LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133111.D
Acq On : 27 Apr 2023 20:57
Operator : CG\JU
Sample : 02423-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	478	482	488	rVB	105129	125361	3.74%	0.448%
2	5.346	549	554	557	rBV	3307156	3023556	90.20%	10.795%
3	6.375	724	729	732	rBV	3220680	3156603	94.17%	11.270%
4	6.734	787	790	793	rBV	1434382	1096154	32.70%	3.914%
5	7.298	881	886	889	rBV	2336913	1877590	56.02%	6.704%
6	8.022	1005	1009	1011	rBV	1622073	1418957	42.33%	5.066%
7	8.045	1011	1013	1020	rVB4	38290	48123	1.44%	0.172%
8	9.092	1188	1191	1194	rBV	3996103	3351919	100.00%	11.967%
9	9.628	1279	1282	1287	rBV	51658	50508	1.51%	0.180%
10	9.769	1300	1306	1310	rBV	1830699	1421583	42.41%	5.076%
11	10.316	1396	1399	1405	rVB3	41056	45907	1.37%	0.164%
12	10.481	1423	1427	1431	rVB	430920	325298	9.70%	1.161%
13	10.557	1436	1440	1443	rBV	1365420	1219822	36.39%	4.355%
14	10.680	1458	1461	1469	rVB5	52029	75562	2.25%	0.270%
15	10.786	1477	1479	1486	rVB	34926	45151	1.35%	0.161%
16	11.104	1530	1533	1535	rBV3	34308	39964	1.19%	0.143%
17	11.251	1554	1558	1560	rBV	1394406	1128556	33.67%	4.029%
18	11.275	1560	1562	1565	rVV	537752	391516	11.68%	1.398%
19	11.322	1567	1570	1573	rVB2	145971	135709	4.05%	0.485%
20	11.357	1573	1576	1580	rBV3	32492	46407	1.38%	0.166%
21	11.751	1640	1643	1645	rBV	87921	73560	2.19%	0.263%
22	11.786	1645	1649	1653	rVV2	293502	341801	10.20%	1.220%
23	11.827	1653	1656	1659	rVV2	54258	64290	1.92%	0.230%
24	11.863	1659	1662	1664	rVV	176081	171725	5.12%	0.613%
25	11.886	1664	1666	1672	rVB	81964	69133	2.06%	0.247%
26	12.045	1691	1693	1695	rBV	74214	64345	1.92%	0.230%
27	12.063	1695	1696	1702	rVB3	62916	67293	2.01%	0.240%
28	12.304	1734	1737	1739	rBV	102784	94656	2.82%	0.338%
29	12.333	1740	1742	1744	rVV3	56192	65762	1.96%	0.235%
30	12.380	1748	1750	1755	rVV2	65341	76560	2.28%	0.273%
31	12.463	1760	1764	1767	rBV	1113811	982449	29.31%	3.508%
32	12.686	1797	1802	1806	rBV	984937	1009264	30.11%	3.603%
33	12.810	1820	1823	1824	rBV	81748	73364	2.19%	0.262%
34	12.839	1824	1828	1831	rVV	2956004	2553367	76.18%	9.116%
35	13.016	1856	1858	1862	rVB2	146131	147430	4.40%	0.526%
36	13.086	1867	1870	1872	rVB	100750	95903	2.86%	0.342%

```
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133111.D
Acq On    : 27 Apr 2023  20:57
Operator  : CG\JU
Sample    : O2423-03
Misc      :
ALS Vial  : 23   Sample Multiplier: 1

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-BF042123.M
Title     : ASP BNA STANDARDS FOR 5 POINT CALIBRATION
```

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

37	13.122	1873	1876	1879	rBV2	131112	136648	4.08%	0.488%
38	13.210	1889	1891	1894	rVB	81974	65801	1.96%	0.235%
39	13.886	2001	2006	2008	rBV2	1130884	1437790	42.89%	5.133%
40	13.910	2008	2010	2013	rVB	466225	369112	11.01%	1.318%
41	14.904	2176	2179	2182	rBV	324810	451754	13.48%	1.613%
42	15.310	2245	2248	2251	rBV	546377	572320	17.07%	2.043%

Sum of corrected areas: 28008573

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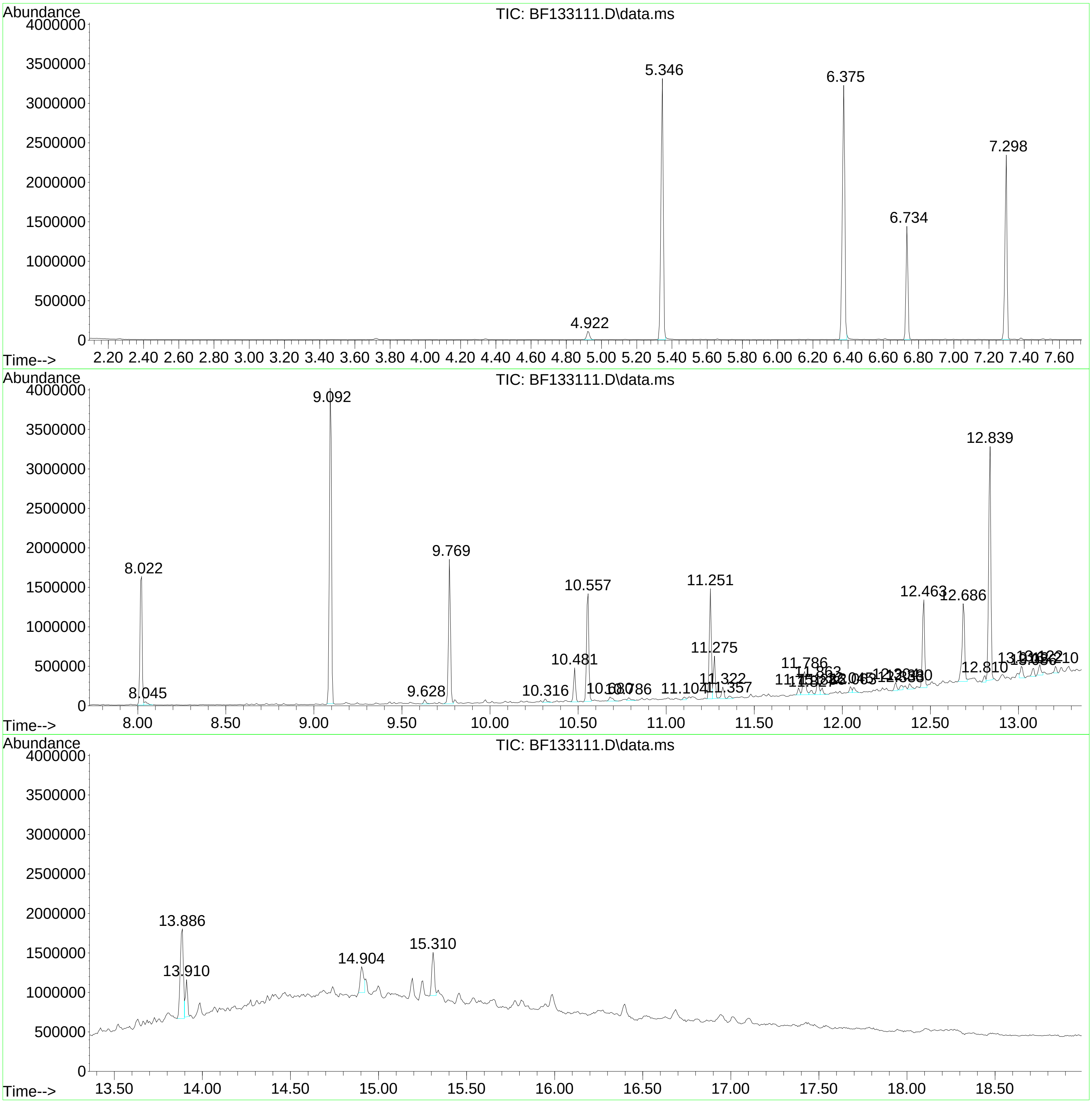
Operator : CG\JU
Sample : O2423-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF042723\
Data File : BF133111.D
Acq On : 27 Apr 2023 20:57
Operator : CG\JU
Sample : 02423-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

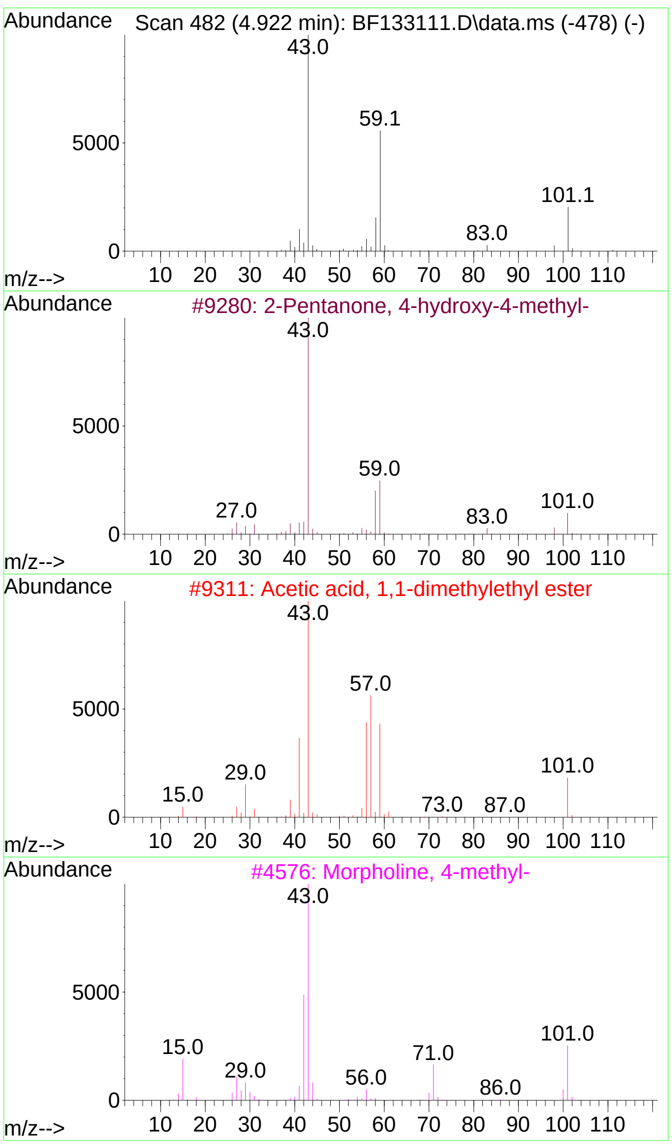
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

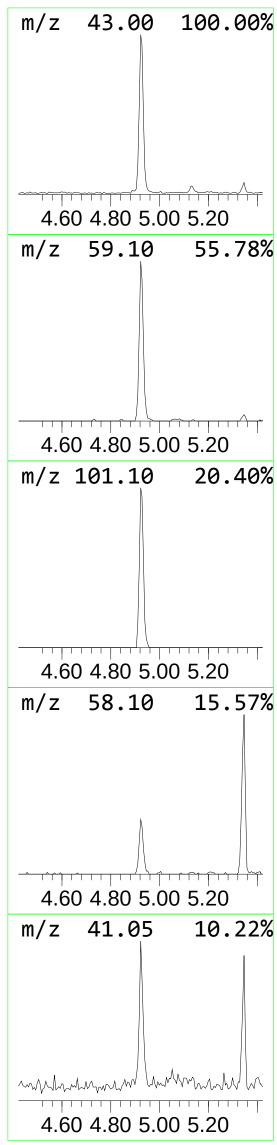
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	2.29 ng	125361	1,4-Dichlorobenzene-d4	6.734

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133111.D
Acq On : 27 Apr 2023 20:57
Operator : CG\JU
Sample : 02423-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

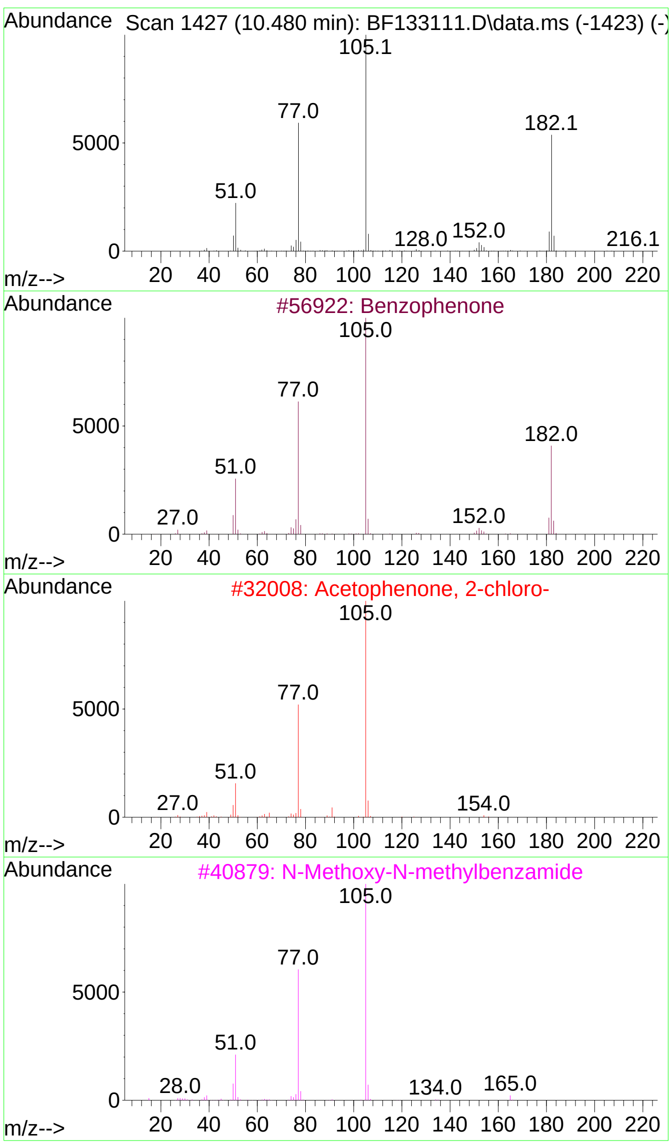
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

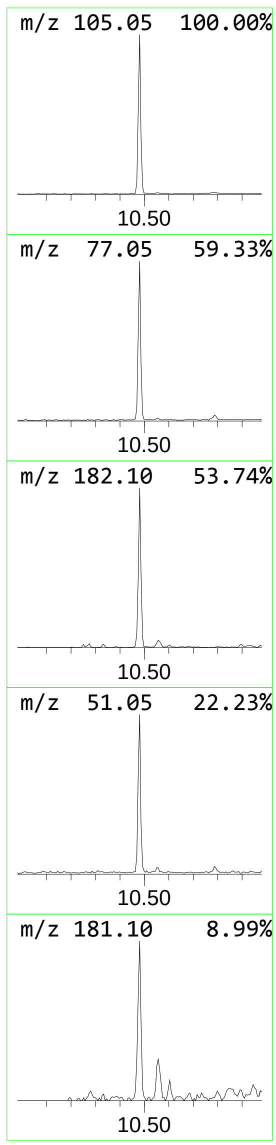
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	4.58 ng	325298	Acenaphthene-d10	9.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133111.D
Acq On : 27 Apr 2023 20:57
Operator : CG\JU
Sample : O2423-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

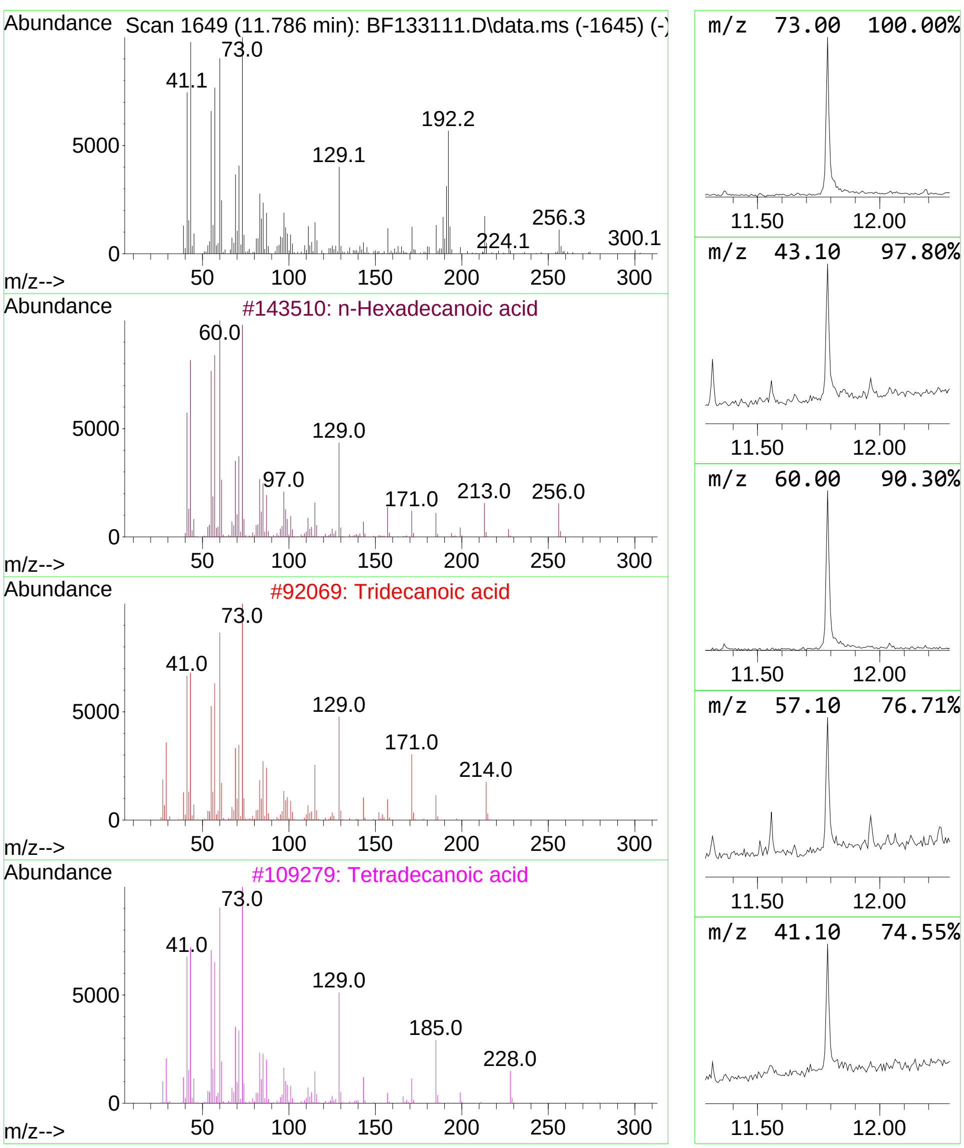
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	6.06 ng	341801	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133111.D
Acq On    : 27 Apr 2023  20:57
Operator  : CG\JU
Sample    : 02423-03
Misc      :
ALS Vial  : 23   Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title  : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

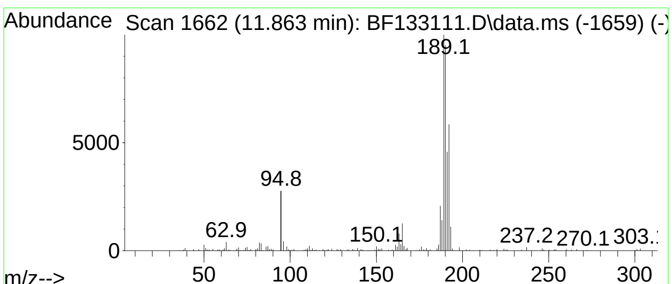
TIC Library    : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P
```

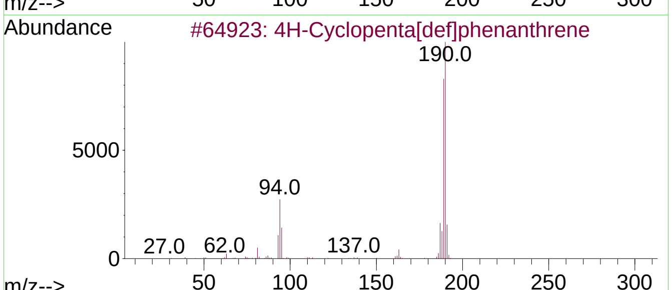
Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

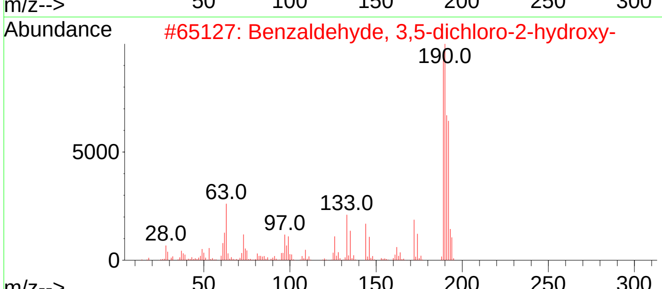
```
*********************************************************************
Peak Number  4  4H-Cyclopenta[def]phenanthrene  Concentration Rank  3
```

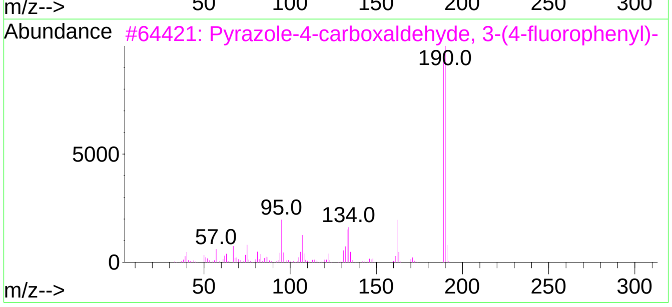
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.04 ng	171725	Phenanthrene-d10	11.251

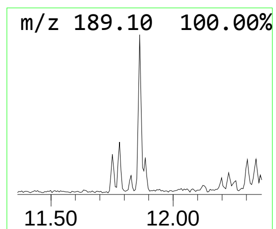
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	47
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	46
4	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	30
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30

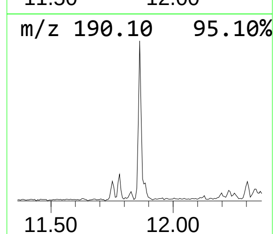


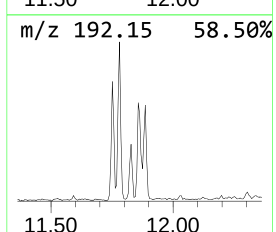


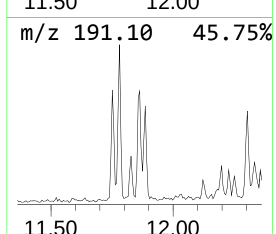


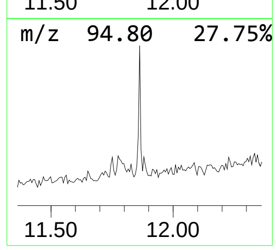












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Data File : BF133111.D
Acq On : 27 Apr 2023 20:57
Operator : CG\JU
Sample : O2423-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPD-1WC-23-04-18

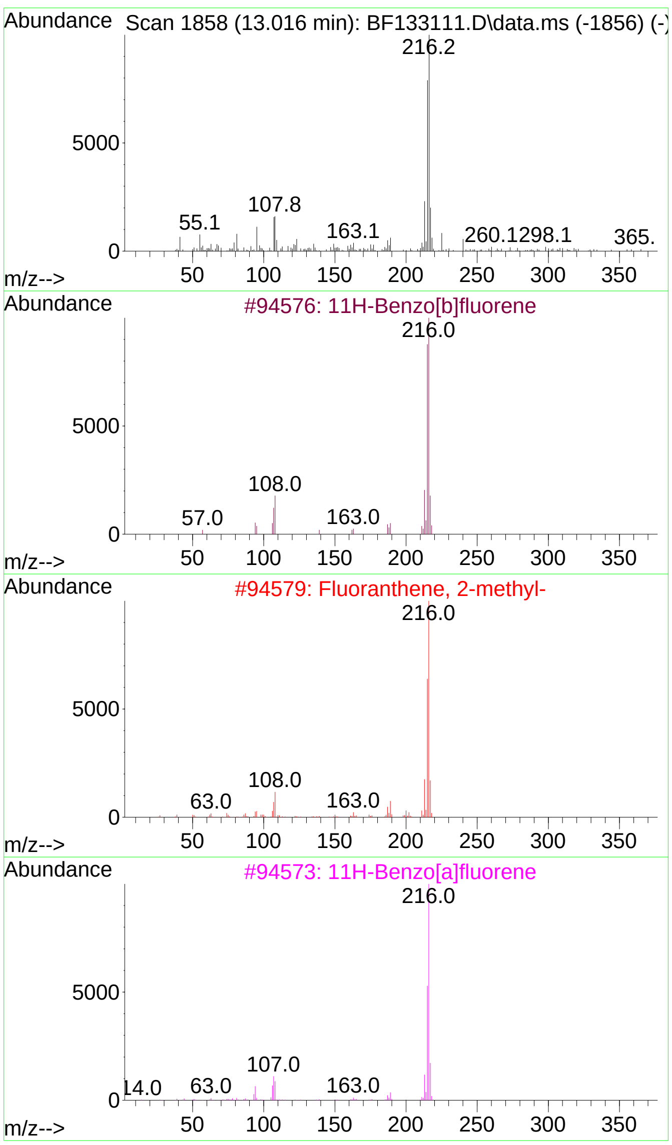
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

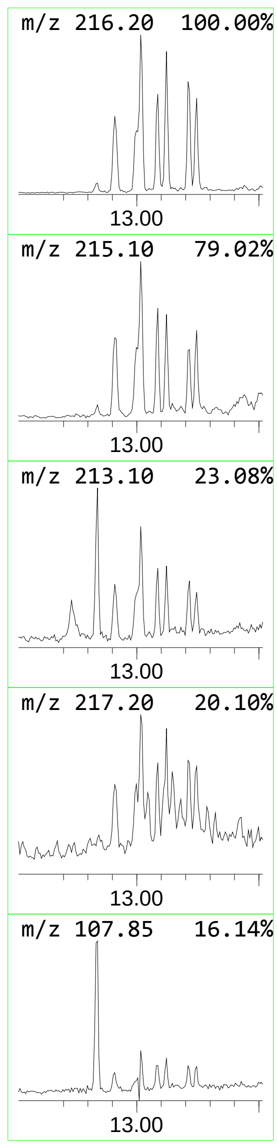
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.016	2.05 ng	147430	Chrysene-d12	13.886

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	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133111.D
Acq On : 27 Apr 2023 20:57
Operator : CG\JU
Sample : O2423-03
Misc :
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Instrument :
BNA_F
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SPD-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
2-Pentanone, 4-...	4.922	2.3	ng	125361	1	6.734	1096150	20.0
Benzophenone	10.480	4.6	ng	325298	3	9.769	1421580	20.0
n-Hexadecanoic ...	11.786	6.1	ng	341801	4	11.251	1128560	20.0
4H-Cyclopenta[d...	11.863	3.0	ng	171725	4	11.251	1128560	20.0
11H-Benzo[b]flu...	13.016	2.0	ng	147430	5	13.886	1437790	20.0