	Perylene-d12	24.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Bromo-1,2,3,4-tetrahydro-phen...	276	C14H13BrO	1000190-54-9	64
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	46
3	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	41
4	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	41
5	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091515\
Data File : BF081629.D
Acq On : 15 Sep 2015 14:48
Operator : UM/IZ
Sample : G3597-08 2X
Misc :
ALS Vial : 6 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...	4.48	34.8	ng	586023	1	8.21	336684	20.0
unknown7.73	7.73	62.4	ng	1049870	1	8.21	336684	20.0
Dodecanoic acid	20.50	3.4	ng	74509	4	18.74	441726	20.0
unknown24.33	24.33	2.1	ng	37439	6	24.81	352386	20.0
10-Bromo-1,2,3,4-...	25.74	2.2	ng	37990	6	24.81	352386	20.0