LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110117\
Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

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-BF102317.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	4.981	489	492	505	rBV	29499	47709	8.70%	0.587%
2	5.404	561	564	589	rBV	186054	336101	61.30%	4.136%
3	6.428	735	738	753	rBV	224927	366801	66.90%	4.514%
4	6.551	756	759	775	rVB	389504	432849	78.94%	5.327%
5	6.775	794	797	811	rVB	357507	358847	65.44%	4.416%
6	6.934	821	824	838	rBV	341914	328588	59.93%	4.044%
7	7.351	892	895	916	rBV	184905	224234	40.89%	2.760%
8	8.063	1013	1016	1019	rBV	589255	495564	90.38%	6.099%
9	8.628	1110	1112	1118	rBB	8314	8775	1.60%	0.108%
10	8.786	1136	1139	1145	rBB	11065	11607	2.12%	0.143%
11	8.881	1153	1155	1160	rBB	8595	8525	1.55%	0.105%
12	9.133	1195	1198	1208	rVB	566982	489317	89.24%	6.022%
13	9.481	1254	1257	1260	rBV	7419	7088	1.29%	0.087%
14	9.539	1264	1267	1274	rVB	104019	88111	16.07%	1.084%
15	9.686	1289	1292	1298	rBB2	8221	7176	1.31%	0.088%
16	9.822	1311	1315	1319	rBV	640303	530290	96.71%	6.526%
17	9.857	1319	1321	1324	rVB	27583	23321	4.25%	0.287%
18	10.033	1347	1351	1355	rBV	17082	17020	3.10%	0.209%
19	10.375	1406	1409	1415	rVB	34062	33203	6.06%	0.409%
20	10.539	1434	1437	1442	rVB	43938	41509	7.57%	0.511%
21	10.622	1447	1451	1462	rBB	213700	220078	40.14%	2.709%
22	10.928	1499	1503	1506	rBV	7719	7622	1.39%	0.094%
23	11.145	1537	1540	1542	rBV	8301	8328	1.52%	0.102%
24	11.163	1542	1543	1547	rVB	7958	6855	1.25%	0.084%
25	11.222	1551	1553	1556	rVB	8417	7194	1.31%	0.089%
26	11.322	1566	1570	1572	rBV	543117	460810	84.04%	5.671%
27	11.345	1572	1574	1579	rVV	285514	227151	41.43%	2.796%
28	11.404	1579	1584	1591	rVB	58329	59250	10.81%	0.729%
29	11.575	1606	1613	1619	rBV2	19673	24149	4.40%	0.297%
30	11.839	1654	1658	1660	rBV	34066	31667	5.78%	0.390%
31	11.869	1660	1663	1669	rVB	41599	42067	7.67%	0.518%
32	11.922	1669	1672	1675	rBV	17170	14870	2.71%	0.183%
33	11.957	1675	1678	1681	rVV	48991	54825	10.00%	0.675%
34	11.980	1681	1682	1686	rVB	21017	14201	2.59%	0.175%

LSC Area Percent Report

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Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.145	1708	1710	1715	rVB	16538	14610	2.66%	0.180%
36	12.210	1718	1721	1725	rBV	8678	10650	1.94%	0.131%
37	12.422	1753	1757	1760	rBV	16831	17014	3.10%	0.209%
38	12.469	1760	1765	1767	rVV4	6092	8327	1.52%	0.102%
39	12.539	1775	1777	1781	rVB	11768	11641	2.12%	0.143%
40	12.604	1784	1788	1794	rBV	288050	270399	49.31%	3.328%
41	12.716	1805	1807	1810	rBV	5481	6682	1.22%	0.082%
42	12.780	1816	1818	1820	rBV	7455	6308	1.15%	0.078%
43	12.839	1825	1828	1829	rVV	42419	35055	6.39%	0.431%
44	12.863	1829	1832	1838	rVV	237753	232456	42.39%	2.861%
45	12.921	1838	1842	1847	rVB	12378	14689	2.68%	0.181%
46	13.016	1853	1858	1862	rBV	377395	339240	61.87%	4.175%
47	13.063	1864	1866	1870	rVB	7999	7824	1.43%	0.096%
48	13.121	1870	1876	1880	rVB3	17397	32511	5.93%	0.400%
49	13.174	1880	1885	1888	rVB4	6132	8970	1.64%	0.110%
50	13.216	1888	1892	1894	rBV3	16565	24549	4.48%	0.302%
51	13.245	1894	1897	1901	rVB2	30730	34285	6.25%	0.422%
52	13.321	1907	1910	1913	rVB	18718	17183	3.13%	0.211%
53	13.369	1913	1918	1923	rBV3	24975	35947	6.56%	0.442%
54	13.433	1926	1929	1932	rVB3	5946	6159	1.12%	0.076%
55	13.480	1932	1937	1940	rBV3	12950	17048	3.11%	0.210%
56	13.521	1940	1944	1950	rVB3	13316	17939	3.27%	0.221%
57	13.639	1962	1964	1970	rVB4	5257	7277	1.33%	0.090%
58	13.692	1970	1973	1977	rBV4	7461	11802	2.15%	0.145%
59	13.880	2001	2005	2010	rBV2	16993	23394	4.27%	0.288%
60	14.010	2023	2027	2028	rBV	15981	17525	3.20%	0.216%
61	14.027	2028	2030	2034	rVV	19366	24000	4.38%	0.295%
62	14.068	2034	2037	2040	rVV	15230	20676	3.77%	0.254%
63	14.121	2043	2046	2048	rVV4	16608	23170	4.23%	0.285%
64	14.151	2048	2051	2056	rVB2	28256	35509	6.48%	0.437%
65	14.321	2071	2080	2084	rBV2	377449	548321	100.00%	6.748%
66	14.357	2084	2086	2090	rVB	88707	101339	18.48%	1.247%
67	14.433	2095	2099	2100	rVV4	6894	7464	1.36%	0.092%
68	14.463	2101	2104	2109	rVB2	15244	18644	3.40%	0.229%
69	14.545	2116	2118	2125	rVB6	18348	24385	4.45%	0.300%
70	14.610	2126	2129	2133	rVB4	9069	9980	1.82%	0.123%
71	14.651	2133	2136	2138	rBV	6676	7514	1.37%	0.092%

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Misc :
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Instrument : BNA_F
ClientSampleId : Q3-COMP

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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.792	2158	2160	2163	rBV3	7653	7145	1.30%	0.088%
73	14.851	2163	2170	2174	rBV	30052	52231	9.53%	0.643%
74	14.892	2174	2177	2182	rVB5	16102	21358	3.90%	0.263%
75	14.945	2182	2186	2188	rBV5	10312	18799	3.43%	0.231%
76	15.021	2196	2199	2201	rBV4	9193	9993	1.82%	0.123%
77	15.045	2201	2203	2207	rVB5	10988	11281	2.06%	0.139%
78	15.321	2248	2250	2253	rBV4	6850	9288	1.69%	0.114%
79	15.368	2255	2258	2262	rBV4	25278	37344	6.81%	0.460%
80	15.721	2314	2318	2321	rBV2	83435	126189	23.01%	1.553%
81	15.751	2321	2323	2331	rVB2	51242	71325	13.01%	0.878%
82	15.857	2338	2341	2345	rVB	21113	26448	4.82%	0.325%
83	16.080	2375	2379	2383	rBV	41441	56452	10.30%	0.695%
84	16.151	2387	2391	2396	rVB	79769	100262	18.29%	1.234%
85	16.215	2397	2402	2407	rBV2	262204	354822	64.71%	4.367%
86	16.904	2515	2519	2527	rVB5	36455	67916	12.39%	0.836%
87	17.351	2591	2595	2599	rBV5	20548	31330	5.71%	0.386%
88	17.809	2669	2673	2678	rBV	21856	37040	6.76%	0.456%

Sum of corrected areas: 8125411

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110117\
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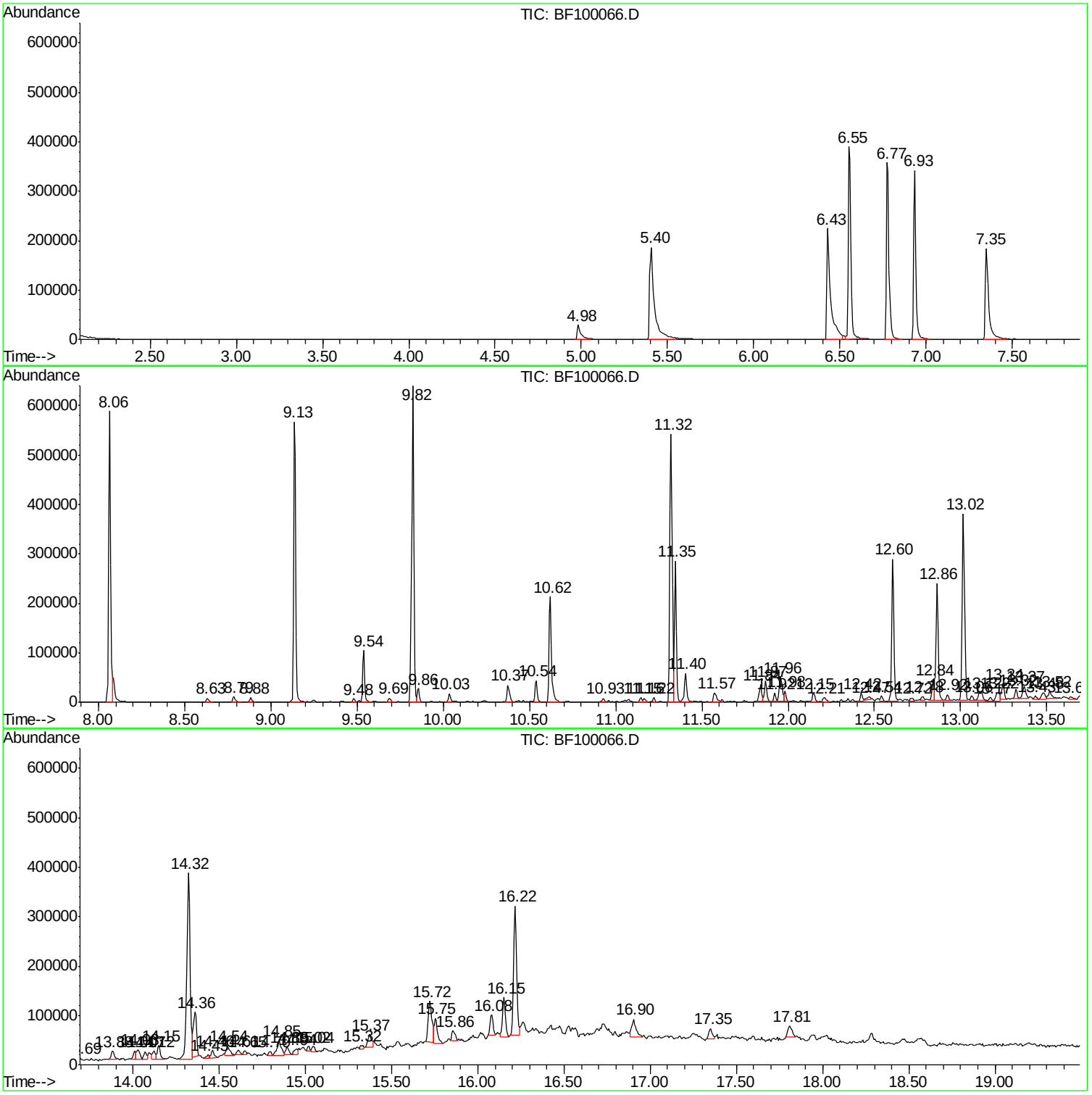
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110117\
Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

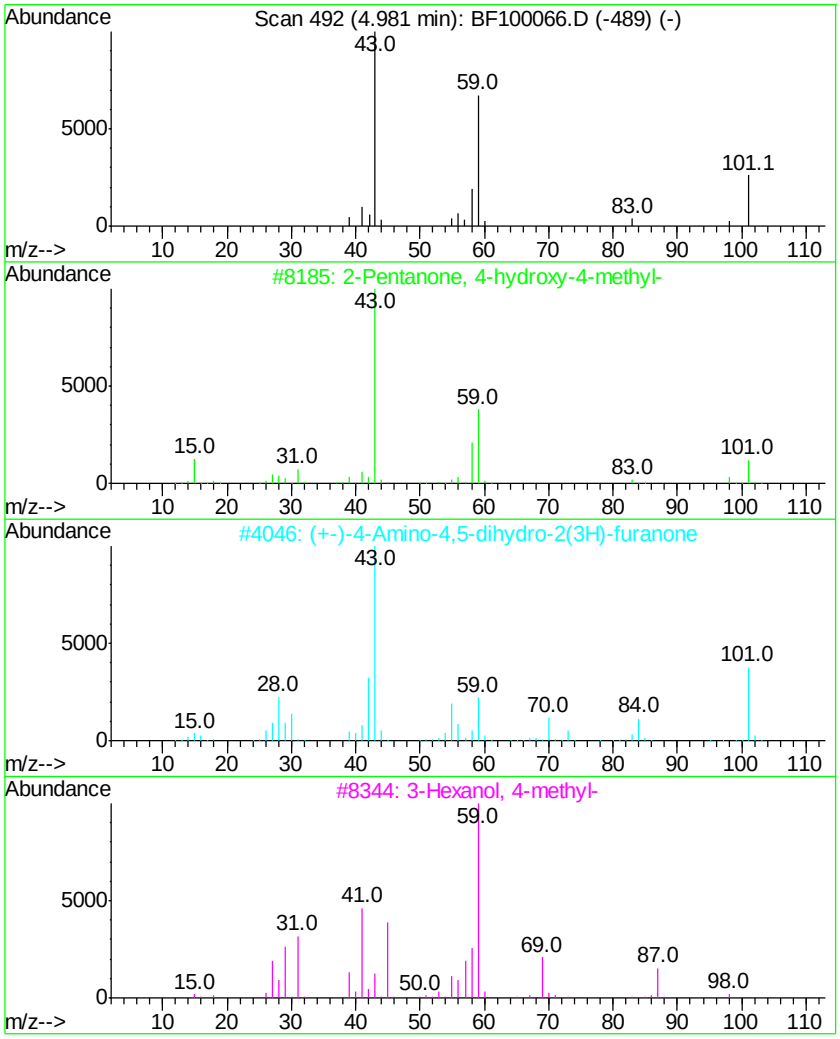
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

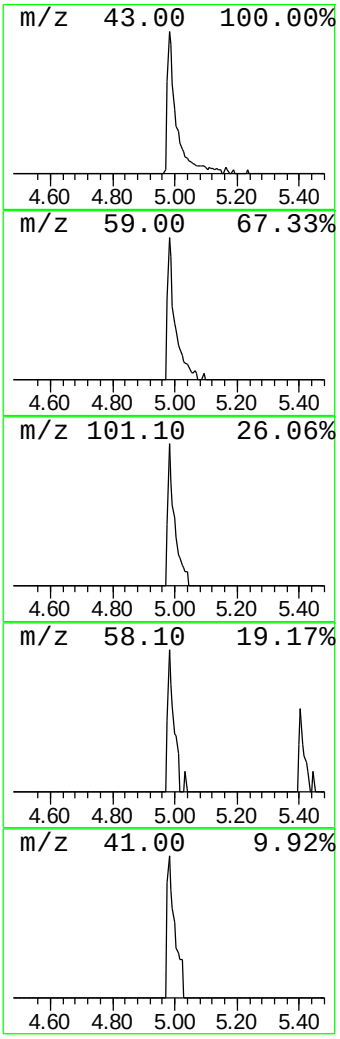
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	2.66 ng	47709	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4	Acetone	58	C3H6O	000067-64-1	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110117\
Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

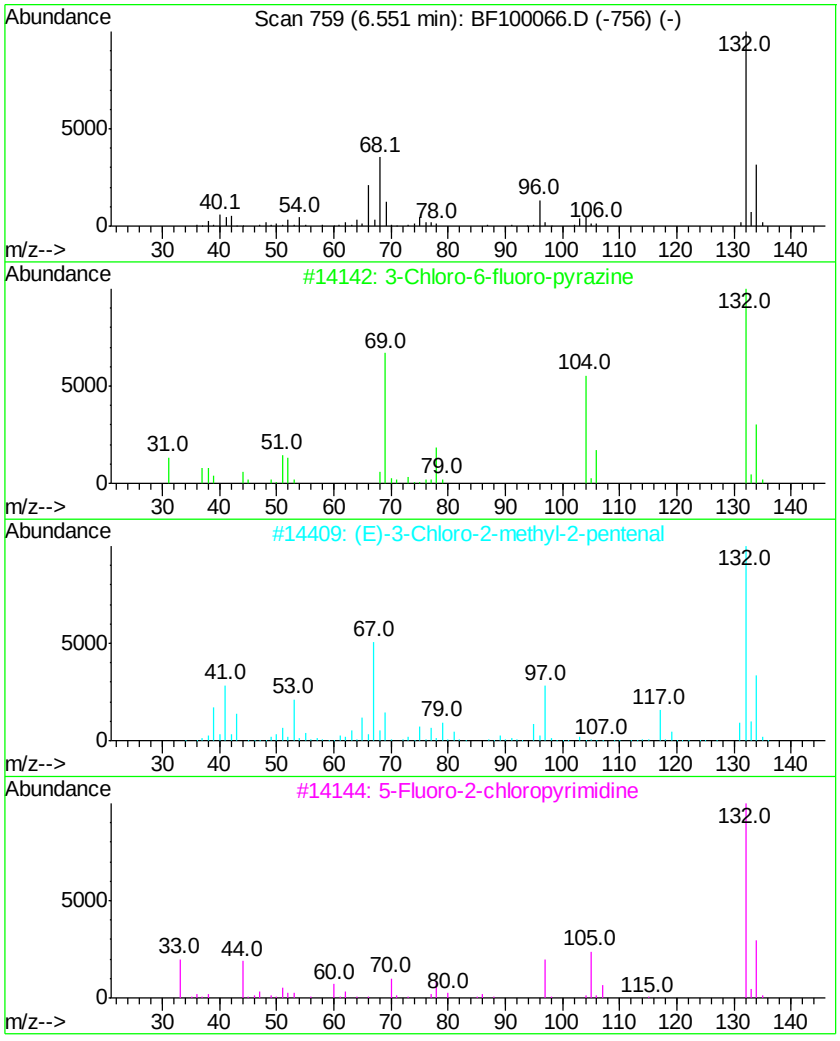
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

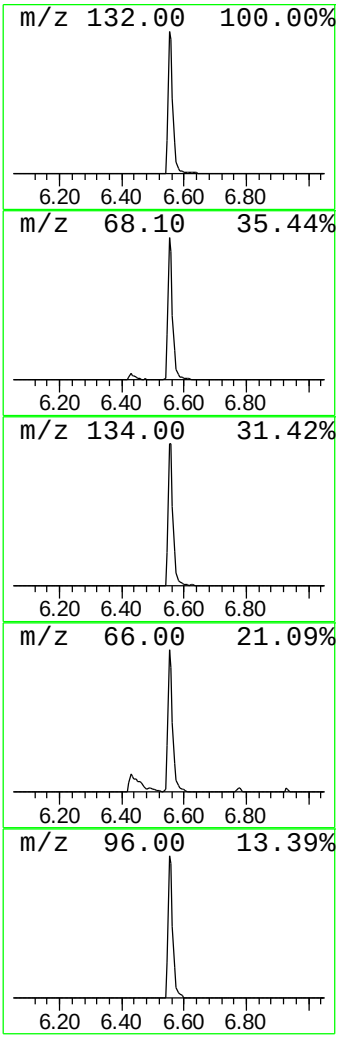
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	24.12 ng	432849	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Aminoindan	133	C9H11N	034698-41-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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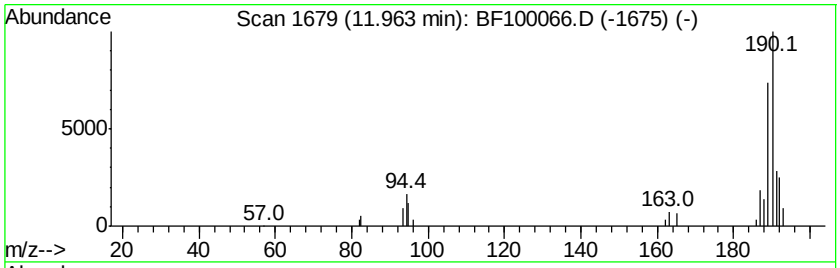
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

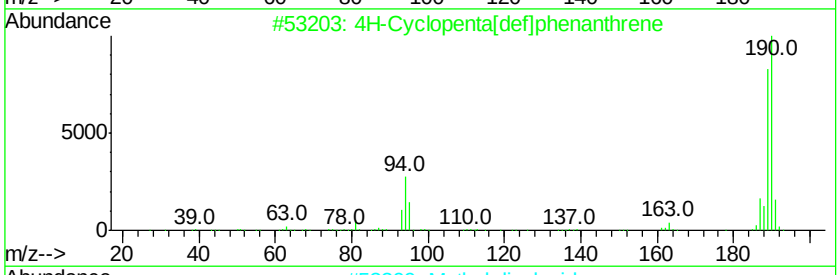
****

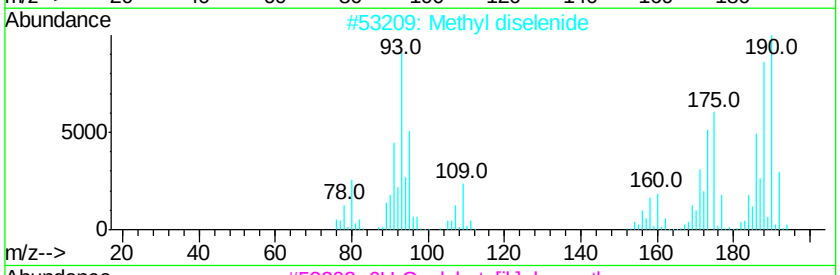
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

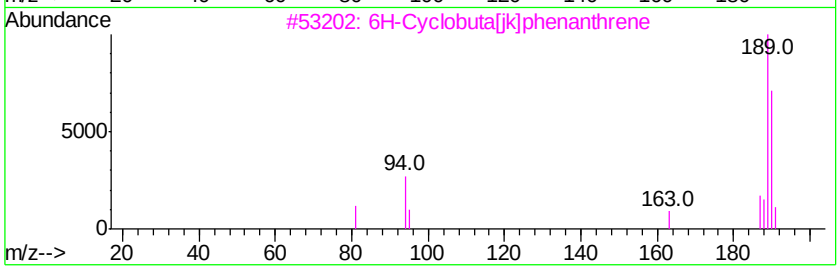
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.38 ng	54825	Phenanthrene-d10	11.32

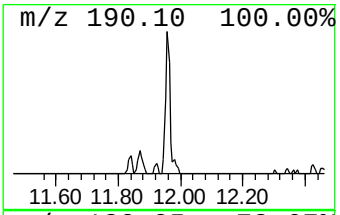
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2	Methyl diselenide	190	C2H6Se2	007101-31-7	49
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	10

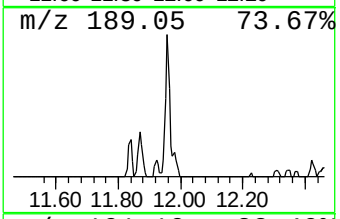


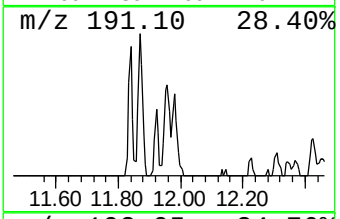


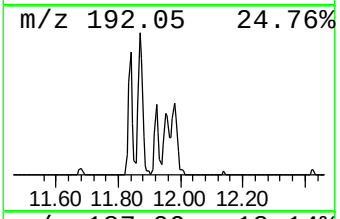


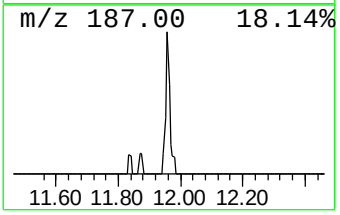












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

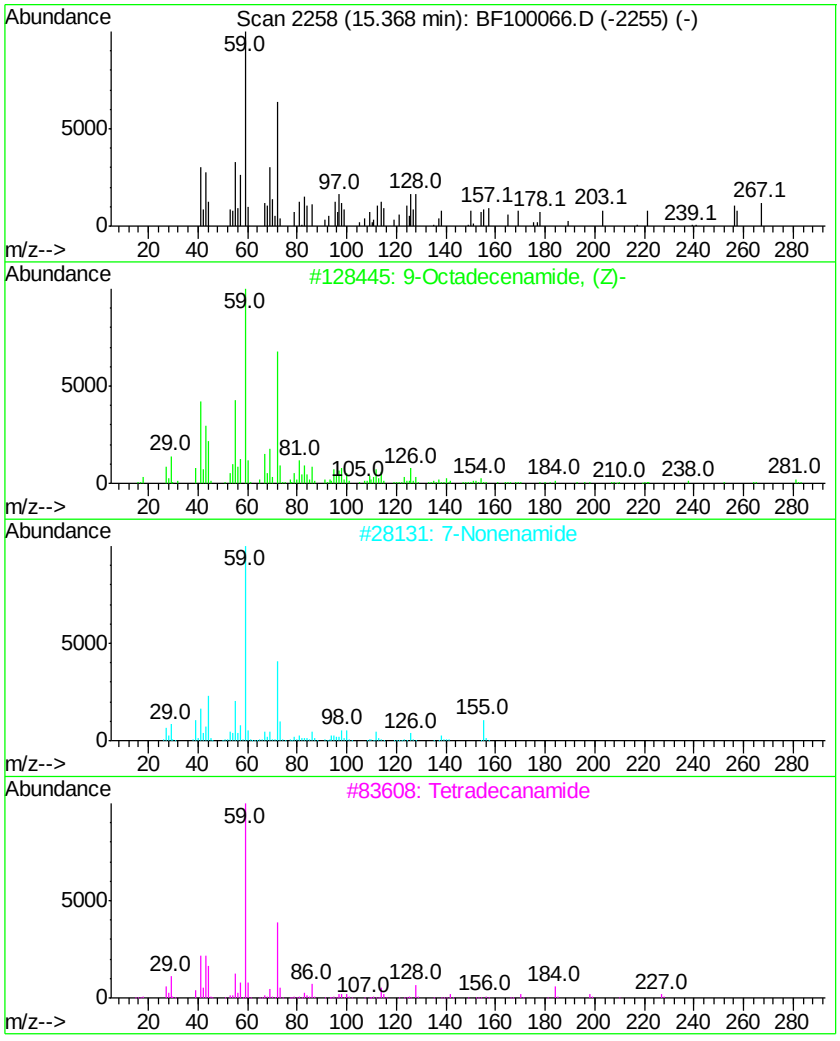
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

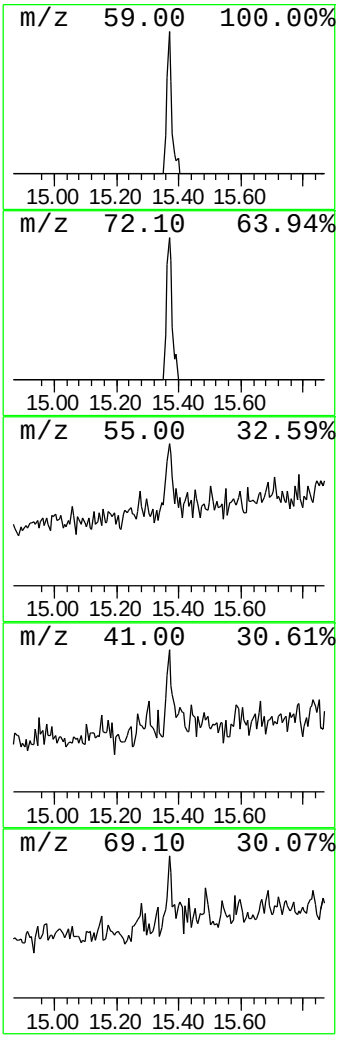
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.10 ng	37344	Perylene-d12	16.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
2	7-Nonenamide	155	C9H17NO	090949-53-4	50
3	Tetradecanamide	227	C14H29NO	000638-58-4	42
4	Dodecanamide	199	C12H25NO	001120-16-7	42
5	Nonanamide	157	C9H19NO	001120-07-6	40





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110117\
Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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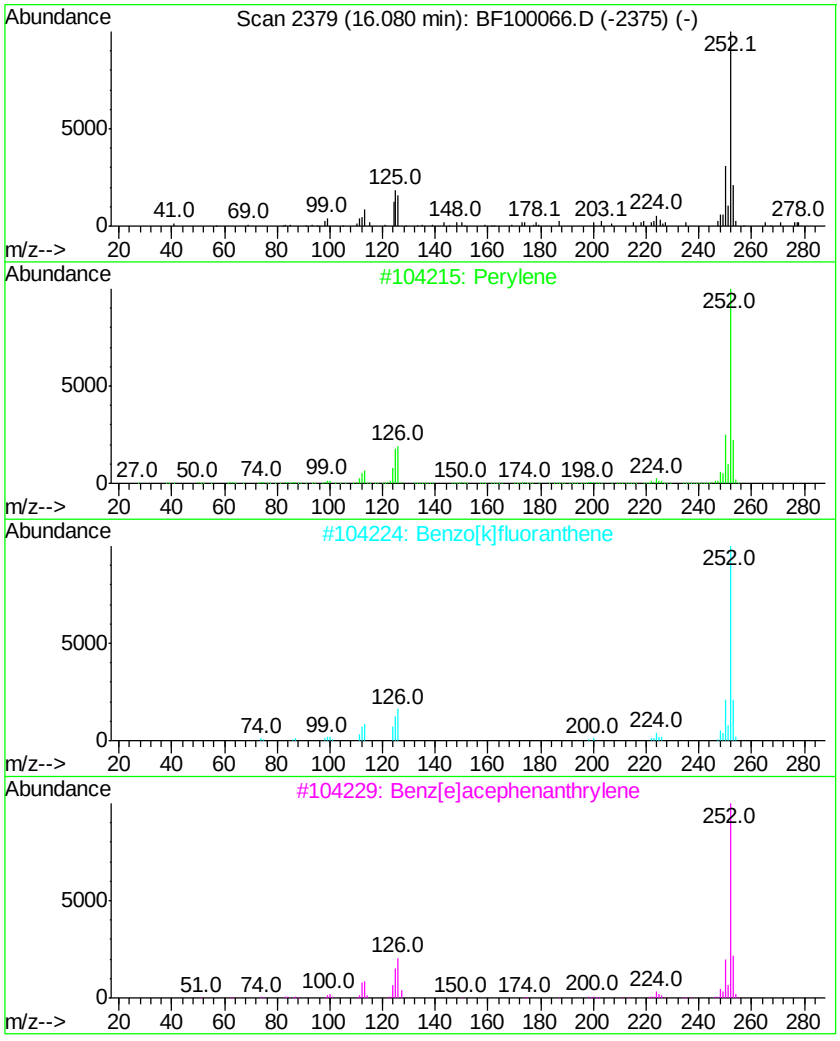
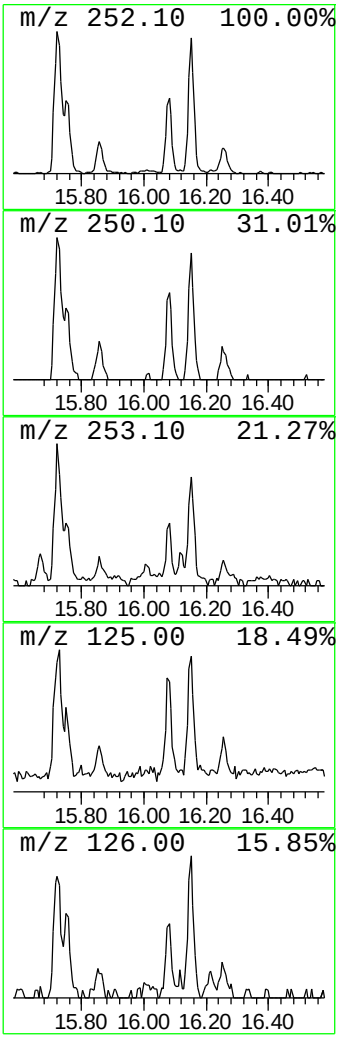
Peak Number 6 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.18 ng	56452	Perylene-d12	16.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[e]pyrene	252	C20H12	000192-97-2	87





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110117\
Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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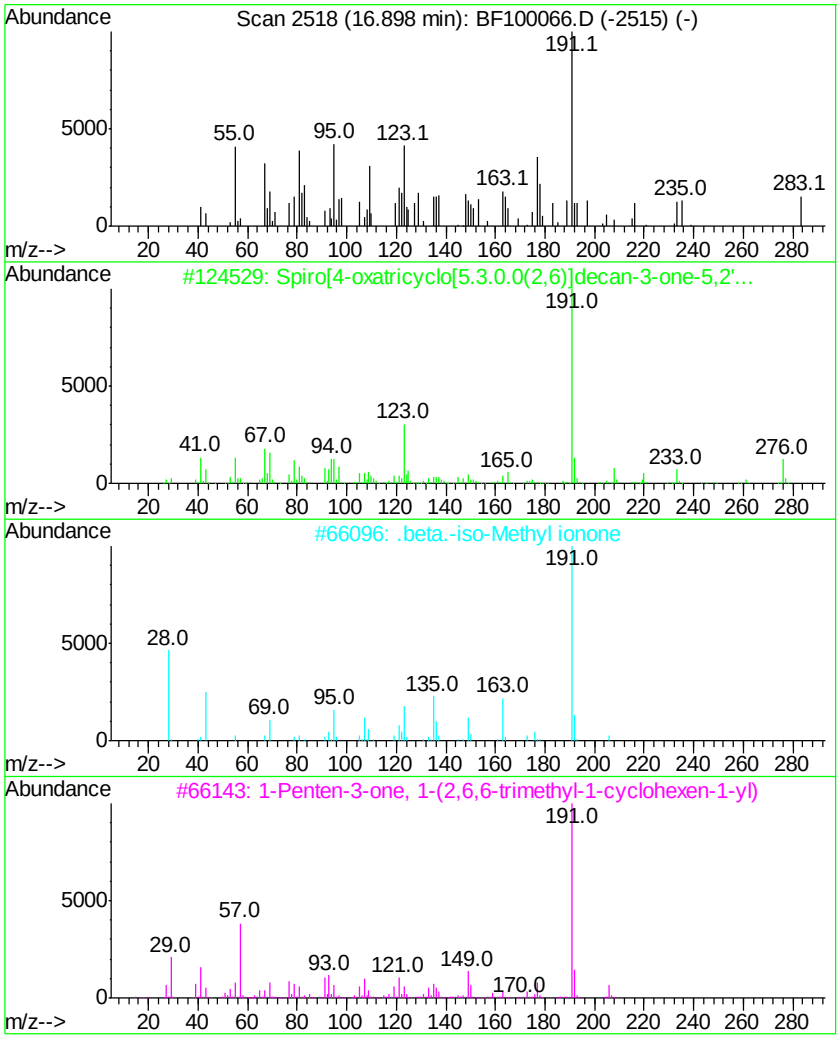
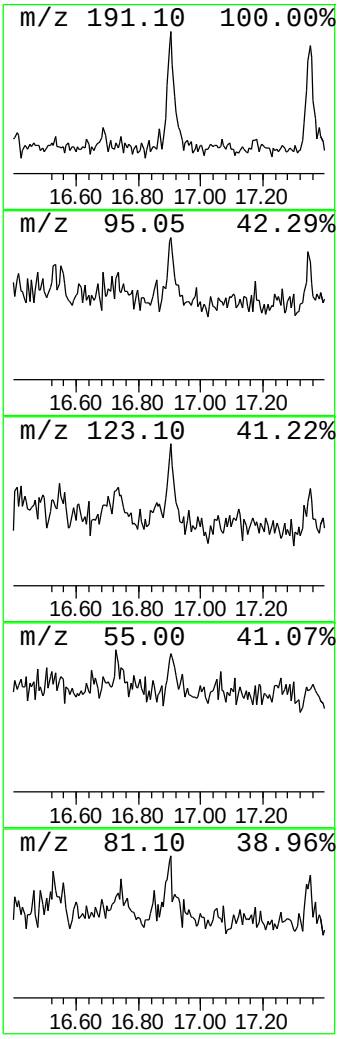
Peak Number 8 unknown16.90 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	3.83 ng	67916	Perylene-d12	16.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[4-oxatricyclo[5.3.0.0(2,6)...	276	C18H28O2	1000156-82-9	38
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	35
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35
4	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	16
5	Pentanoic acid, 4-methyl-2-(2,5-...	278	C13H18N4O3	1000294-63-5	16





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF110117\
Data File : BF100066.D
Acq On : 2 Nov 2017 1:00
Operator : SJ/JU
Sample : I6079-14 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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
2-Pentanone, 4-hy...	4.98	2.7	ng	47709	1	6.78	358847	20.0
unknown6.55	6.55	24.1	ng	432849	1	6.78	358847	20.0
4H-Cyclopenta[def...	11.96	2.4	ng	54825	4	11.32	460810	20.0
9-Octadecenamide,...	15.37	2.1	ng	37344	6	16.22	354822	20.0
Perylene	16.08	3.2	ng	56452	6	16.22	354822	20.0
unknown16.90	16.90	3.8	ng	67916	6	16.22	354822	20.0