LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	5.016	495	498	522	rBV	539321	939936	25.06%	2.537%
2	5.422	563	567	593	rBV	2912088	3655445	97.45%	9.867%
3	6.445	736	741	758	rBV	2967492	3751271	100.00%	10.126%
4	6.569	758	762	769	rVV	3215073	3315294	88.38%	8.949%
5	6.798	797	801	809	rBV	843803	796708	21.24%	2.151%
6	6.951	823	827	840	rBV	2824622	2773960	73.95%	7.488%
7	7.369	893	898	915	rBV	2238023	2327227	62.04%	6.282%
8	8.080	1015	1019	1020	rBV	965400	912213	24.32%	2.462%
9	8.098	1020	1022	1029	rVV	1153911	1092746	29.13%	2.950%
10	8.157	1029	1032	1040	rVB	40212	51411	1.37%	0.139%
11	8.792	1137	1140	1147	rBV	132622	129508	3.45%	0.350%
12	8.892	1154	1157	1163	rVB	70661	66491	1.77%	0.179%
13	9.151	1196	1201	1205	rBV	3284410	3233686	86.20%	8.729%
14	9.222	1210	1213	1216	rVV	43931	39302	1.05%	0.106%
15	9.257	1216	1219	1224	rVB	61823	58784	1.57%	0.159%
16	9.545	1265	1268	1275	rVB	425616	432111	11.52%	1.166%
17	9.698	1290	1294	1299	rBV	253836	228708	6.10%	0.617%
18	9.751	1299	1303	1306	rVV	101913	77037	2.05%	0.208%
19	9.833	1311	1317	1321	rVV	949877	854321	22.77%	2.306%
20	9.869	1321	1323	1330	rVB	63478	61545	1.64%	0.166%
21	10.039	1349	1352	1356	rBV	185817	172820	4.61%	0.466%
22	10.251	1385	1388	1391	rVB	101587	84008	2.24%	0.227%
23	10.380	1407	1410	1419	rVB	265852	270425	7.21%	0.730%
24	10.627	1447	1452	1465	rBV	1531273	1545396	41.20%	4.172%
25	10.721	1465	1468	1479	rVB	87715	95617	2.55%	0.258%
26	10.933	1498	1504	1515	rVB5	25905	44832	1.20%	0.121%
27	11.221	1551	1553	1557	rVB	65017	51749	1.38%	0.140%
28	11.321	1567	1570	1572	rBV	783914	706742	18.84%	1.908%
29	11.345	1572	1574	1579	rVV	1020859	960884	25.61%	2.594%
30	11.404	1579	1584	1589	rVB	312618	309988	8.26%	0.837%
31	11.563	1607	1611	1615	rBV	167559	159085	4.24%	0.429%
32	11.827	1649	1656	1659	rBV2	62065	95034	2.53%	0.257%
33	11.857	1659	1661	1666	rVB	68843	70024	1.87%	0.189%
34	11.939	1672	1675	1678	rBV	138789	129389	3.45%	0.349%

LSC Area Percent Report

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Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.121	1703	1706	1709	rVB	45791	38347	1.02%	0.104%
36	12.539	1773	1777	1781	rBV	896491	783314	20.88%	2.114%
37	12.639	1790	1794	1799	rVB	105365	95578	2.55%	0.258%
38	12.774	1810	1817	1822	rBV	607936	673044	17.94%	1.817%
39	12.904	1835	1839	1843	rBV	2497056	2514390	67.03%	6.787%
40	12.980	1849	1852	1857	rBV3	24911	43281	1.15%	0.117%
41	13.098	1865	1872	1877	rBV	114360	154395	4.12%	0.417%
42	13.162	1880	1883	1887	rVV	111938	108720	2.90%	0.293%
43	13.721	1975	1978	1980	rBV	46126	46034	1.23%	0.124%
44	13.745	1980	1982	1984	rVV	52852	48777	1.30%	0.132%
45	13.786	1984	1989	1999	rVB5	316846	468688	12.49%	1.265%
46	13.968	2015	2020	2023	rBV2	953910	1194702	31.85%	3.225%
47	13.998	2023	2025	2031	rVB	264876	245540	6.55%	0.663%
48	15.015	2194	2198	2200	rBV	173824	242322	6.46%	0.654%
49	15.315	2246	2249	2256	rVB	98091	124088	3.31%	0.335%
50	15.374	2256	2259	2263	rBV	141072	186458	4.97%	0.503%
51	15.439	2266	2270	2274	rBV	492744	584895	15.59%	1.579%

Sum of corrected areas: 37046270

LSC Report - Integrated Chromatogram

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Data File : BF101611.D
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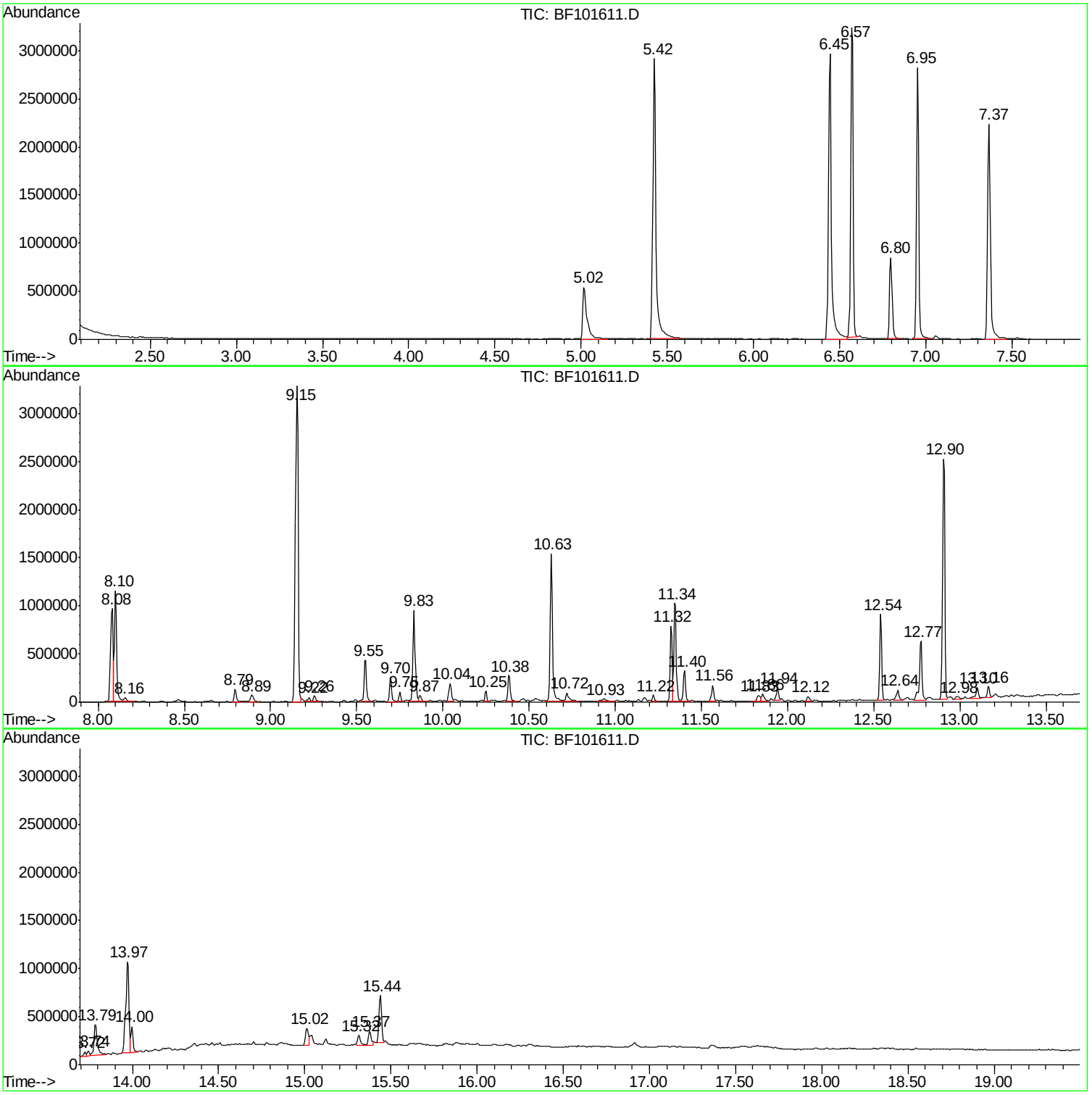
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

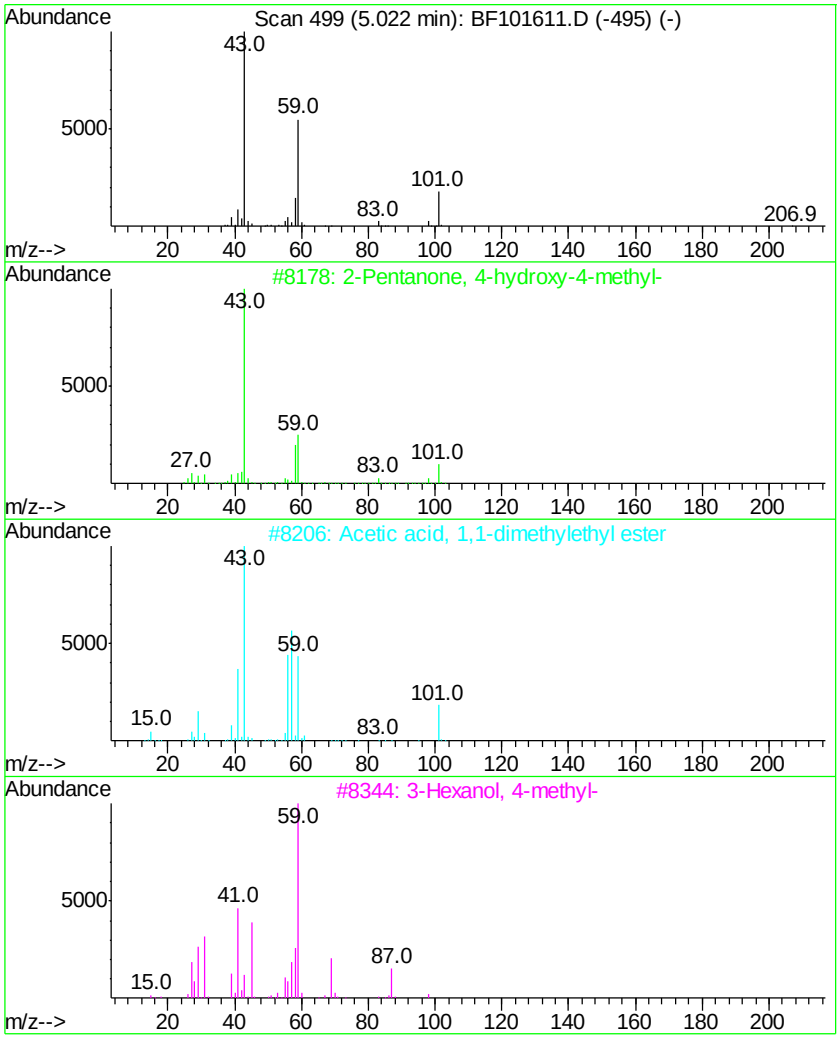
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

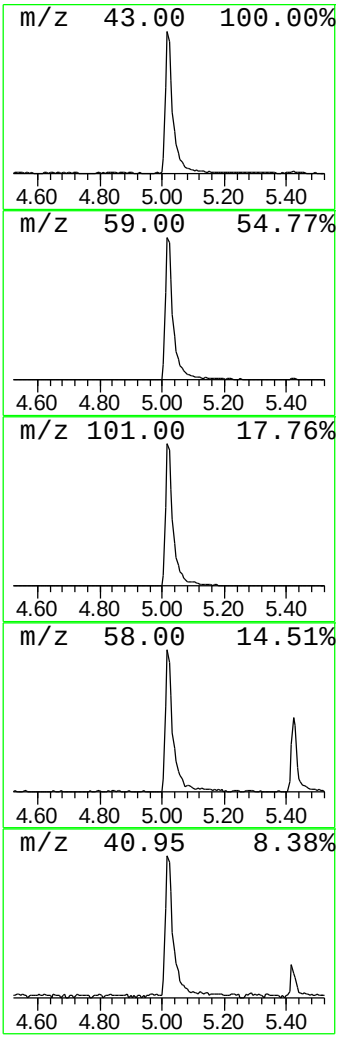
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	23.60 ng	939936	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

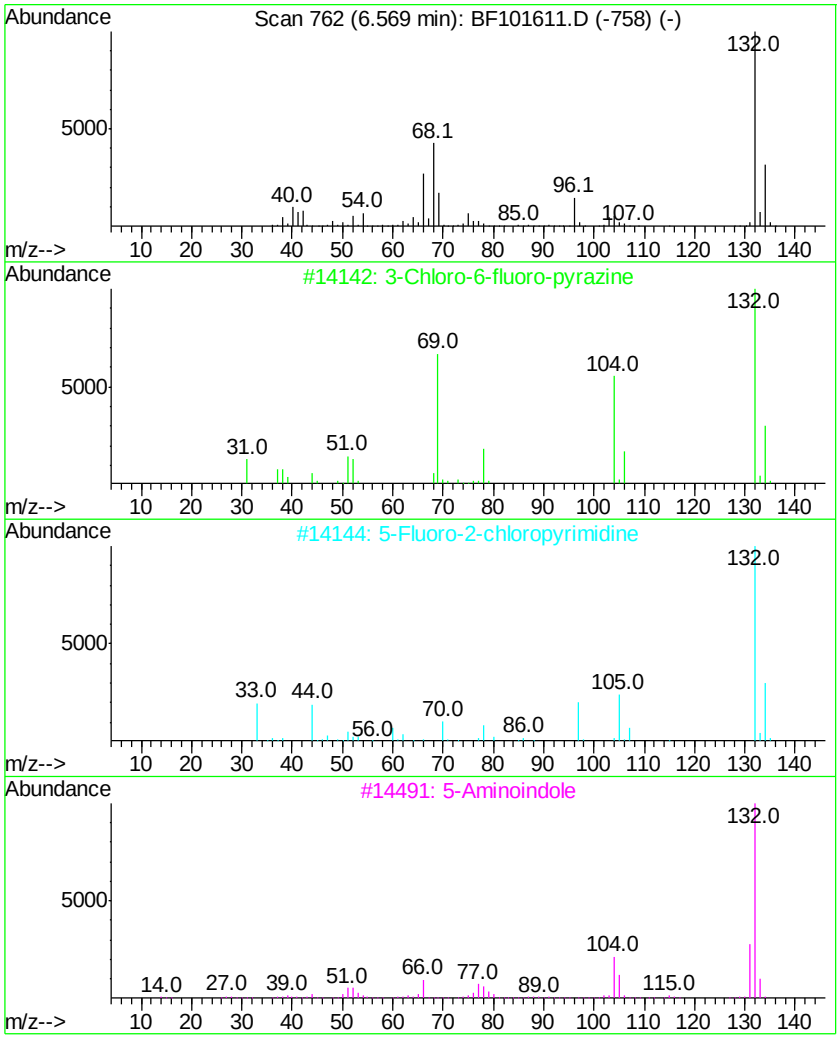
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

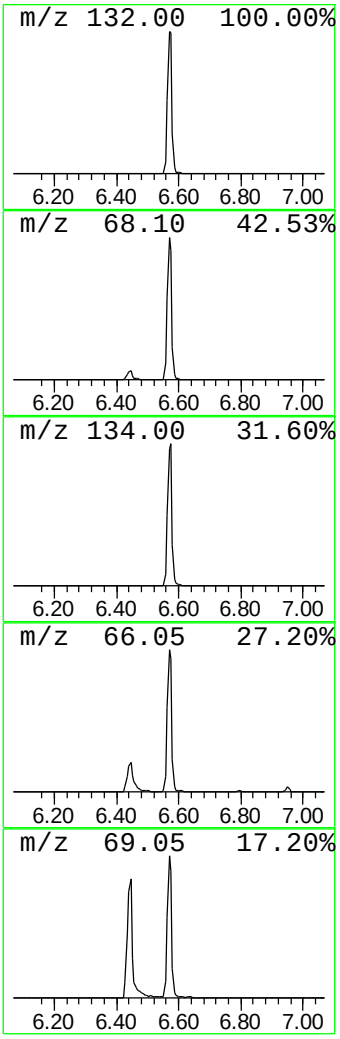
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	83.22 ng	3315290	1,4-Dichlorobenzene-d4	6.80

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

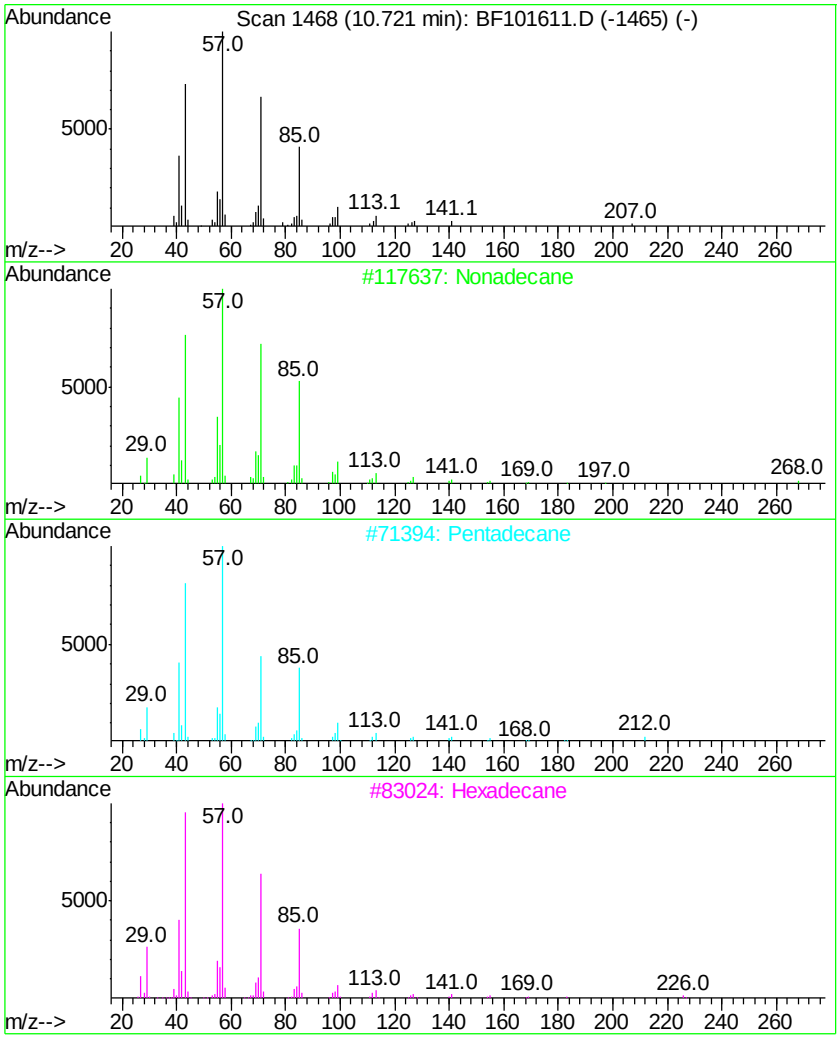
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

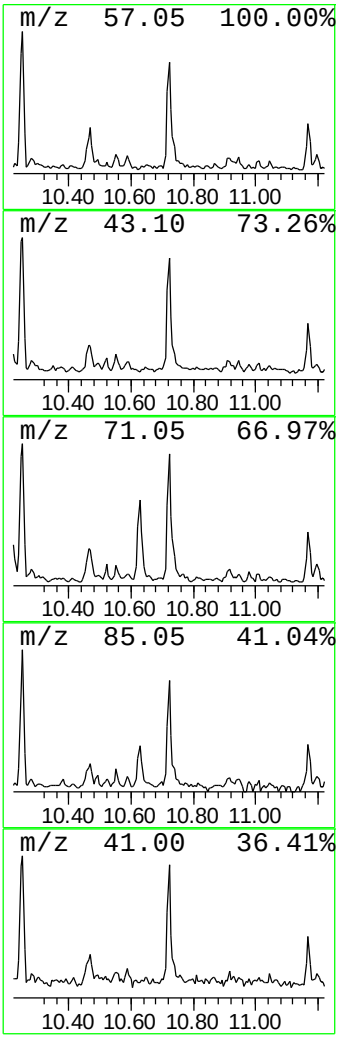
****

Peak Number 4 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.71 ng	95617	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Pentadecane	212	C15H32	000629-62-9	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Tetradecane	198	C14H30	000629-59-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

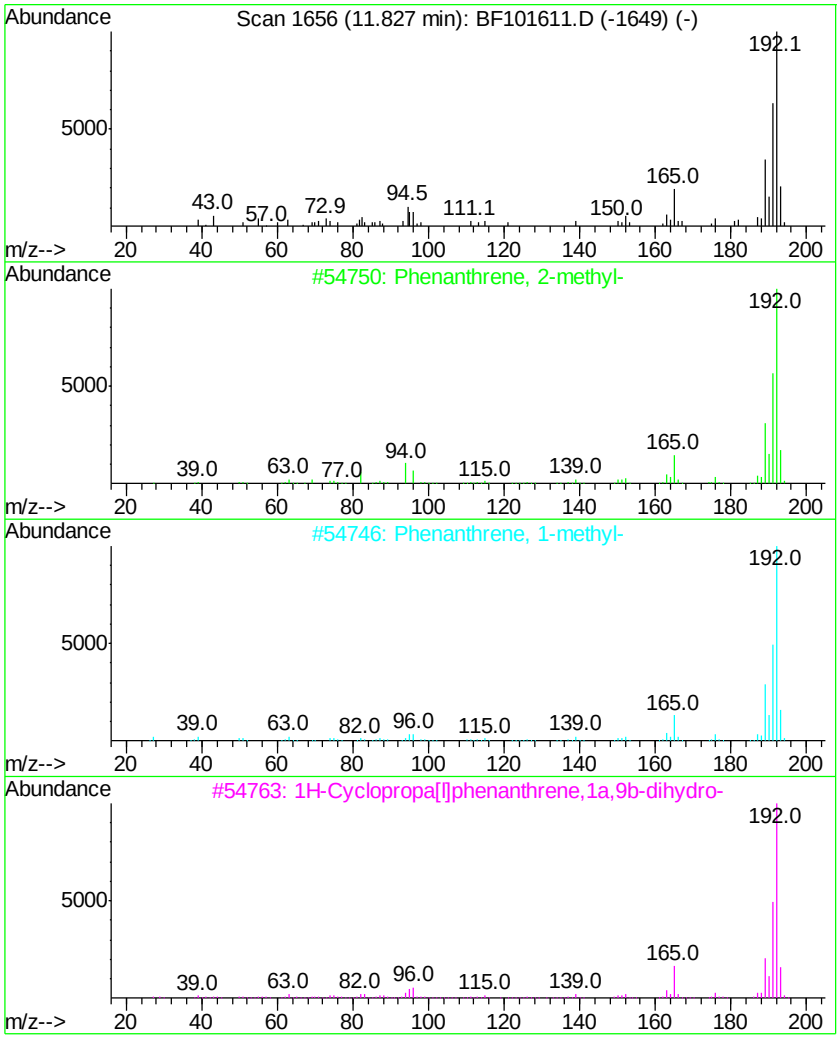
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

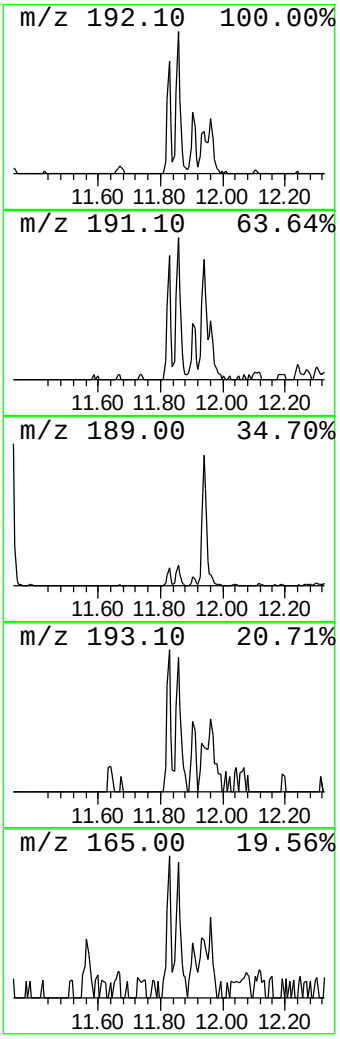
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.69 ng	95034	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93





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Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

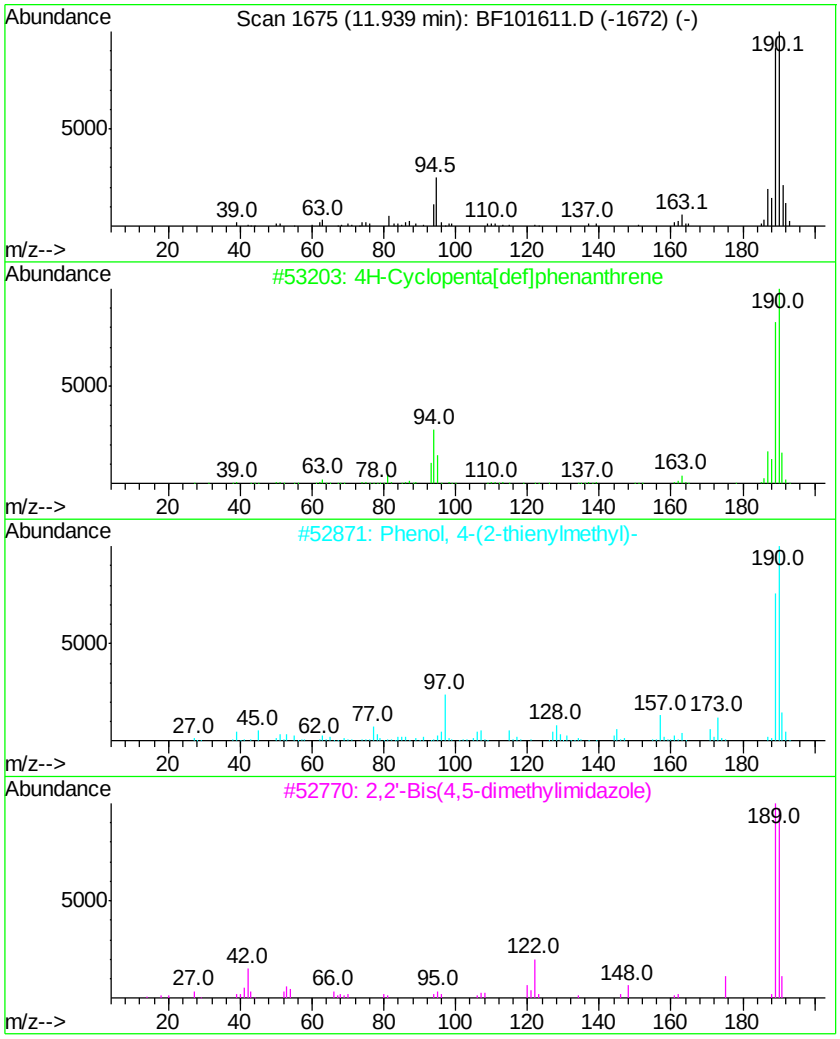
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

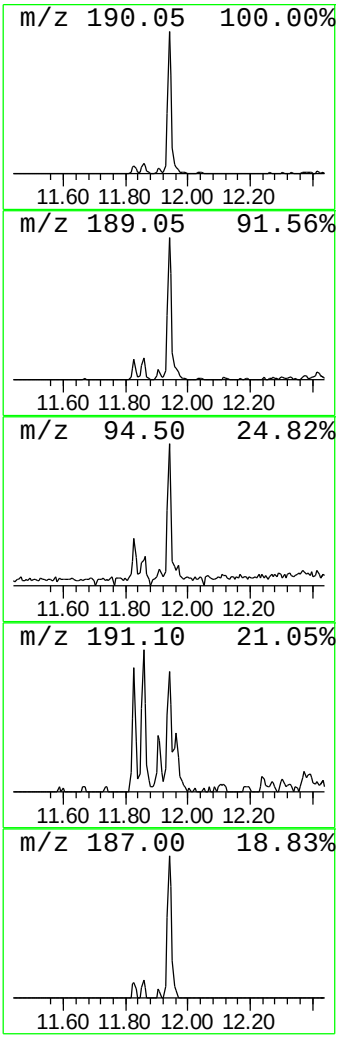
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.66 ng	129389	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	97
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	42
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	23





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Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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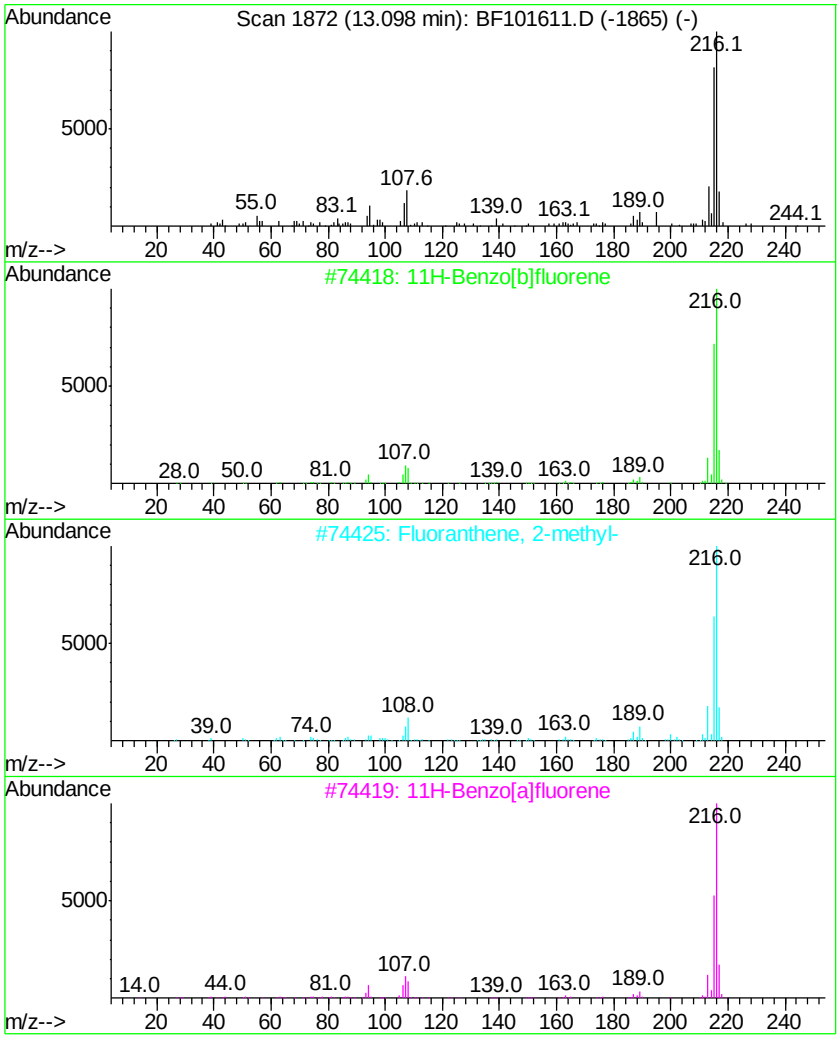
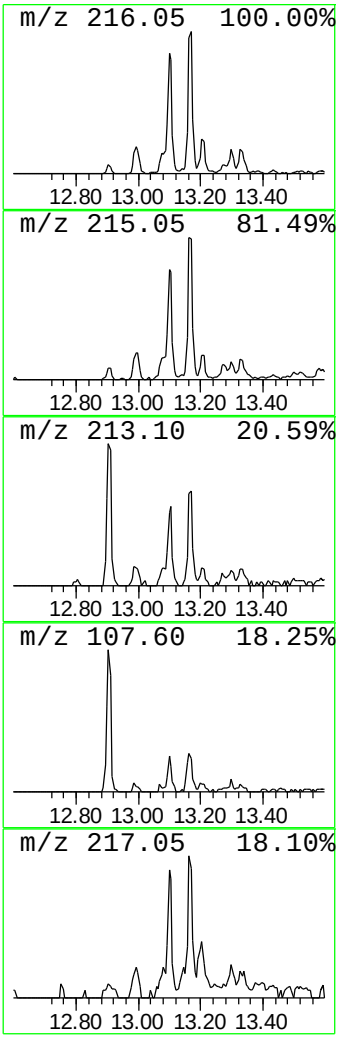
Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	2.58 ng	154395	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93





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Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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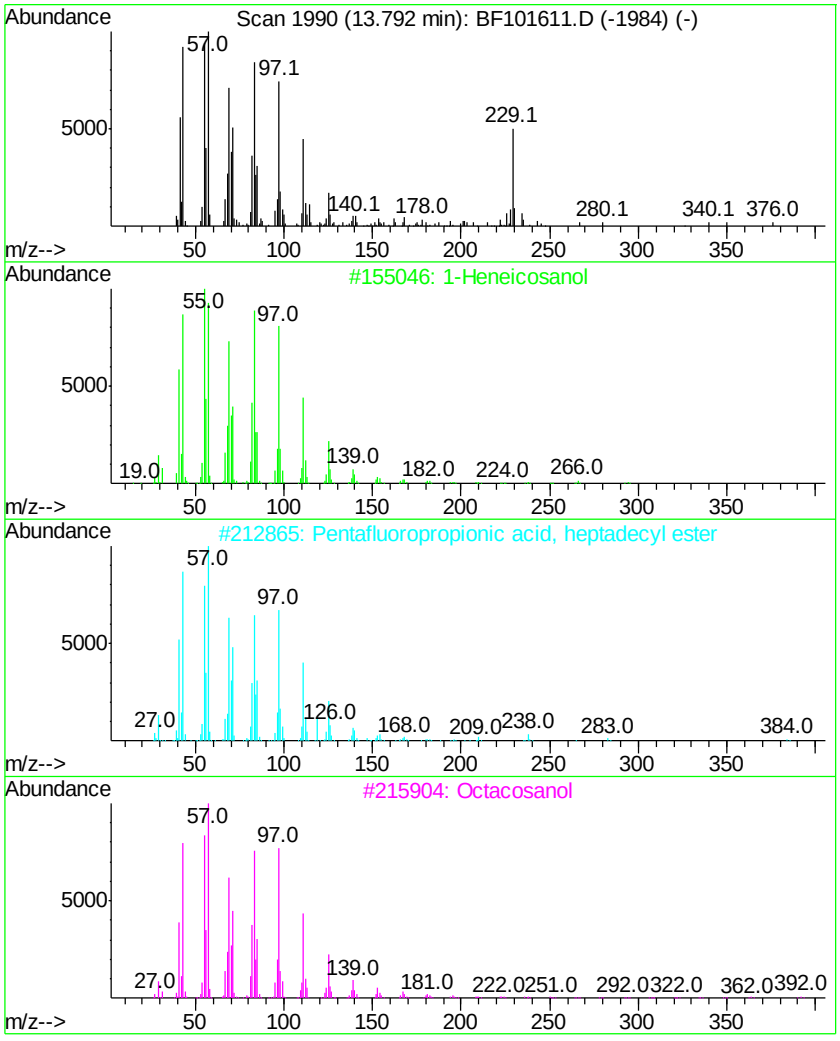
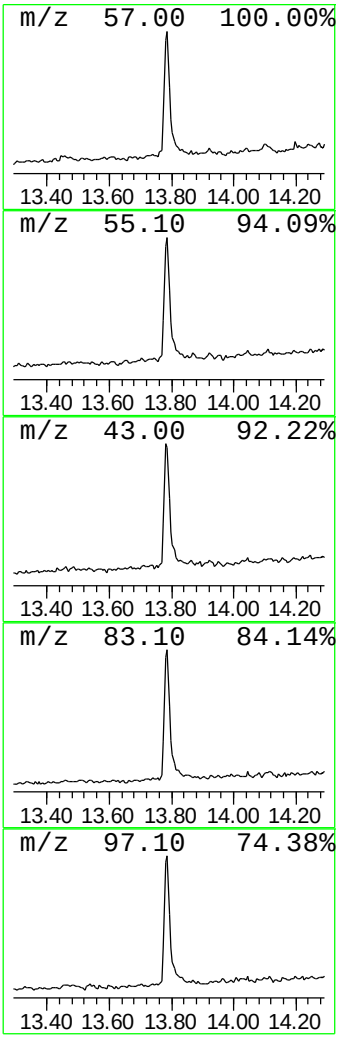
Peak Number 9 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.85 ng	468688	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
3	Octacosanol	410	C28H58O	000557-61-9	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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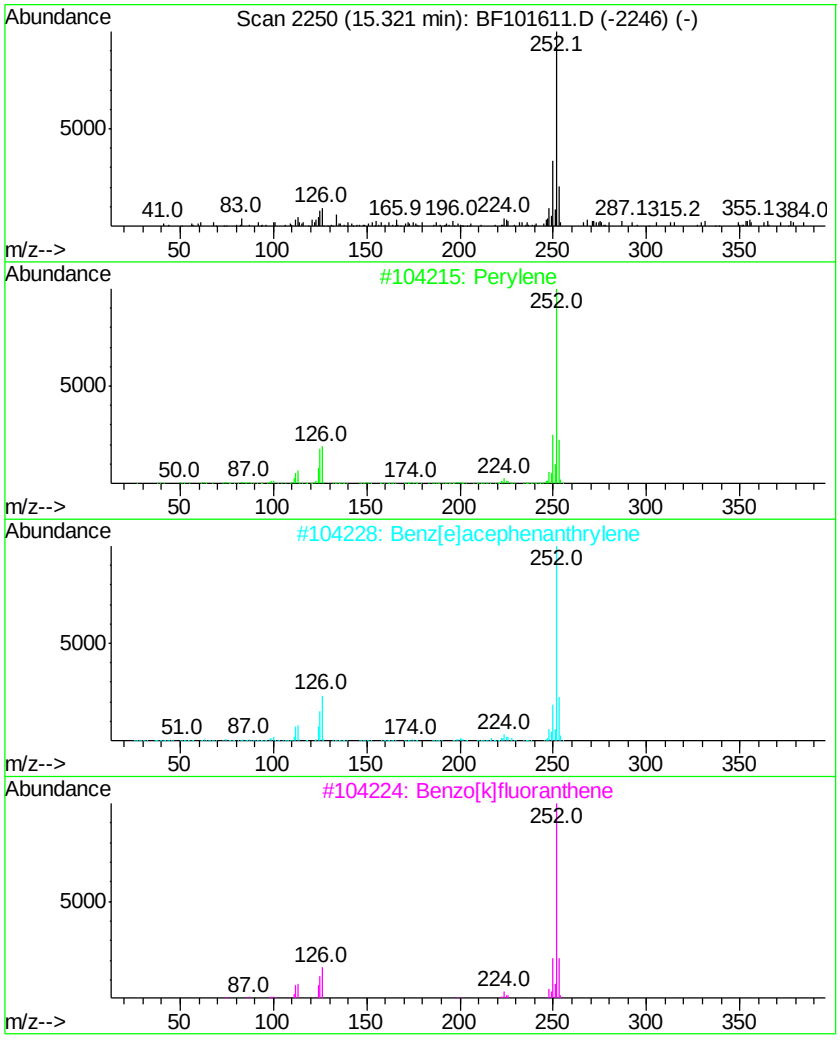
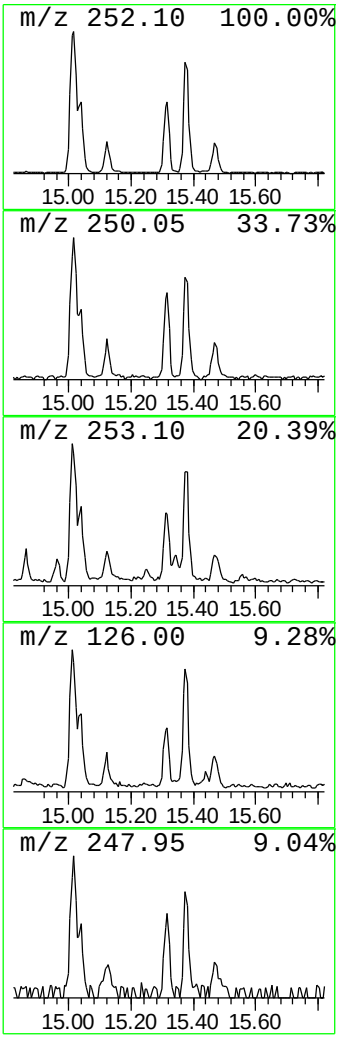
Peak Number 10 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	4.24 ng	124088	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
5	Benzo[e]pyrene	252	C20H12	000192-97-2	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
Data File : BF101611.D
Acq On : 21 Dec 2017 17:12
Operator : SJ/JU
Sample : I6993-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.02	23.6	ng	939936	1	6.80	796708	20.0
unknown6.57	6.57	83.2	ng	3315290	1	6.80	796708	20.0
Nonadecane	10.72	2.7	ng	95617	4	11.32	706742	20.0
Phenanthrene, 2-m...	11.83	2.7	ng	95034	4	11.32	706742	20.0
4H-Cyclopenta[def...	11.94	3.7	ng	129389	4	11.32	706742	20.0
11H-Benzo[b]fluorene	13.10	2.6	ng	154395	5	13.97	1194700	20.0
1-Heneicosanol	13.79	7.8	ng	468688	5	13.97	1194700	20.0
Perylene	15.32	4.2	ng	124088	6	15.44	584895	20.0