LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135853.D
Acq On : 18 Oct 2023 18:11
Operator : CG\JU
Sample : 04767-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

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-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.357	381	386	390	rBV3	10712	18738	1.16%	0.130%
2	4.957	485	488	504	rBV	329050	404286	25.11%	2.807%
3	5.381	557	560	587	rBV	751141	1022251	63.48%	7.098%
4	6.393	729	732	752	rBV	1431022	1610266	100.00%	11.180%
5	6.734	787	790	800	rBV	565161	548979	34.09%	3.812%
6	7.304	884	887	900	rBV	1032032	959221	59.57%	6.660%
7	7.992	1002	1004	1005	rBV	38209	29551	1.84%	0.205%
8	8.016	1005	1008	1011	rVV	860414	708364	43.99%	4.918%
9	8.039	1011	1012	1016	rVV	115899	93756	5.82%	0.651%
10	8.069	1016	1017	1020	rVV	35527	29491	1.83%	0.205%
11	8.104	1020	1023	1030	rVB6	13851	21326	1.32%	0.148%
12	8.304	1048	1057	1063	rBV8	12226	28468	1.77%	0.198%
13	8.434	1074	1079	1086	rVB2	28433	30387	1.89%	0.211%
14	8.604	1105	1108	1112	rBV	72086	56101	3.48%	0.390%
15	8.704	1121	1125	1128	rVB4	15724	20154	1.25%	0.140%
16	8.739	1128	1131	1137	rBV	38481	41856	2.60%	0.291%
17	8.834	1145	1147	1150	rBV	27530	21452	1.33%	0.149%
18	9.092	1188	1191	1201	rBV	1902086	1578483	98.03%	10.960%
19	9.169	1201	1204	1207	rVV	54832	45990	2.86%	0.319%
20	9.210	1207	1211	1214	rVV2	28313	29366	1.82%	0.204%
21	9.292	1223	1225	1232	rVB3	10790	18349	1.14%	0.127%
22	9.369	1234	1238	1242	rBV2	26396	37891	2.35%	0.263%
23	9.434	1246	1249	1252	rBV	31085	36334	2.26%	0.252%
24	9.557	1267	1270	1275	rVB	14803	19033	1.18%	0.132%
25	9.628	1278	1282	1288	rBV3	66125	87452	5.43%	0.607%
26	9.704	1292	1295	1298	rBV	33136	27375	1.70%	0.190%
27	9.775	1303	1307	1311	rBV	1225773	1028265	63.86%	7.139%
28	9.986	1337	1343	1346	rBV2	28202	35206	2.19%	0.244%
29	10.204	1377	1380	1382	rVB2	24877	19056	1.18%	0.132%
30	10.333	1397	1402	1408	rVB2	19977	24738	1.54%	0.172%
31	10.575	1439	1443	1455	rBV	412568	456321	28.34%	3.168%
32	10.680	1458	1461	1466	rBV2	29773	40673	2.53%	0.282%
33	11.128	1534	1537	1540	rBV2	30880	26445	1.64%	0.184%
34	11.157	1540	1542	1549	rVB3	18496	26710	1.66%	0.185%
35	11.269	1558	1561	1564	rBV	876198	779310	48.40%	5.411%
36	11.292	1564	1565	1571	rVV	188009	172064	10.69%	1.195%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
Q-2(5-10)

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-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.351	1572	1575	1582	rVB	75367	81884	5.09%	0.569%
38	11.527	1600	1605	1608	rBV3	16653	25087	1.56%	0.174%
39	11.557	1608	1610	1613	rVV2	28985	27665	1.72%	0.192%
40	11.586	1613	1615	1624	rVB	86294	91292	5.67%	0.634%
41	11.780	1645	1648	1650	rBV	17460	18587	1.15%	0.129%
42	11.804	1650	1652	1659	rVV3	61464	94095	5.84%	0.653%
43	11.892	1664	1667	1670	rBV	39780	41500	2.58%	0.288%
44	12.075	1696	1698	1704	rBV	17688	23131	1.44%	0.161%
45	12.327	1737	1741	1744	rBV4	15640	26716	1.66%	0.185%
46	12.392	1749	1752	1757	rVB	162512	156185	9.70%	1.084%
47	12.498	1767	1770	1777	rBV	212045	201688	12.53%	1.400%
48	12.598	1784	1787	1794	rBV2	35550	43820	2.72%	0.304%
49	12.727	1803	1809	1815	rVB	183254	192222	11.94%	1.335%
50	12.863	1828	1832	1836	rBV	1287980	1181049	73.34%	8.200%
51	13.939	2010	2015	2018	rBV2	469791	537393	33.37%	3.731%
52	13.963	2018	2019	2026	rVB	89411	76882	4.77%	0.534%
53	14.027	2027	2030	2036	rVB	37134	45130	2.80%	0.313%
54	14.110	2042	2044	2050	rVB6	16334	26239	1.63%	0.182%
55	14.163	2050	2053	2056	rBV4	16366	23392	1.45%	0.162%
56	14.404	2086	2094	2098	rBV8	35453	108373	6.73%	0.752%
57	14.568	2120	2122	2126	rVB	25166	23646	1.47%	0.164%
58	14.686	2140	2142	2147	rVB5	18494	24978	1.55%	0.173%
59	14.768	2153	2156	2161	rVB	61105	62080	3.86%	0.431%
60	14.986	2189	2193	2197	rBV	86728	134362	8.34%	0.933%
61	15.104	2210	2213	2219	rVB	22463	29300	1.82%	0.203%
62	15.292	2242	2245	2252	rBV	50301	63682	3.95%	0.442%
63	15.357	2252	2256	2261	rBV	77734	96066	5.97%	0.667%
64	15.415	2261	2266	2271	rBV	379473	500369	31.07%	3.474%
65	16.757	2490	2494	2501	rVB3	44057	84657	5.26%	0.588%
66	16.933	2518	2524	2532	rVB2	51359	108679	6.75%	0.755%
67	17.386	2596	2601	2610	rVB2	48683	118937	7.39%	0.826%

Sum of corrected areas: 14402794

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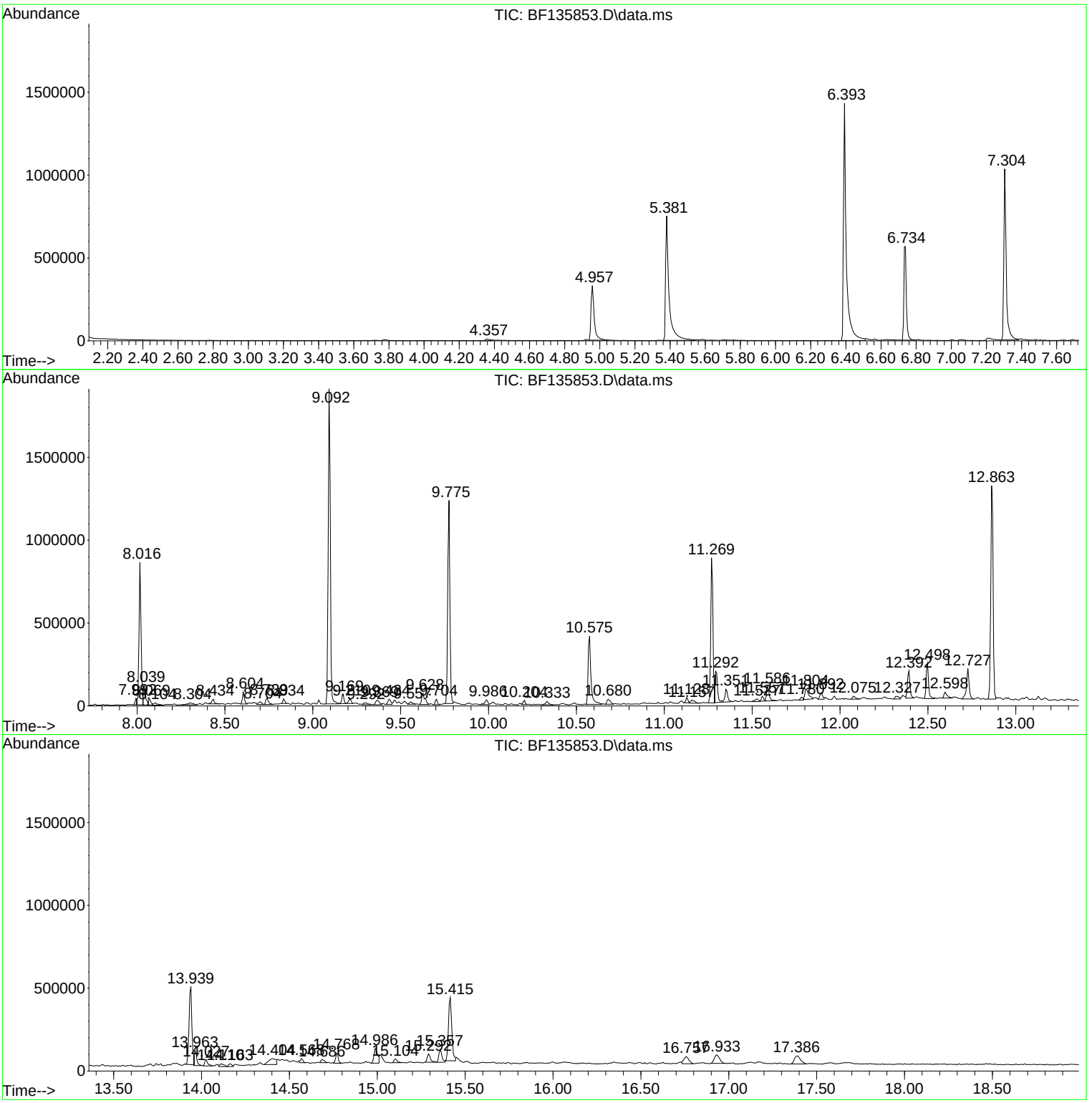
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

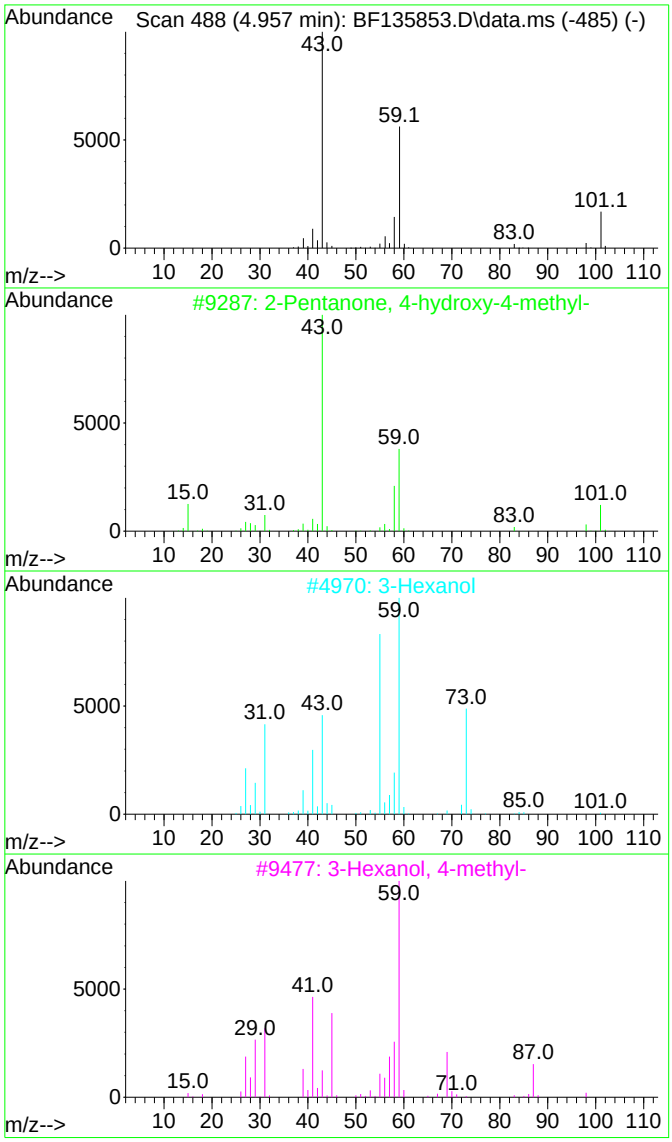
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

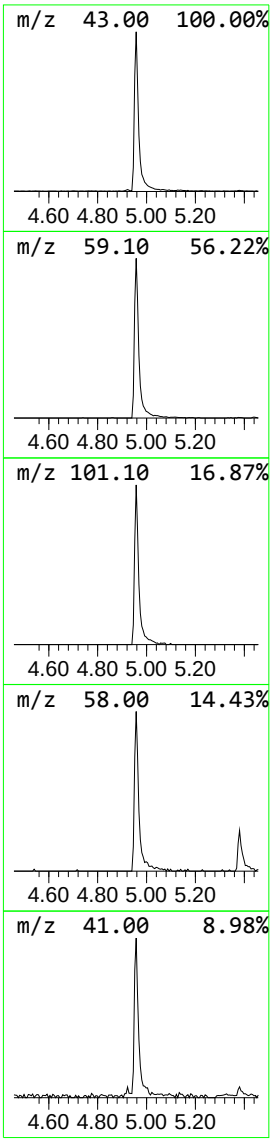
****

Peak Number 1 unknown4.957 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	14.73 ng	404286	1,4-Dichlorobenzene-d4	6.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Data File : BF135853.D
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Operator : CG\JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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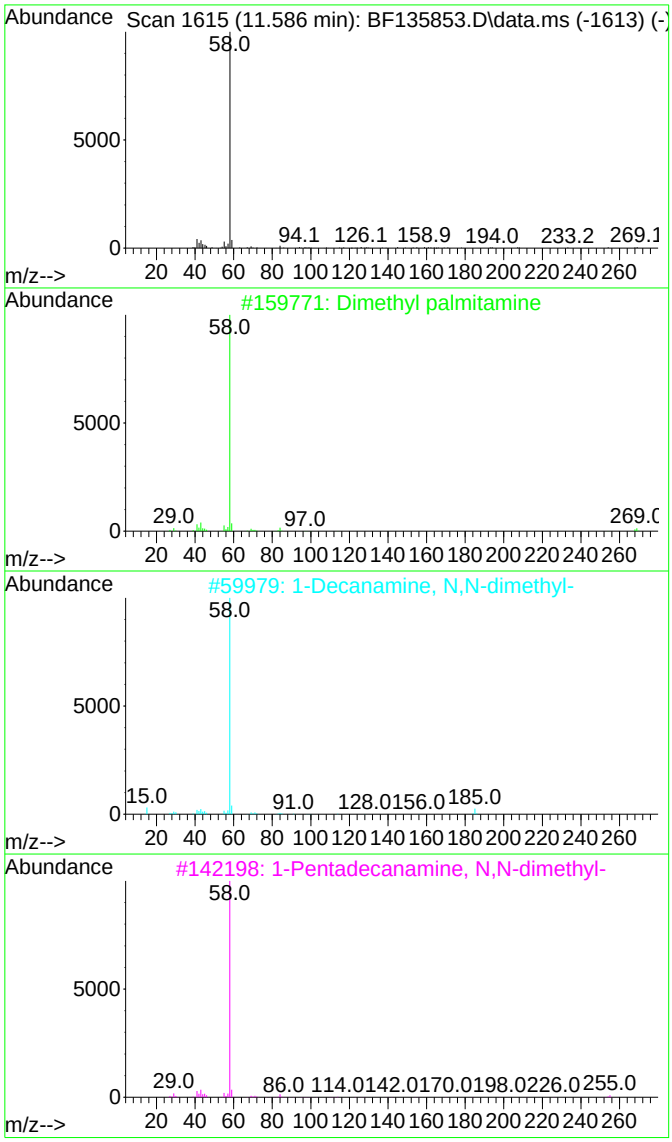
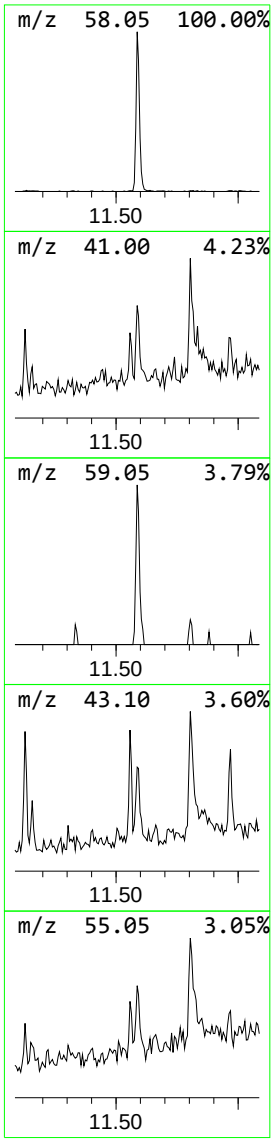
Peak Number 2 Dimethyl palmitamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.586	2.34 ng	91292	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl palmitamine	269	C18H39N	000112-69-6	80
2	1-Decanamine, N,N-dimethyl-	185	C12H27N	001120-24-7	72
3	1-Pentadecanamine, N,N-dimethyl-	255	C17H37N	017678-60-3	72
4	Dimantine	297	C20H43N	000124-28-7	72
5	1-Nonadecanamine, N,N-dimethyl-	311	C21H45N	049859-87-2	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
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Sample : 04767-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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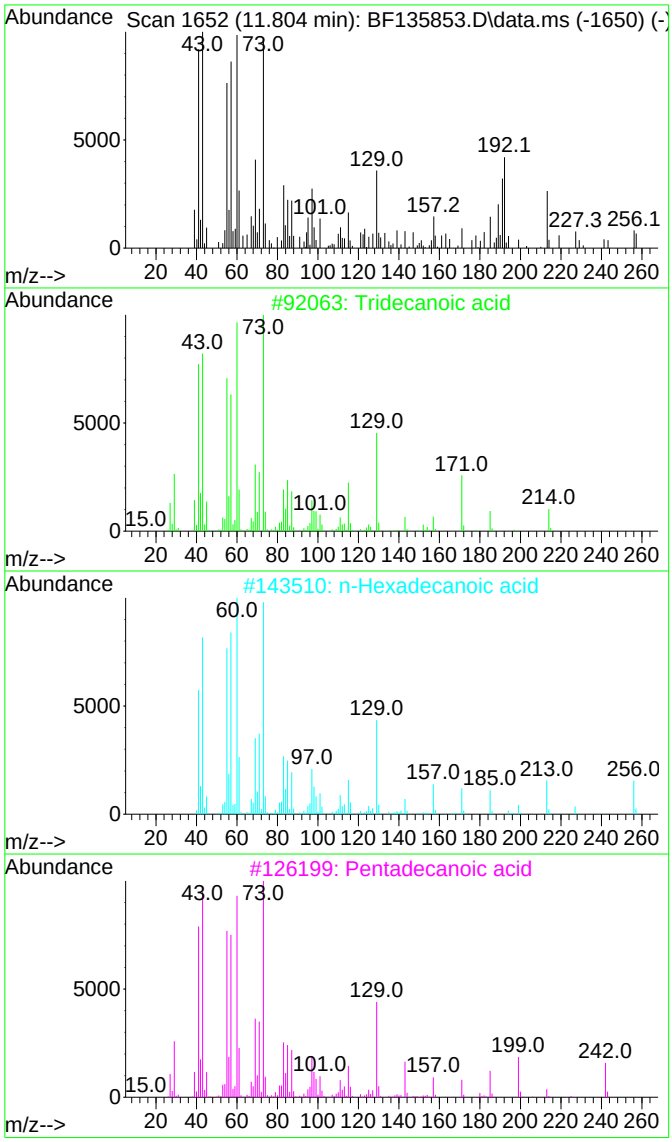
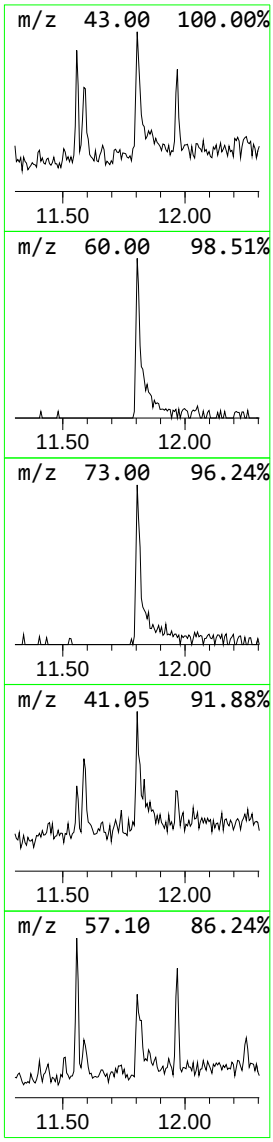
Peak Number 3 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.41 ng	94095	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	53
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
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Sample : 04767-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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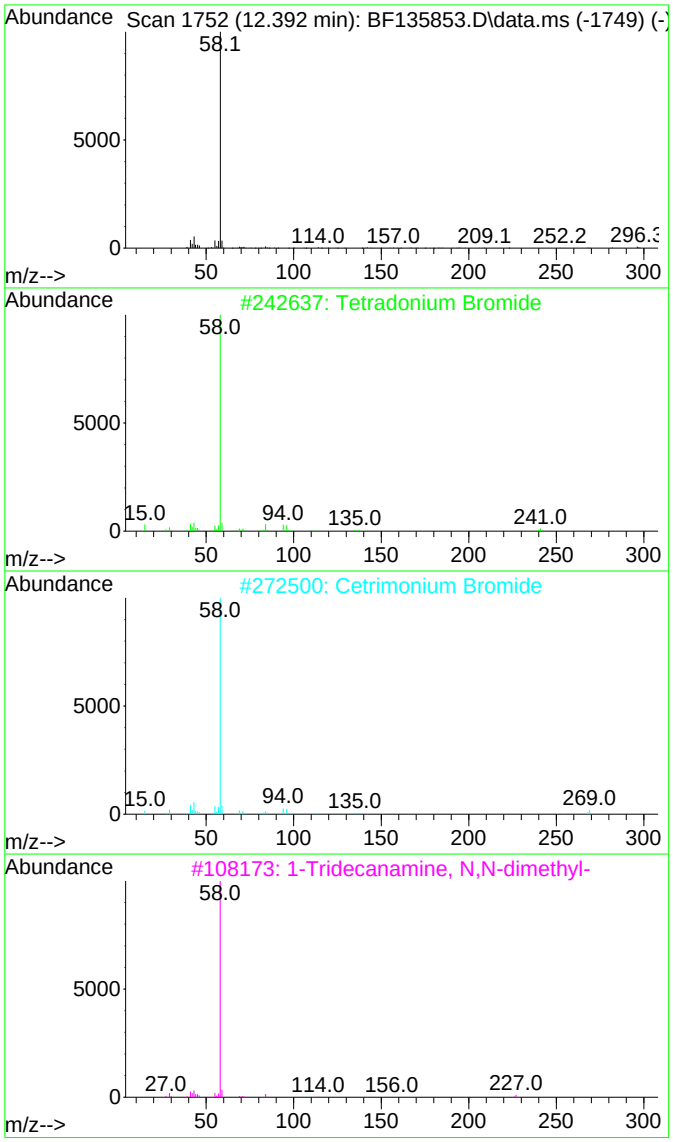
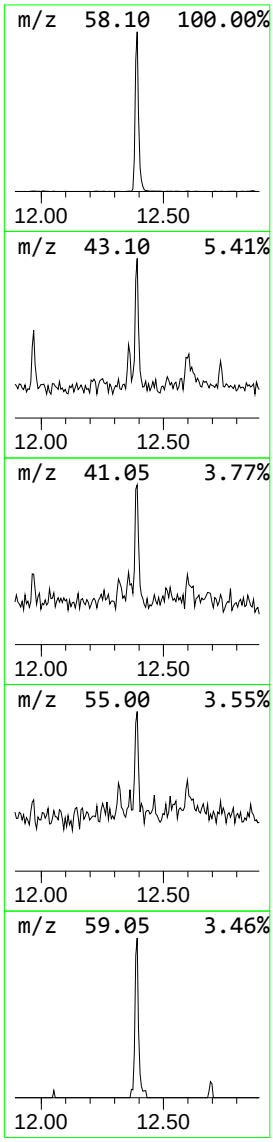
Peak Number 4 Tetradonium Bromide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	4.01 ng	156185	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradonium Bromide	335	C17H38BrN	001119-97-7	72
2	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	72
3	1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	72
4	1-Nonadecanamine, N,N-dimethyl-	311	C21H45N	049859-87-2	72
5	Dimethyl palmitamine	269	C18H39N	000112-69-6	72





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Data File : BF135853.D
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Sample : 04767-08
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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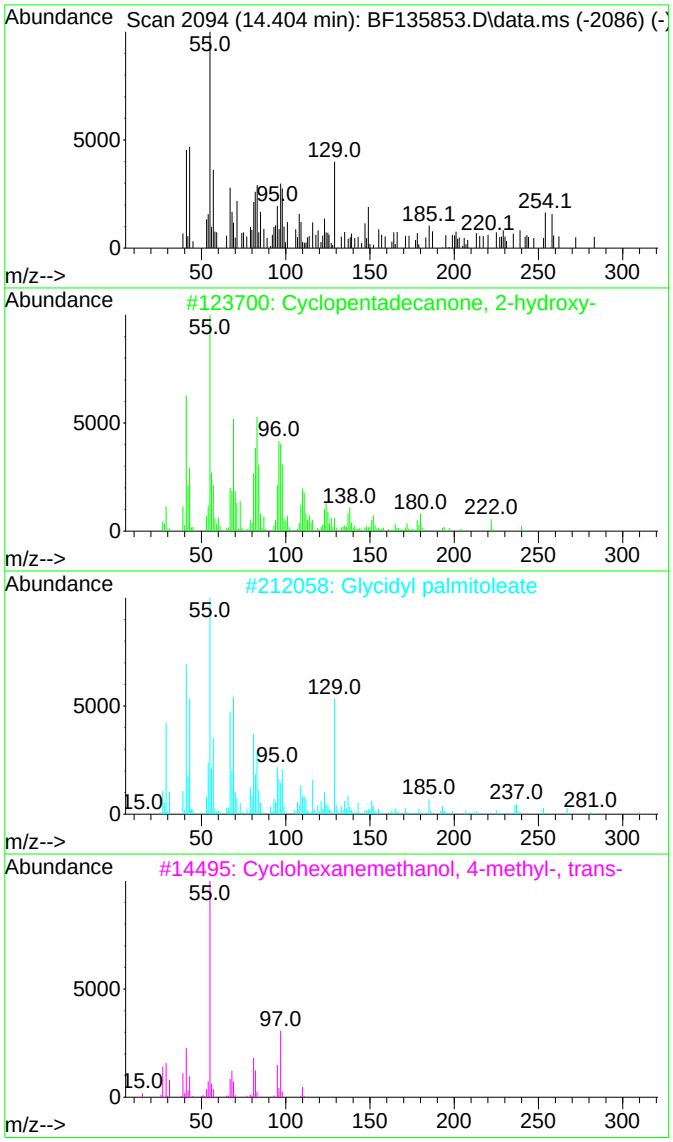
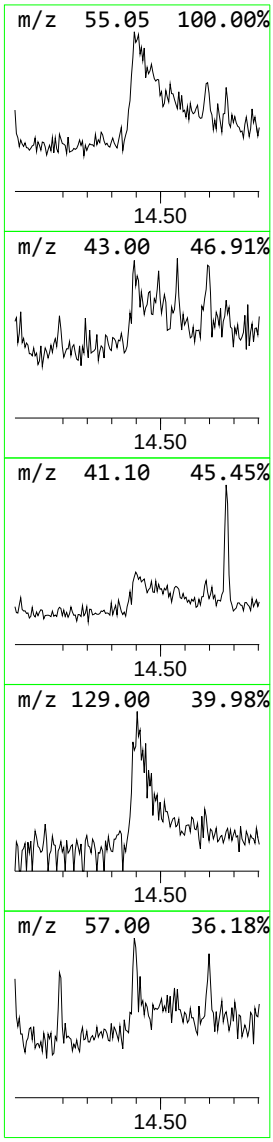
Peak Number 5 unknown14.404 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.404	4.03 ng	108373	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	16
2	Glycidyl palmitoleate	310	C19H34O3	213738-77-3	14
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	14
4	cis-11-Hexadecenal	238	C16H30O	053939-28-9	12
5	E-9-Hexadecenal	238	C16H30O	1000130-90-3	12





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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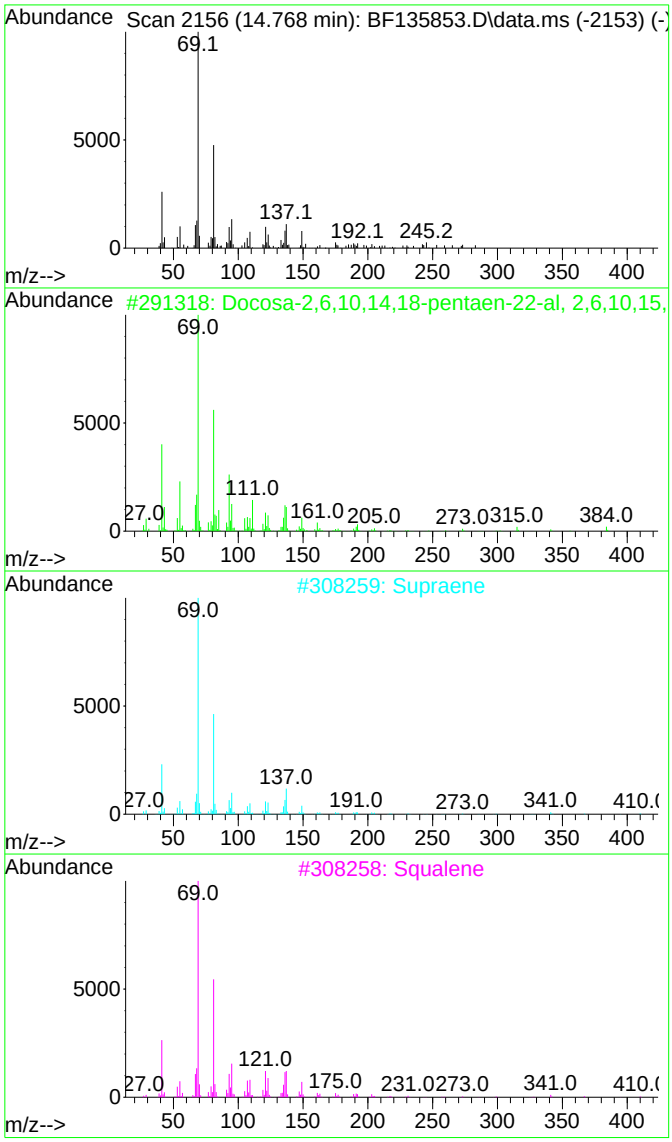
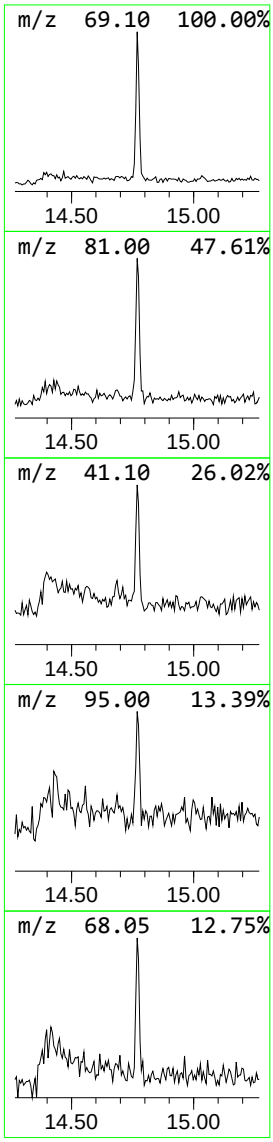
Peak Number 6 Docosa-2,6,10,14,18-pentaen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	2.48 ng	62080	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
2	Supraene	410	C30H50	007683-64-9	83
3	Squalene	410	C30H50	000111-02-4	83
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53





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Data File : BF135853.D
Acq On : 18 Oct 2023 18:11
Operator : CG\JU
Sample : 04767-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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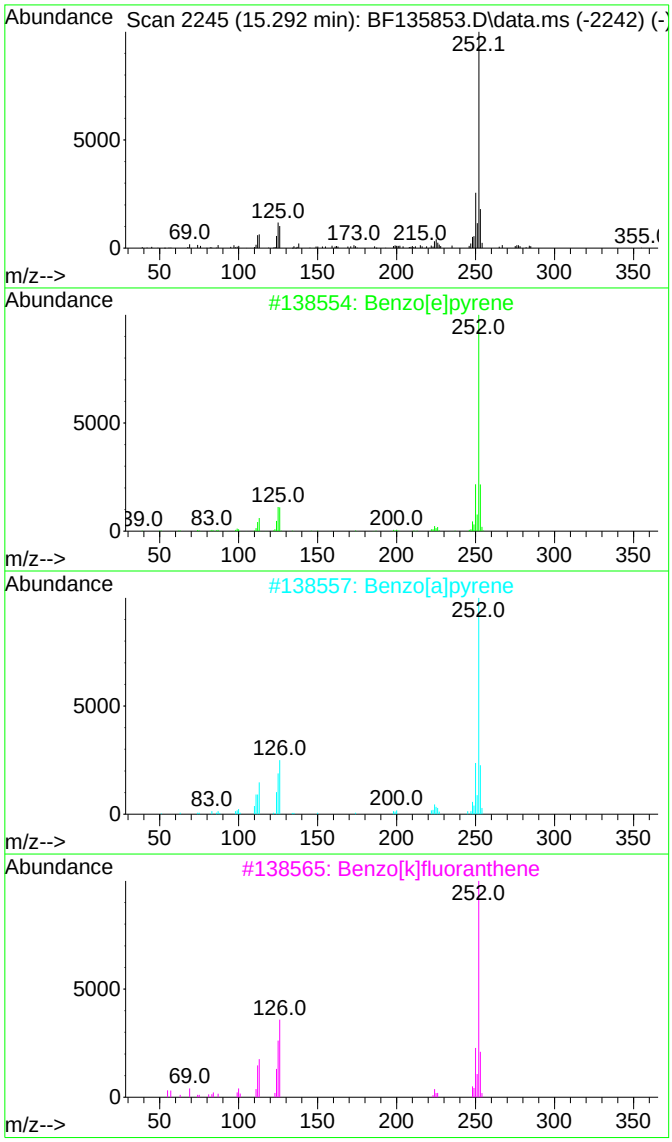
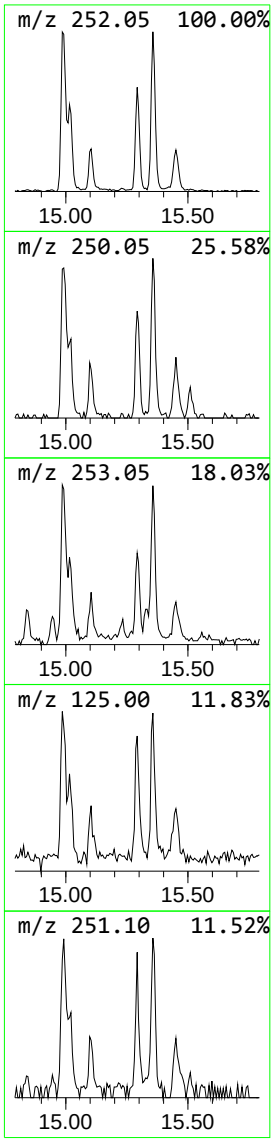
Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.55 ng	63682	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135853.D
Acq On : 18 Oct 2023 18:11
Operator : CG\JU
Sample : 04767-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

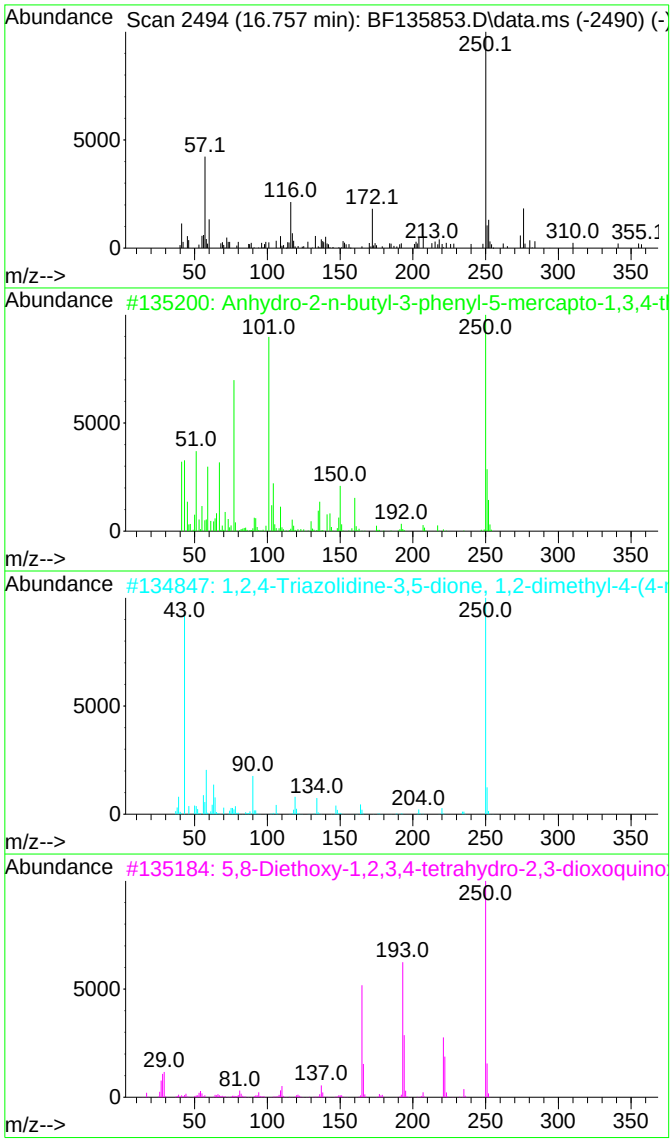
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

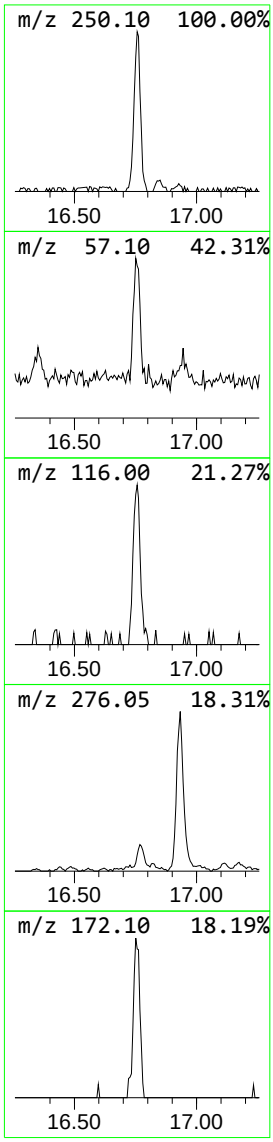
****

Peak Number 8 unknown16.757 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.757	3.38 ng	84657	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anhydro-2-n-butyl-3-phenyl-5-mer...	250	C12H14N2S2	1000254-97-9	47
2	1,2,4-Triazolidine-3,5-dione, 1,...	250	C10H10N4O4	1000350-49-8	47
3	5,8-Diethoxy-1,2,3,4-tetrahydro-...	250	C12H14N2O4	092959-72-3	37
4	2-Phenylbenzo[d]imidazo[2,1-b]th...	250	C15H10N2S	017833-07-7	28
5	4-Iodothioanisole	250	C7H7IS	035371-03-0	28





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135853.D
Acq On : 18 Oct 2023 18:11
Operator : CG\JU
Sample : 04767-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q-2(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.957	4.957	14.7	ng	404286	1	6.740	548979	20.0
Dimethyl palmit...	11.586	2.3	ng	91292	4	11.269	779310	20.0
Tridecanoic acid	11.804	2.4	ng	94095	4	11.269	779310	20.0
Tetradonium Bro...	12.392	4.0	ng	156185	4	11.269	779310	20.0
unknown14.404	14.404	4.0	ng	108373	5	13.939	537393	20.0
Docosa-2,6,10,1...	14.769	2.5	ng	62080	6	15.416	500369	20.0
Benzo[e]pyrene	15.292	2.5	ng	63682	6	15.416	500369	20.0
unknown16.757	16.757	3.4	ng	84657	6	15.416	500369	20.0