LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-10-OW(2-2.5)

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-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	4.999	492	495	510	rBV	24397	54027	4.45%	0.345%
2	5.404	561	564	590	rBV	452442	831355	68.50%	5.308%
3	6.428	735	738	757	rBV	535423	891742	73.48%	5.693%
4	6.557	757	760	775	rVB	804058	888408	73.20%	5.672%
5	6.787	796	799	815	rBV	902145	906396	74.69%	5.787%
6	6.940	822	825	841	rBV	580394	593230	48.88%	3.787%
7	7.357	893	896	915	rBV	373371	529042	43.59%	3.378%
8	8.069	1014	1017	1038	rVB	1285041	1213618	100.00%	7.748%
9	9.139	1196	1199	1208	rBV	872200	755406	62.24%	4.823%
10	9.210	1208	1211	1216	rVB	18883	18005	1.48%	0.115%
11	9.545	1260	1268	1273	rBV	50862	66127	5.45%	0.422%
12	9.739	1297	1301	1304	rVB	43973	35358	2.91%	0.226%
13	9.822	1311	1315	1319	rBV2	1345405	1200806	98.94%	7.666%
14	9.857	1319	1321	1327	rVB	32033	33522	2.76%	0.214%
15	10.039	1348	1352	1354	rBV3	14104	19492	1.61%	0.124%
16	10.063	1354	1356	1360	rVB3	12244	13457	1.11%	0.086%
17	10.239	1383	1386	1389	rVB	54016	40294	3.32%	0.257%
18	10.381	1406	1410	1416	rVB	23968	27767	2.29%	0.177%
19	10.457	1416	1423	1426	rBV4	16623	24056	1.98%	0.154%
20	10.533	1434	1436	1441	rVB2	12206	13169	1.09%	0.084%
21	10.616	1447	1450	1464	rBV	399348	486862	40.12%	3.108%
22	10.710	1464	1466	1472	rVV	43002	42108	3.47%	0.269%
23	11.157	1540	1542	1546	rVB3	21744	19936	1.64%	0.127%
24	11.316	1565	1569	1571	rBV	1272476	1166211	96.09%	7.446%
25	11.339	1571	1573	1577	rVV	216722	199466	16.44%	1.273%
26	11.398	1579	1583	1590	rVB	75576	86924	7.16%	0.555%
27	11.563	1608	1611	1613	rBV2	23487	20701	1.71%	0.132%
28	11.822	1651	1655	1658	rBV2	43670	56105	4.62%	0.358%
29	11.851	1658	1660	1665	rVB	38397	33133	2.73%	0.212%
30	11.898	1665	1668	1671	rBV	20433	19004	1.57%	0.121%
31	11.933	1671	1674	1677	rBV	75268	72517	5.98%	0.463%
32	12.110	1701	1704	1709	rBV	29447	31444	2.59%	0.201%
33	12.169	1711	1714	1721	rVB4	13547	17487	1.44%	0.112%
34	12.369	1745	1748	1751	rBV2	22331	24290	2.00%	0.155%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-10-OW(2-2.5)

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.475	1759	1766	1770	rVB3	14458	28843	2.38%	0.184%
36	12.533	1772	1776	1781	rBV	530590	497486	40.99%	3.176%
37	12.686	1799	1802	1804	rBV	23076	22387	1.84%	0.143%
38	12.763	1808	1815	1821	rVV	436898	510528	42.07%	3.259%
39	12.816	1821	1824	1828	rVB2	24050	23901	1.97%	0.153%
40	12.892	1834	1837	1842	rVB	685295	569270	46.91%	3.634%
41	12.939	1842	1845	1848	rBV	13974	16416	1.35%	0.105%
42	12.974	1848	1851	1857	rBV3	24904	41098	3.39%	0.262%
43	13.092	1868	1871	1876	rVB	59605	66298	5.46%	0.423%
44	13.157	1878	1882	1885	rBV	61931	57457	4.73%	0.367%
45	13.198	1885	1889	1896	rVB3	37762	64544	5.32%	0.412%
46	13.292	1902	1905	1907	rBV	25522	23450	1.93%	0.150%
47	13.322	1907	1910	1914	rVV2	22801	22924	1.89%	0.146%
48	13.369	1915	1918	1919	rBV	18774	15215	1.25%	0.097%
49	13.569	1950	1952	1956	rBV4	9925	15425	1.27%	0.098%
50	13.616	1959	1960	1966	rVB2	19937	21085	1.74%	0.135%
51	13.716	1973	1977	1979	rBV	37018	43407	3.58%	0.277%
52	13.733	1979	1980	1983	rVV	40561	35662	2.94%	0.228%
53	13.774	1983	1987	1994	rVV4	66567	131733	10.85%	0.841%
54	13.827	1994	1996	2000	rVB	30580	32404	2.67%	0.207%
55	13.963	2013	2019	2022	rBV2	1034158	1168908	96.32%	7.463%
56	13.986	2022	2023	2030	rVB	185212	165606	13.65%	1.057%
57	14.074	2035	2038	2040	rBV	36058	31609	2.60%	0.202%
58	14.351	2083	2085	2088	rVB2	31298	28665	2.36%	0.183%
59	14.486	2105	2108	2109	rBV2	24230	31476	2.59%	0.201%
60	14.768	2154	2156	2161	rVB	33255	33523	2.76%	0.214%
61	15.004	2192	2196	2206	rVB	167652	344320	28.37%	2.198%
62	15.304	2243	2247	2251	rBV	97801	133784	11.02%	0.854%
63	15.368	2254	2258	2263	rBV	124344	183359	15.11%	1.171%
64	15.427	2263	2268	2272	rBV	632111	777628	64.08%	4.965%
65	16.904	2516	2519	2525	rVB2	58401	93369	7.69%	0.596%

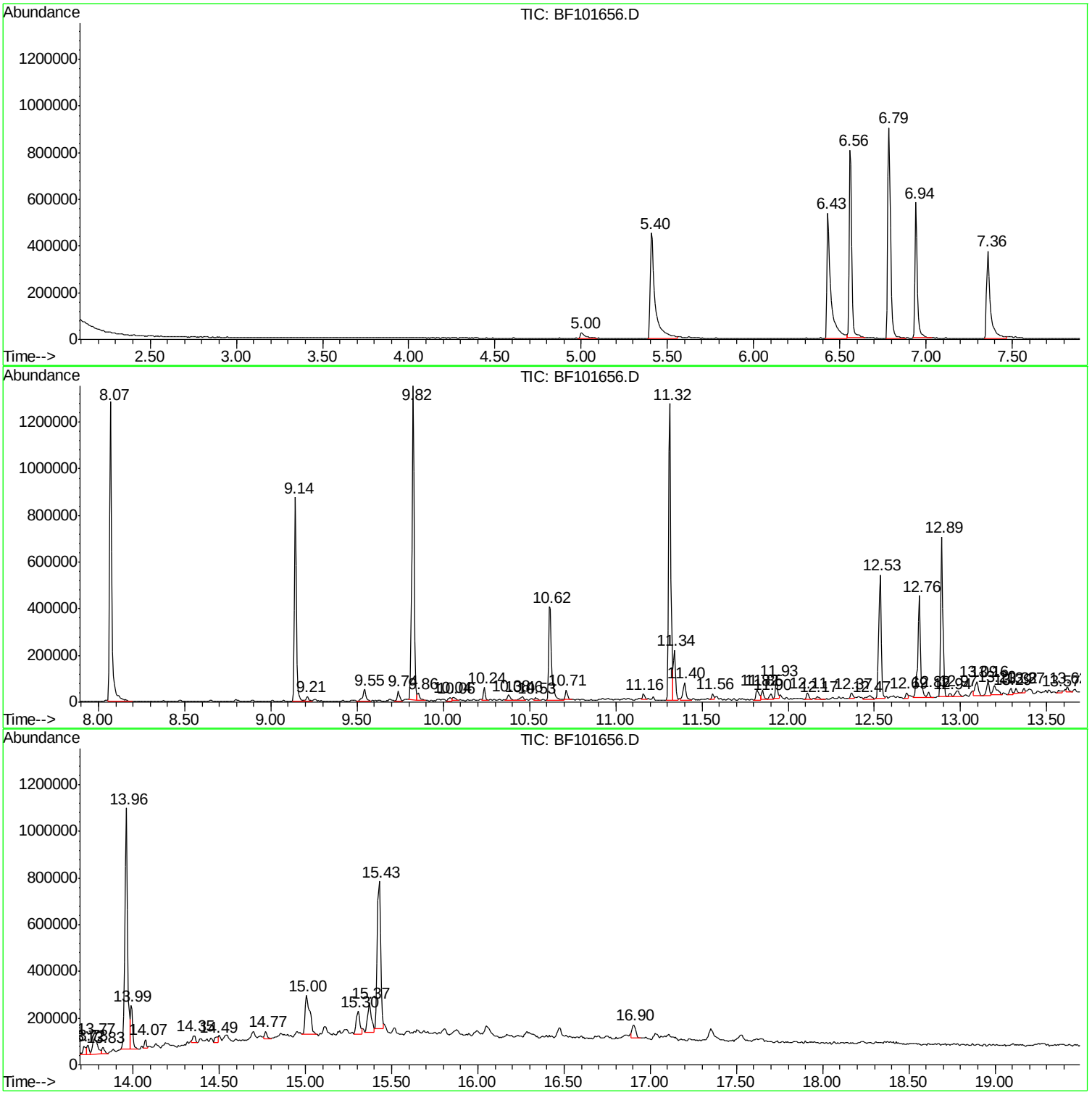
Sum of corrected areas: 15663245

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-10-OW(2-2.5)

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\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-10-OW(2-2.5)

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

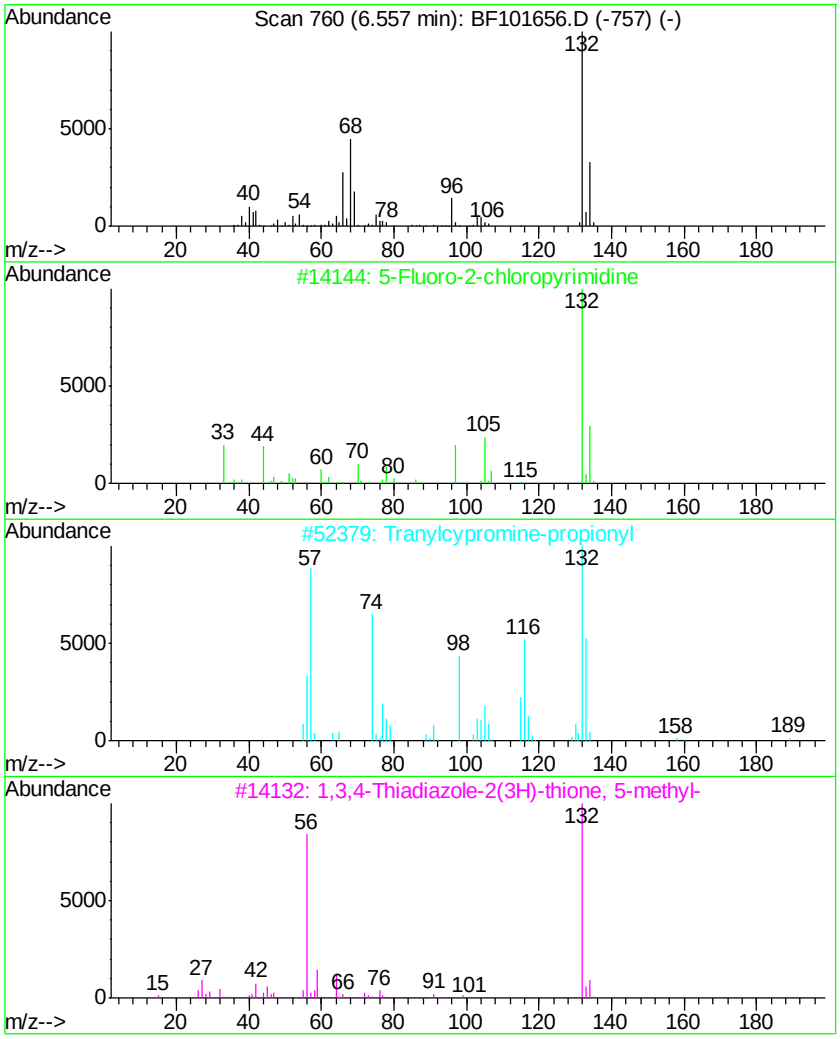
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

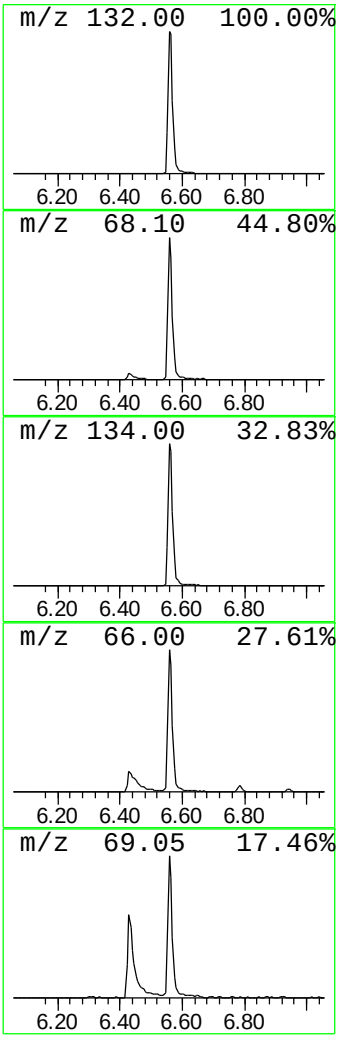
****

Peak Number 1 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	19.60 ng	888408	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-10-OW(2-2.5)

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

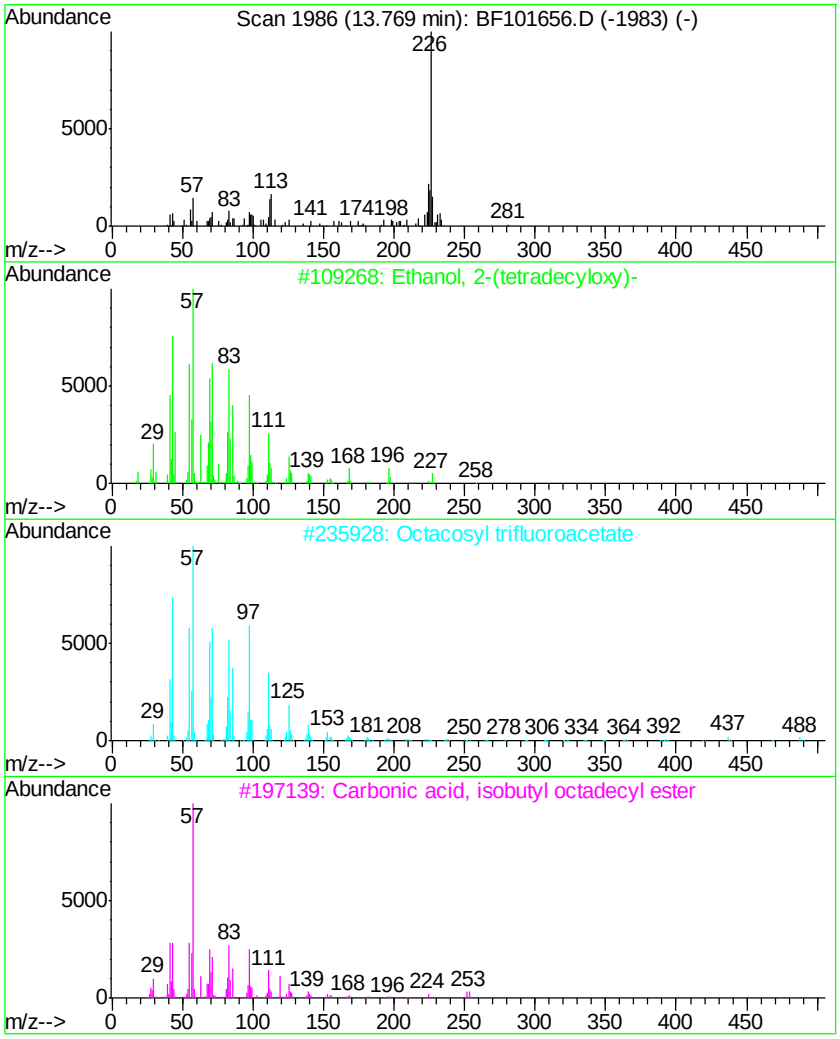
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

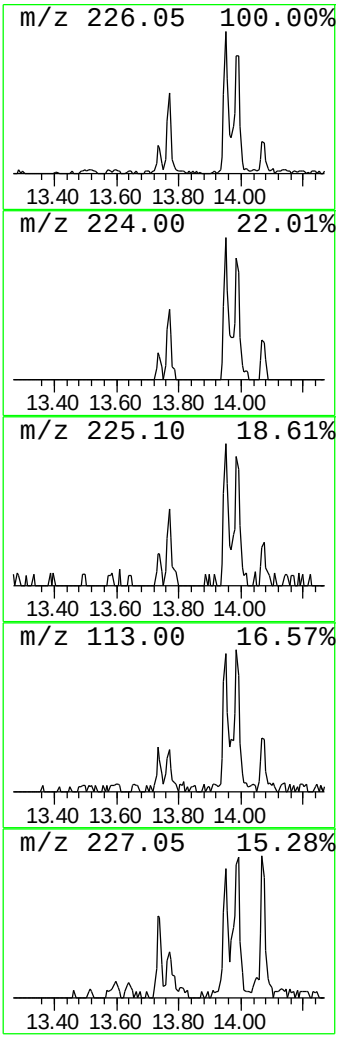
****

Peak Number 3 unknown13.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.25 ng	131733	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	38
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	38
3	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	30
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	30
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	30





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-10-OW(2-2.5)

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

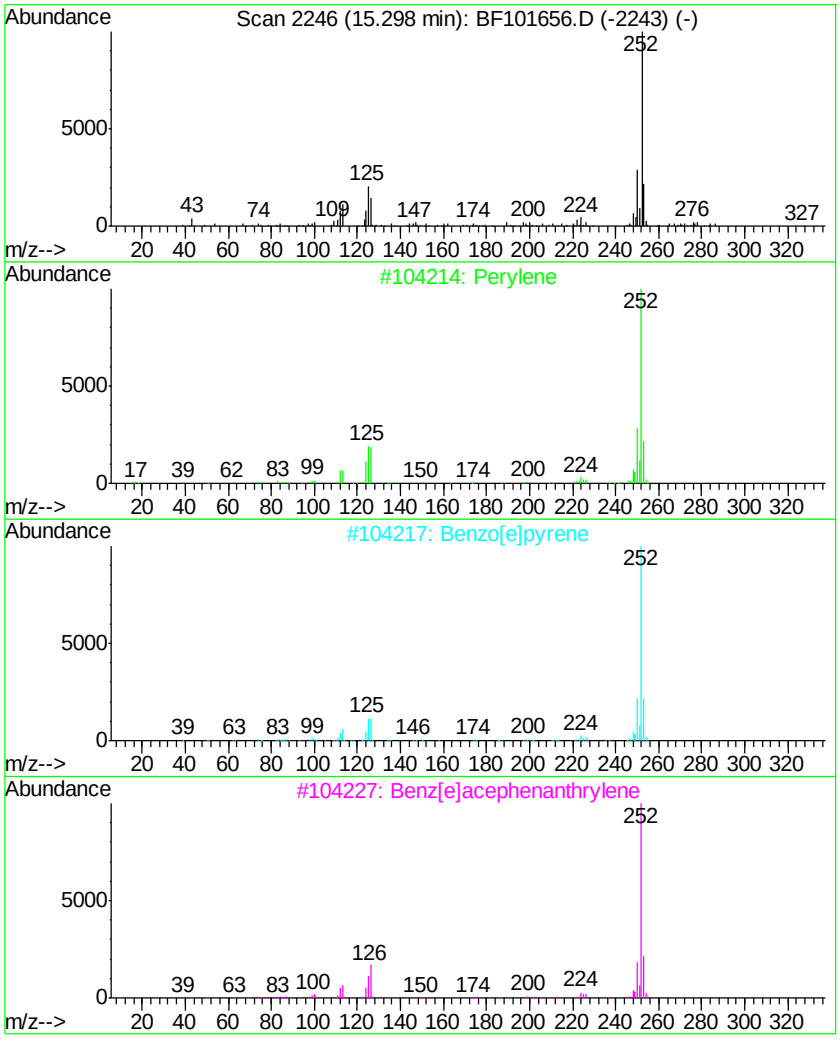
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

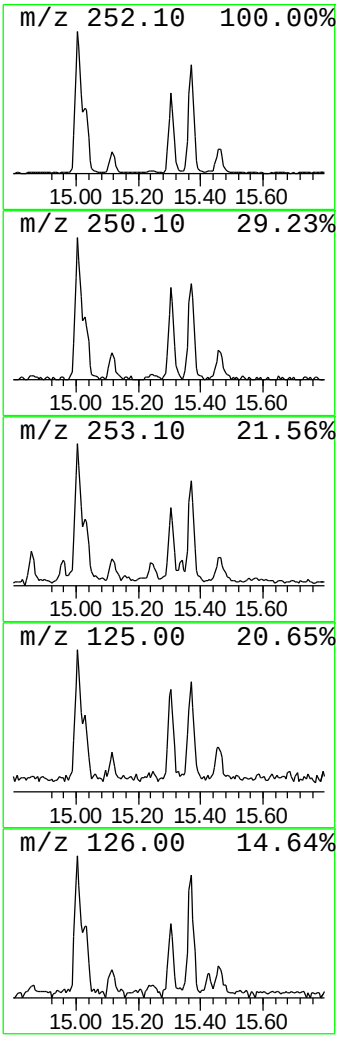
****

Peak Number 4 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	3.44 ng	133784	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	97
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101656.D
Acq On : 22 Dec 2017 16:32
Operator : SJ/JU
Sample : I6890-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-10-OW(2-2.5)

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
unknown6.56	6.56	19.6	ng	888408	1	6.79	906396	20.0
unknown13.77	13.77	2.3	ng	131733	5	13.96	1168910	20.0
Perylene	15.30	3.4	ng	133784	6	15.43	777628	20.0