LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

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-BF061918.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	5.148	475	478	491	rBV	45466	55815	9.13%	0.805%
2	5.566	546	549	571	rBV	346223	431037	70.48%	6.220%
3	6.578	717	721	735	rBV	318439	410705	67.15%	5.926%
4	6.707	739	743	755	rVV	459526	433873	70.94%	6.260%
5	6.925	777	780	789	rBV	302072	286203	46.80%	4.130%
6	7.084	803	807	819	rBB	407205	350672	57.34%	5.060%
7	7.495	873	877	894	rBV	229928	245442	40.13%	3.542%
8	8.213	995	999	1018	rBV	320099	327830	53.60%	4.730%
9	9.283	1178	1181	1191	rBV	408730	445068	72.77%	6.422%
10	9.683	1247	1249	1257	rVB	47522	46189	7.55%	0.666%
11	9.842	1272	1276	1280	rBV	20675	21006	3.43%	0.303%
12	9.977	1295	1299	1311	rVB	357260	335831	54.91%	4.846%
13	10.530	1390	1393	1399	rVB2	10116	11939	1.95%	0.172%
14	10.777	1431	1435	1446	rBV	254458	257700	42.14%	3.718%
15	11.471	1550	1553	1556	rBV	402173	385304	63.00%	5.560%
16	11.495	1556	1557	1561	rVV	103601	82261	13.45%	1.187%
17	11.554	1564	1567	1570	rBV	22583	22385	3.66%	0.323%
18	11.719	1590	1595	1596	rBV2	6478	7746	1.27%	0.112%
19	11.807	1606	1610	1614	rBV2	9427	10378	1.70%	0.150%
20	11.895	1620	1625	1629	rVB3	10148	11765	1.92%	0.170%
21	11.977	1635	1639	1642	rBV	36287	37908	6.20%	0.547%
22	12.007	1642	1644	1649	rVB	43549	36695	6.00%	0.529%
23	12.054	1649	1652	1655	rBV	14348	15971	2.61%	0.230%
24	12.089	1655	1658	1660	rBV2	41785	44736	7.31%	0.646%
25	12.113	1660	1662	1665	rVB	26345	20659	3.38%	0.298%
26	12.266	1686	1688	1691	rBV	15607	16591	2.71%	0.239%
27	12.313	1693	1696	1699	rVB5	12638	15120	2.47%	0.218%
28	12.401	1709	1711	1713	rBV3	9671	10258	1.68%	0.148%
29	12.454	1717	1720	1722	rVV	16815	14041	2.30%	0.203%
30	12.477	1722	1724	1728	rVB3	17621	14140	2.31%	0.204%
31	12.524	1728	1732	1735	rBV	48850	51242	8.38%	0.739%
32	12.566	1735	1739	1741	rVV3	16601	22529	3.68%	0.325%
33	12.583	1741	1742	1744	rVB	14002	7829	1.28%	0.113%
34	12.630	1744	1750	1757	rVB3	18224	36322	5.94%	0.524%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.695	1757	1761	1765	rBV	193362	171029	27.96%	2.468%
36	12.795	1775	1778	1780	rBV	13365	13039	2.13%	0.188%
37	12.842	1783	1786	1789	rBV3	16198	22080	3.61%	0.319%
38	12.865	1789	1790	1794	rVB4	13094	8583	1.40%	0.124%
39	12.907	1794	1797	1798	rBV2	31263	30945	5.06%	0.447%
40	12.930	1798	1801	1806	rVB	193797	199174	32.57%	2.874%
41	12.977	1806	1809	1811	rBV	26596	26166	4.28%	0.378%
42	13.054	1819	1822	1826	rBV	689183	611584	100.00%	8.825%
43	13.083	1826	1827	1833	rVB6	11915	14543	2.38%	0.210%
44	13.148	1833	1838	1842	rBV4	27413	54282	8.88%	0.783%
45	13.189	1843	1845	1849	rBV4	10671	11155	1.82%	0.161%
46	13.236	1849	1853	1854	rBV4	29028	37427	6.12%	0.540%
47	13.254	1854	1856	1861	rVB2	39711	38698	6.33%	0.558%
48	13.318	1865	1867	1870	rBV	13983	11465	1.87%	0.165%
49	13.360	1871	1874	1877	rBV2	31054	32149	5.26%	0.464%
50	13.454	1888	1890	1893	rBV	34437	34009	5.56%	0.491%
51	13.489	1893	1896	1898	rVV	30817	30093	4.92%	0.434%
52	13.601	1913	1915	1918	rBV2	18389	18966	3.10%	0.274%
53	13.883	1961	1963	1965	rBV2	24292	19996	3.27%	0.289%
54	13.942	1969	1973	1978	rBV4	59359	97065	15.87%	1.401%
55	14.136	2001	2006	2009	rBV2	501256	565311	92.43%	8.157%
56	14.160	2009	2010	2016	rVB	92667	64687	10.58%	0.933%
57	14.560	2076	2078	2081	rBV	39396	36329	5.94%	0.524%
58	15.677	2264	2268	2273	rBV	195256	258406	42.25%	3.729%

Sum of corrected areas: 6930371

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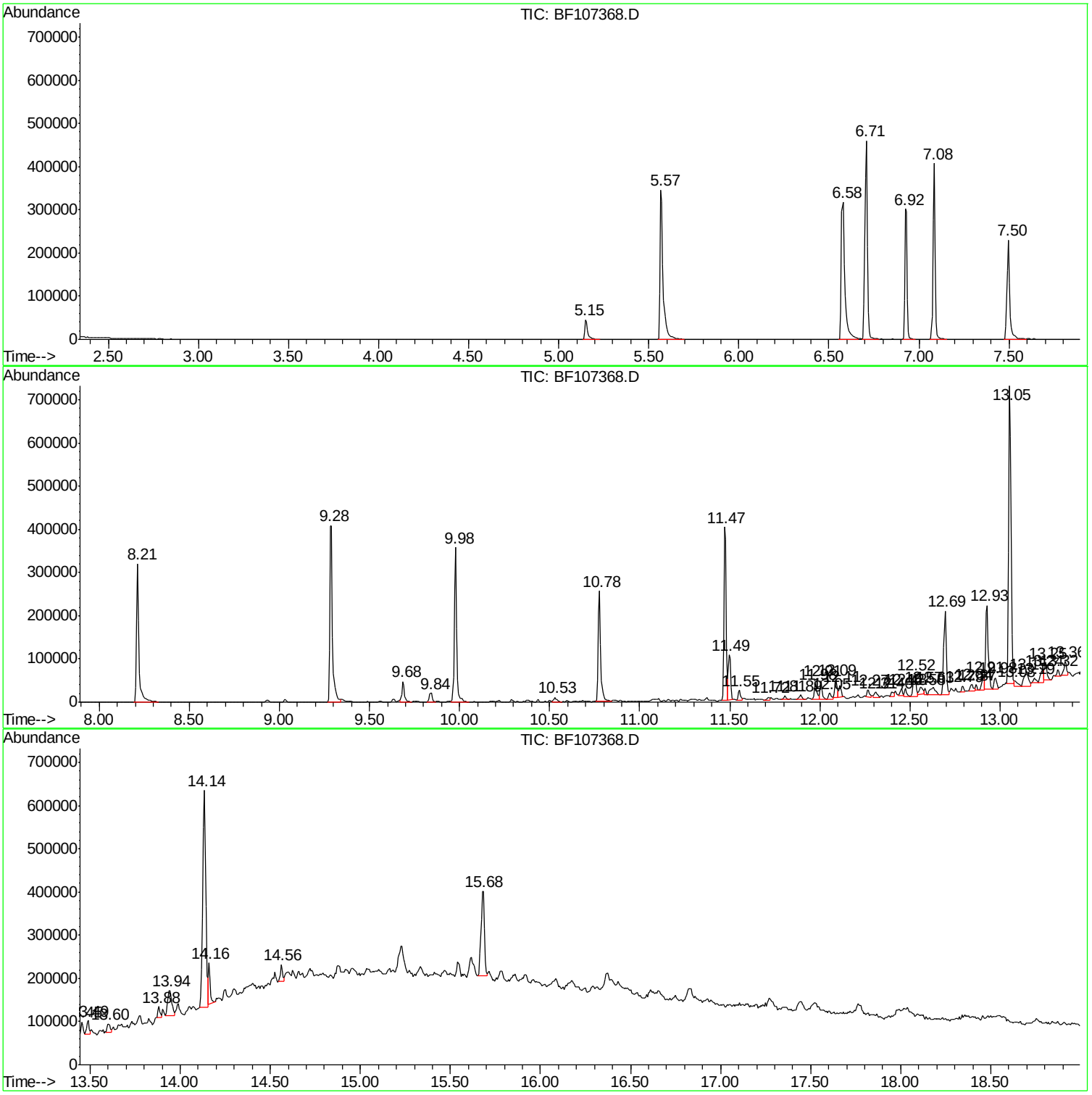
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

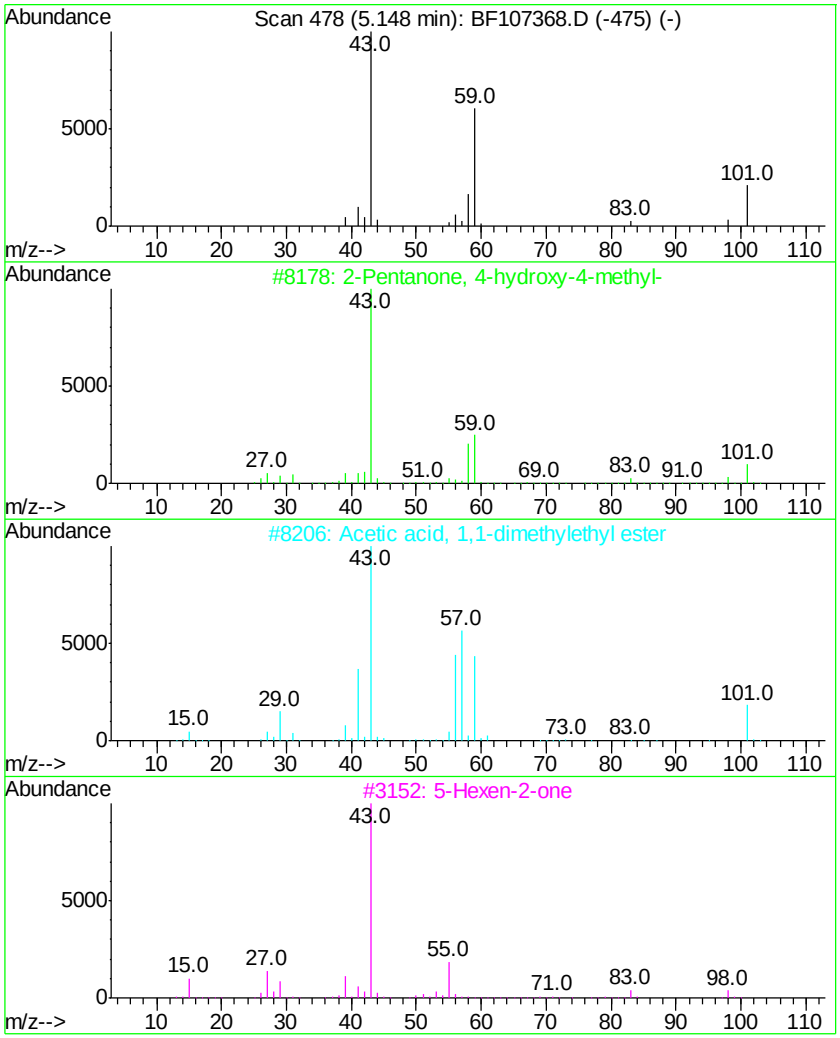
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

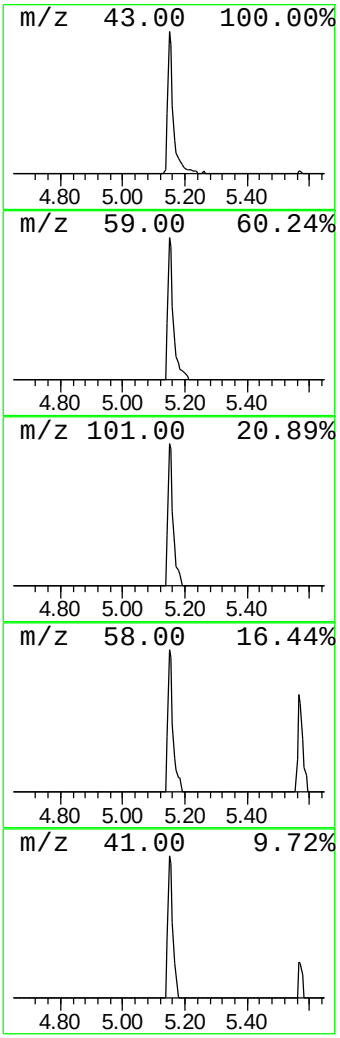
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	3.90 ng	55815	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	3-Octanol	130	C8H18O	000589-98-0	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

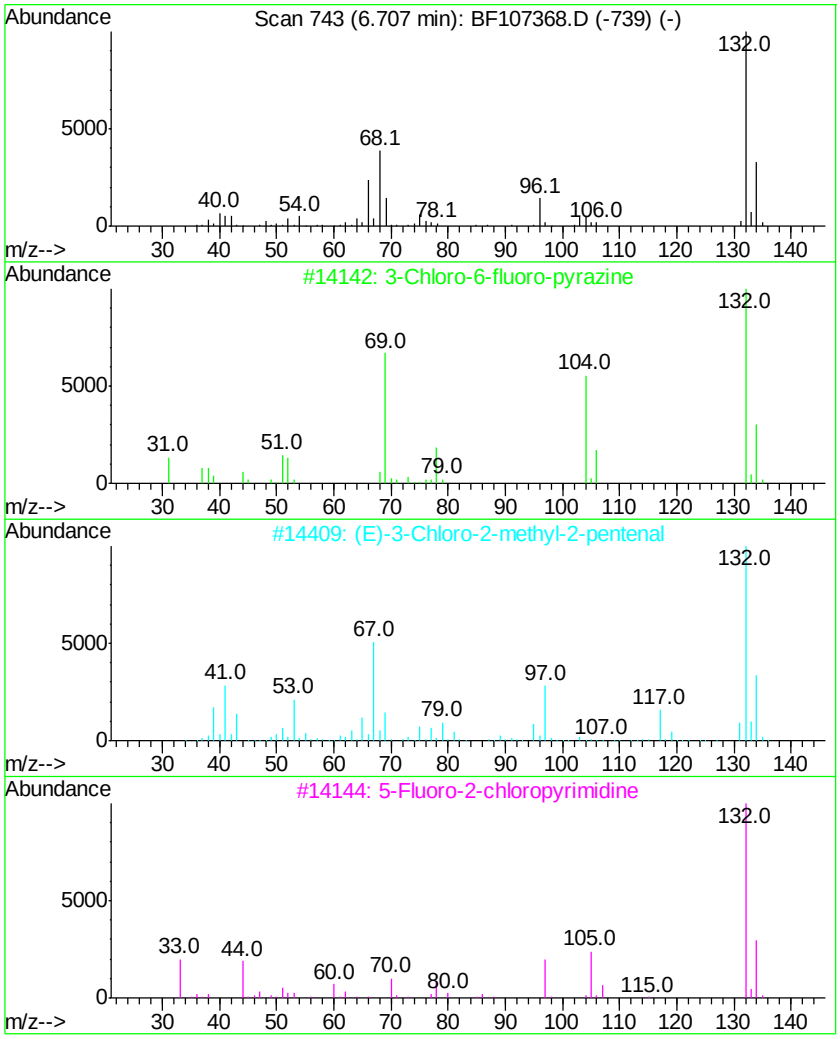
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

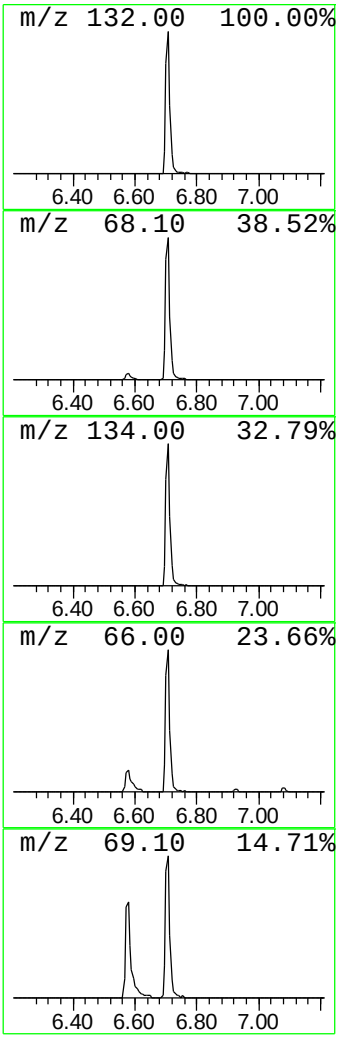
****

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	30.32 ng	433873	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

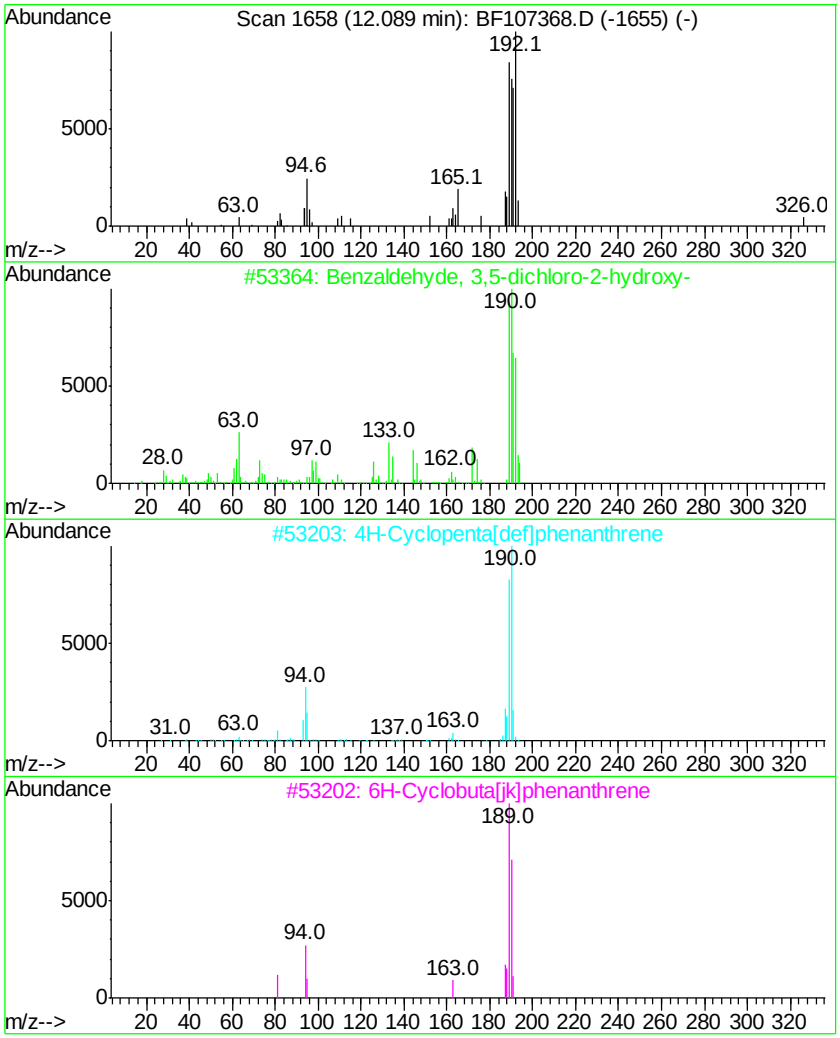
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

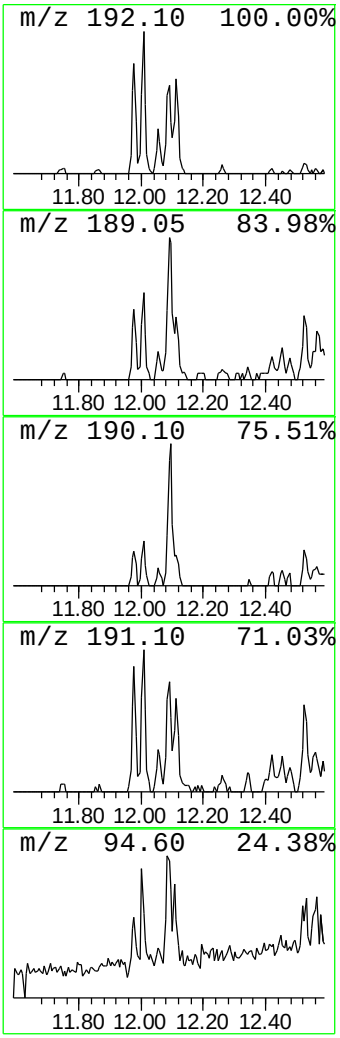
****

Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	2.32 ng	44736	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	58
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

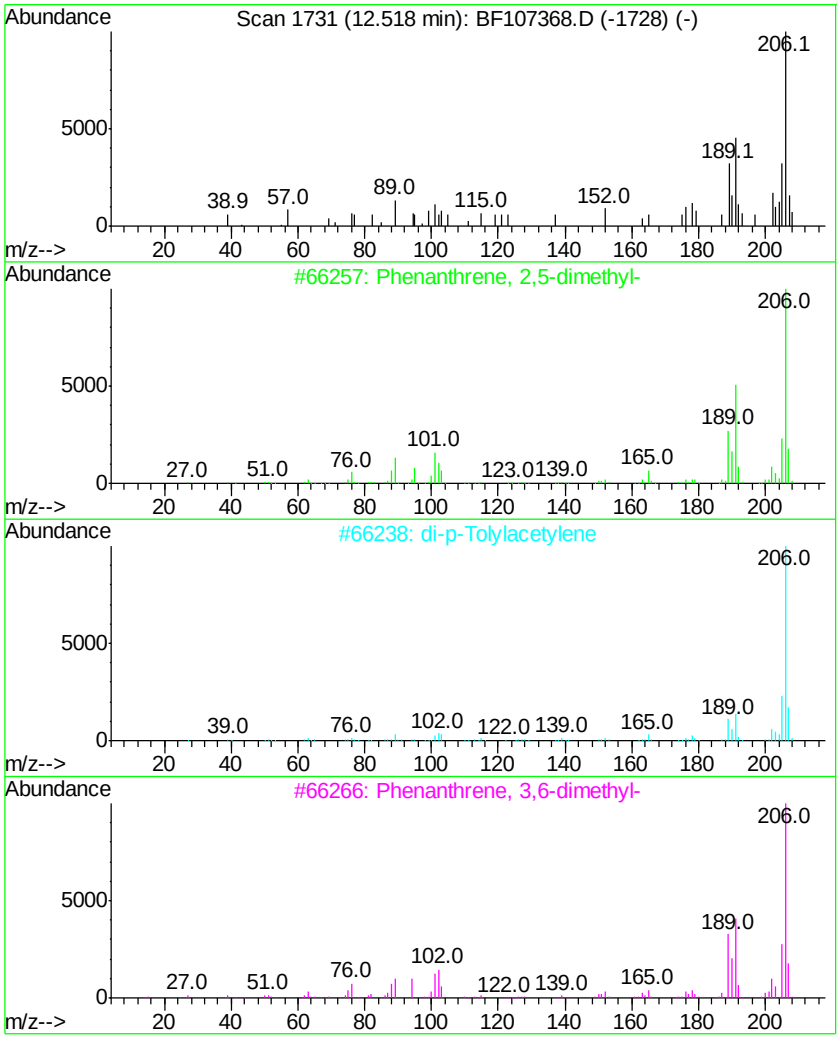
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

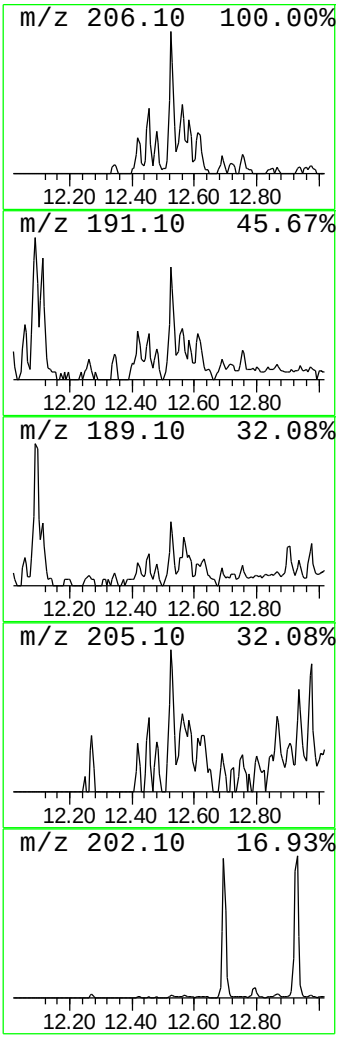
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	2.66 ng	51242	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	94
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

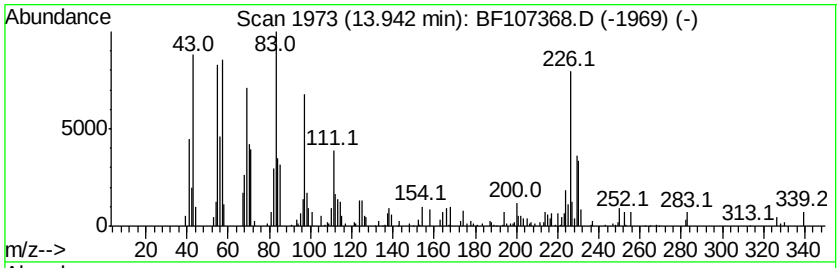
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

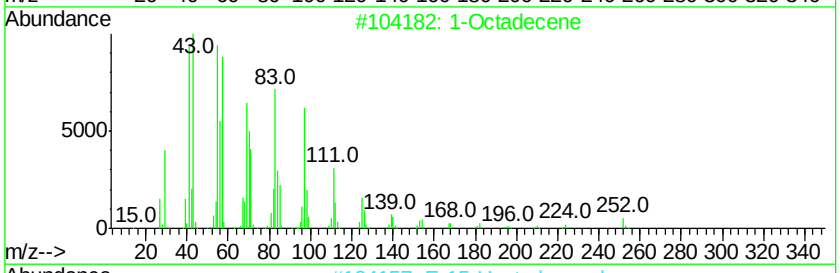
****

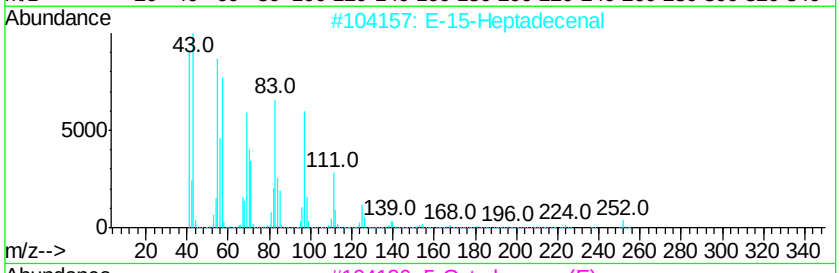
Peak Number 6 1-Octadecene Concentration Rank 4

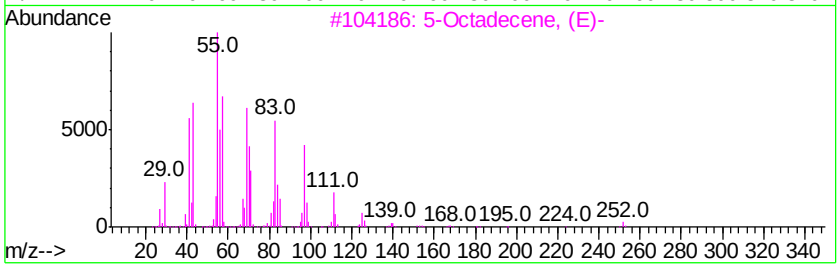
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.43 ng	97065	Chrysene-d12	14.14

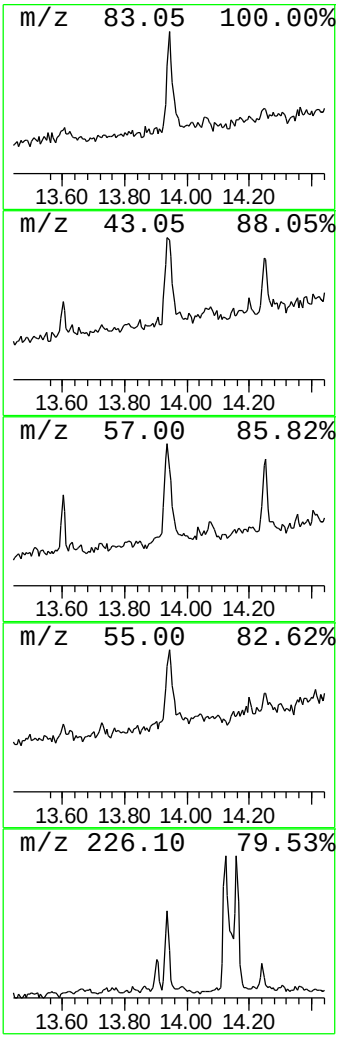
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	95
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	94
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	84
4	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	83
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	68











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071318\
Data File : BF107368.D
Acq On : 13 Jul 2018 15:42
Operator : JU/SJ
Sample : J3825-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-071118-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.15	3.9	ng	55815	1	6.93	286203	20.0
unknown6.71	6.71	30.3	ng	433873	1	6.93	286203	20.0
Benzaldehyde, 3,5...	12.09	2.3	ng	44736	4	11.47	385304	20.0
Phenanthrene, 2,5...	12.52	2.7	ng	51242	4	11.47	385304	20.0
1-Octadecene	13.94	3.4	ng	97065	5	14.14	565311	20.0