LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137075.D
Acq On : 15 Jan 2024 21:03
Operator : CG\JU
Sample : P1139-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137075.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB4	6643	10248	1.69%	0.177%
2	5.004	493	496	505	rBV	22653	27434	4.53%	0.475%
3	5.428	565	568	581	rBV	348709	355797	58.71%	6.161%
4	6.434	736	739	756	rBV	305481	328616	54.22%	5.690%
5	6.787	795	799	808	rVB	233154	208736	34.44%	3.614%
6	7.345	890	894	903	rBV	244035	209887	34.63%	3.634%
7	8.063	1012	1016	1019	rBV	279839	235893	38.92%	4.085%
8	9.133	1195	1198	1207	rBV	516636	413048	68.15%	7.152%
9	9.680	1287	1291	1294	rBV	8363	7095	1.17%	0.123%
10	9.816	1311	1314	1318	rBV	340042	274202	45.24%	4.748%
11	9.851	1318	1320	1323	rVB	12459	9641	1.59%	0.167%
12	10.369	1404	1408	1414	rVB	8038	8175	1.35%	0.142%
13	10.592	1443	1446	1447	rBV	36885	28474	4.70%	0.493%
14	10.610	1447	1449	1460	rVB	263459	257395	42.47%	4.457%
15	10.722	1466	1468	1477	rVB3	5384	9804	1.62%	0.170%
16	11.310	1565	1568	1571	rBV	365953	334922	55.26%	5.799%
17	11.333	1571	1572	1576	rVV	121178	95270	15.72%	1.650%
18	11.386	1579	1581	1584	rVB	25826	21128	3.49%	0.366%
19	11.557	1604	1610	1615	rBV3	7123	14485	2.39%	0.251%
20	11.774	1643	1647	1650	rBV4	8950	11982	1.98%	0.207%
21	11.816	1650	1654	1656	rVV2	48694	60040	9.91%	1.040%
22	11.845	1656	1659	1665	rVV	123548	139744	23.06%	2.420%
23	11.892	1665	1667	1670	rVV	18904	20400	3.37%	0.353%
24	11.927	1670	1673	1676	rVV	39097	47949	7.91%	0.830%
25	11.951	1676	1677	1681	rVB	23616	15138	2.50%	0.262%
26	12.116	1702	1705	1709	rBV	17186	16196	2.67%	0.280%
27	12.151	1709	1711	1716	rVB5	11047	10330	1.70%	0.179%
28	12.368	1744	1748	1751	rBV	23390	26037	4.30%	0.451%
29	12.404	1751	1754	1757	rVV4	14605	19955	3.29%	0.346%
30	12.463	1759	1764	1768	rBV3	14205	18177	3.00%	0.315%
31	12.533	1770	1776	1779	rBV	288353	249408	41.15%	4.319%
32	12.633	1790	1793	1797	rBV3	22060	26082	4.30%	0.452%
33	12.686	1799	1802	1805	rVB3	10303	10342	1.71%	0.179%
34	12.763	1809	1815	1821	rBV	270109	269619	44.49%	4.669%
35	12.816	1821	1824	1827	rVB2	15298	14830	2.45%	0.257%
36	12.904	1831	1839	1843	rBV	705921	606071	100.00%	10.494%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137075.D
Acq On : 15 Jan 2024 21:03
Operator : CG\JU
Sample : P1139-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.986	1848	1853	1856	rBV5	21575	33308	5.50%	0.577%
38	13.068	1864	1867	1868	rBV3	17486	16914	2.79%	0.293%
39	13.092	1869	1871	1874	rVB	33695	35077	5.79%	0.607%
40	13.139	1876	1879	1880	rBV2	9298	11149	1.84%	0.193%
41	13.163	1880	1883	1885	rVB	20241	16166	2.67%	0.280%
42	13.198	1886	1889	1891	rVV2	26066	25204	4.16%	0.436%
43	13.257	1896	1899	1903	rBV6	12026	13979	2.31%	0.242%
44	13.292	1903	1905	1908	rBV	21714	19350	3.19%	0.335%
45	13.321	1908	1910	1917	rVB	19262	24442	4.03%	0.423%
46	13.410	1923	1925	1929	rBV5	8342	9909	1.63%	0.172%
47	13.480	1934	1937	1940	rBV4	12254	17499	2.89%	0.303%
48	13.610	1957	1959	1964	rVB	23089	22630	3.73%	0.392%
49	13.721	1975	1978	1980	rBV	23210	23981	3.96%	0.415%
50	13.745	1980	1982	1984	rVB	21708	16541	2.73%	0.286%
51	13.768	1984	1986	1988	rBV	16941	17227	2.84%	0.298%
52	13.968	2013	2020	2023	rBV2	368537	475743	78.50%	8.238%
53	13.998	2023	2025	2033	rVB	123045	110283	18.20%	1.910%
54	14.063	2033	2036	2037	rBV2	24336	22429	3.70%	0.388%
55	14.362	2085	2087	2091	rVB	25286	19921	3.29%	0.345%
56	15.027	2196	2200	2203	rBV	72643	104867	17.30%	1.816%
57	15.333	2249	2252	2255	rBV2	36618	41514	6.85%	0.719%
58	15.404	2260	2264	2267	rVV	57923	73494	12.13%	1.273%
59	15.462	2270	2274	2278	rBV	162780	211013	34.82%	3.654%

Sum of corrected areas: 5775190

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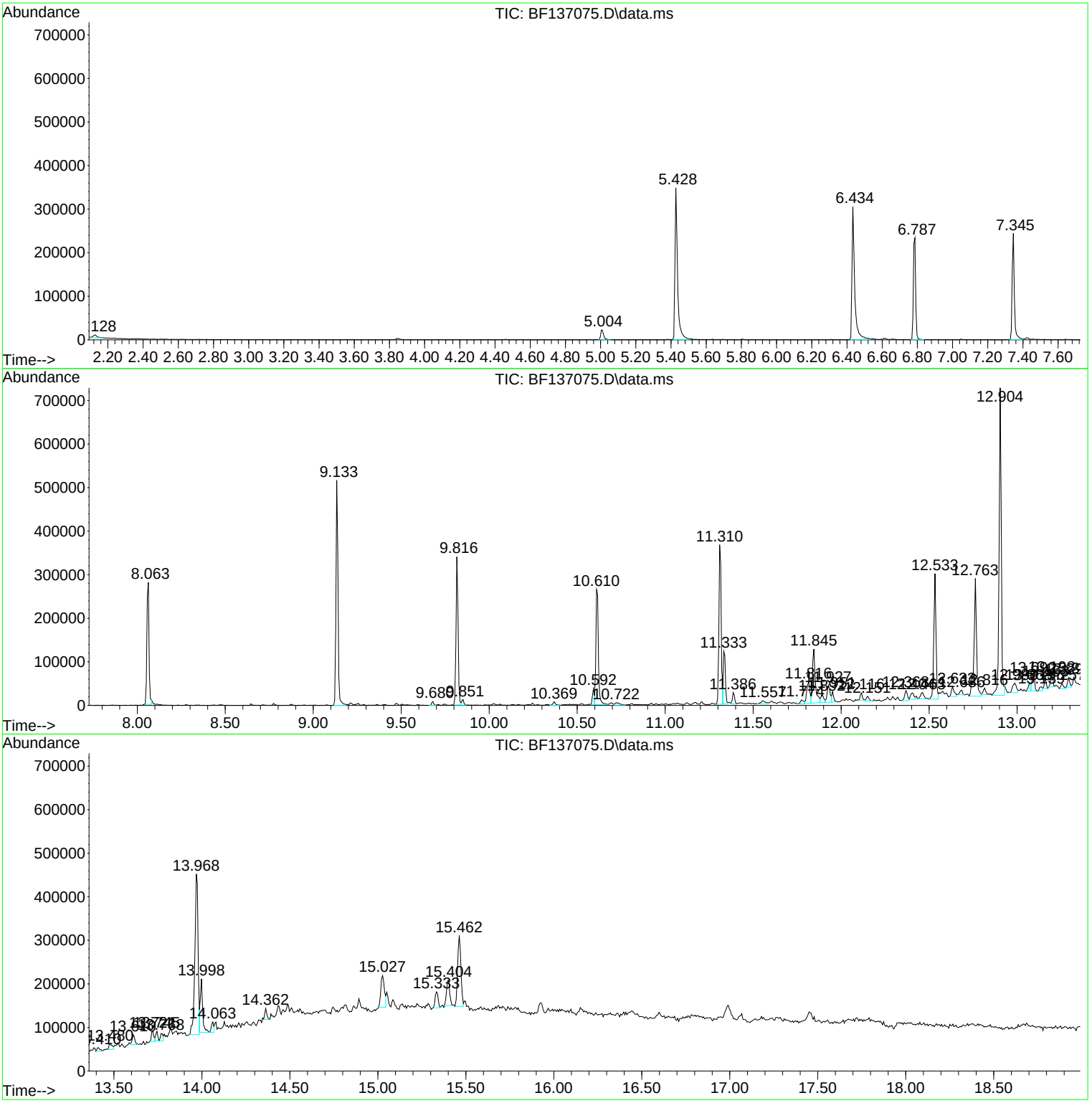
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF011524\
Data File : BF137075.D
Acq On : 15 Jan 2024 21:03
Operator : CG\JU
Sample : P1139-01 2X
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Instrument :
BNA_F
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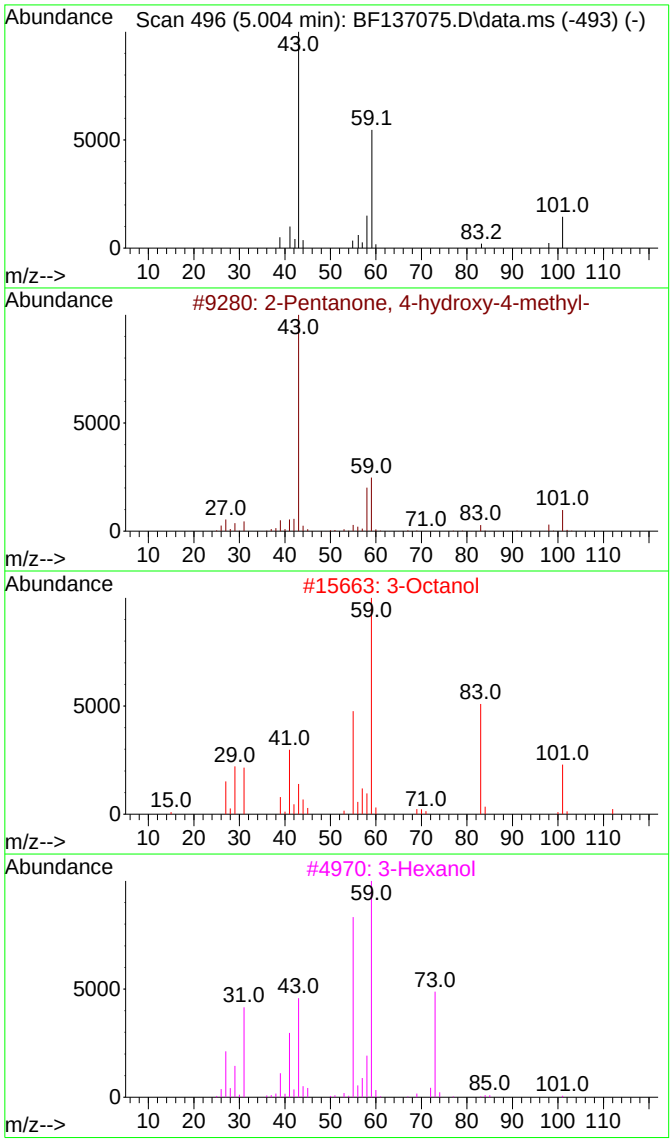
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

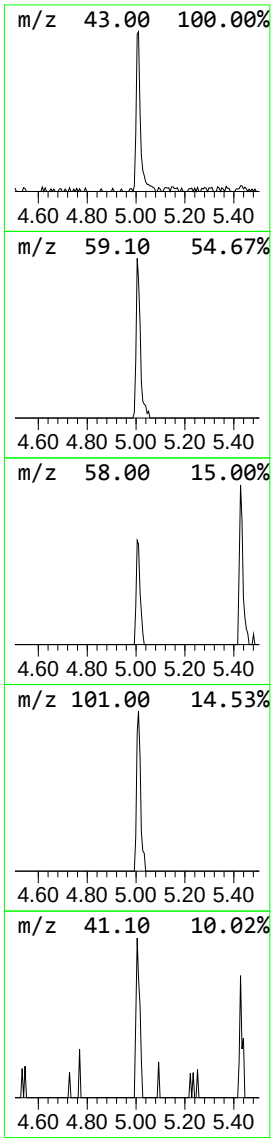
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.63 ng	27434	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Octanol	130	C8H18O	000589-98-0	33
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137075.D
Acq On : 15 Jan 2024 21:03
Operator : CG\JU
Sample : P1139-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

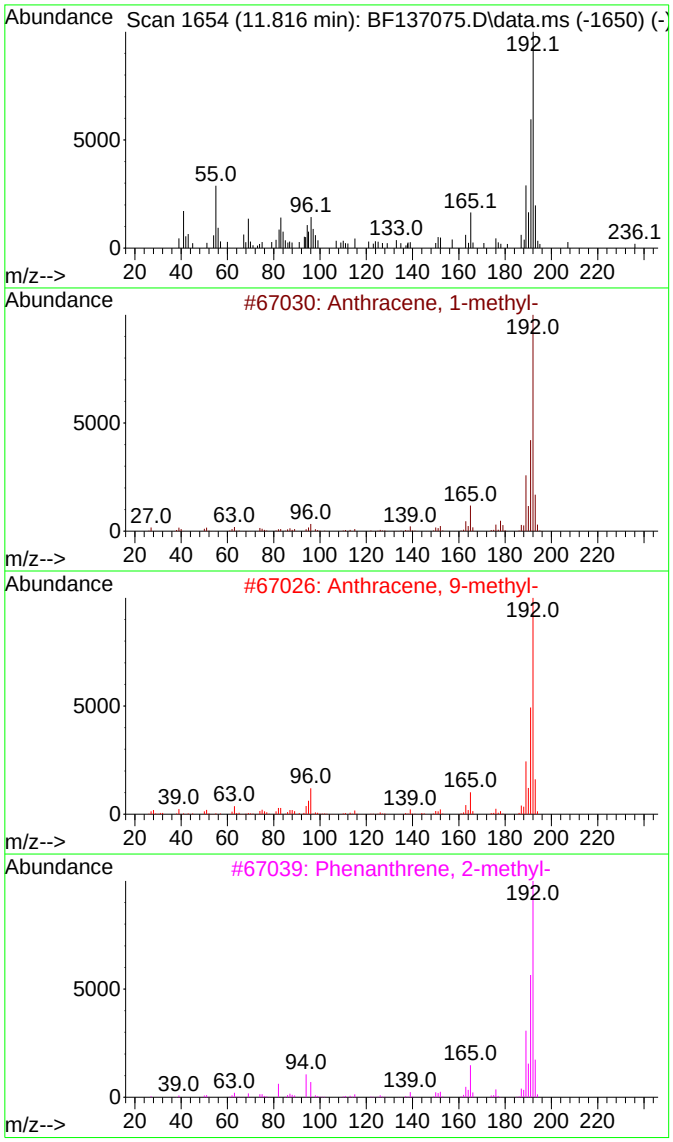
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

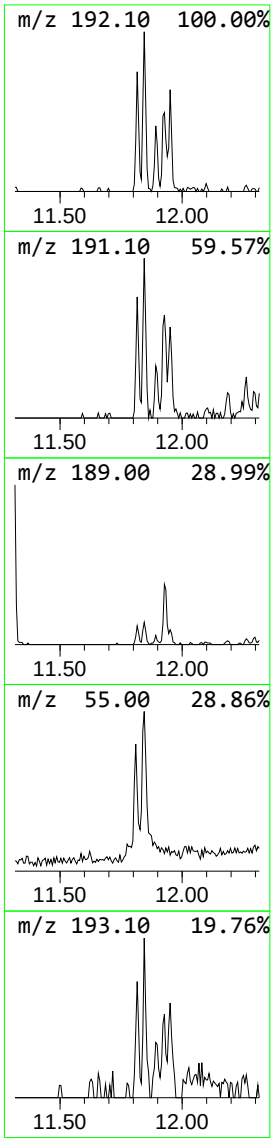
****

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	3.59 ng	60040	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137075.D
Acq On : 15 Jan 2024 21:03
Operator : CG\JU
Sample : P1139-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

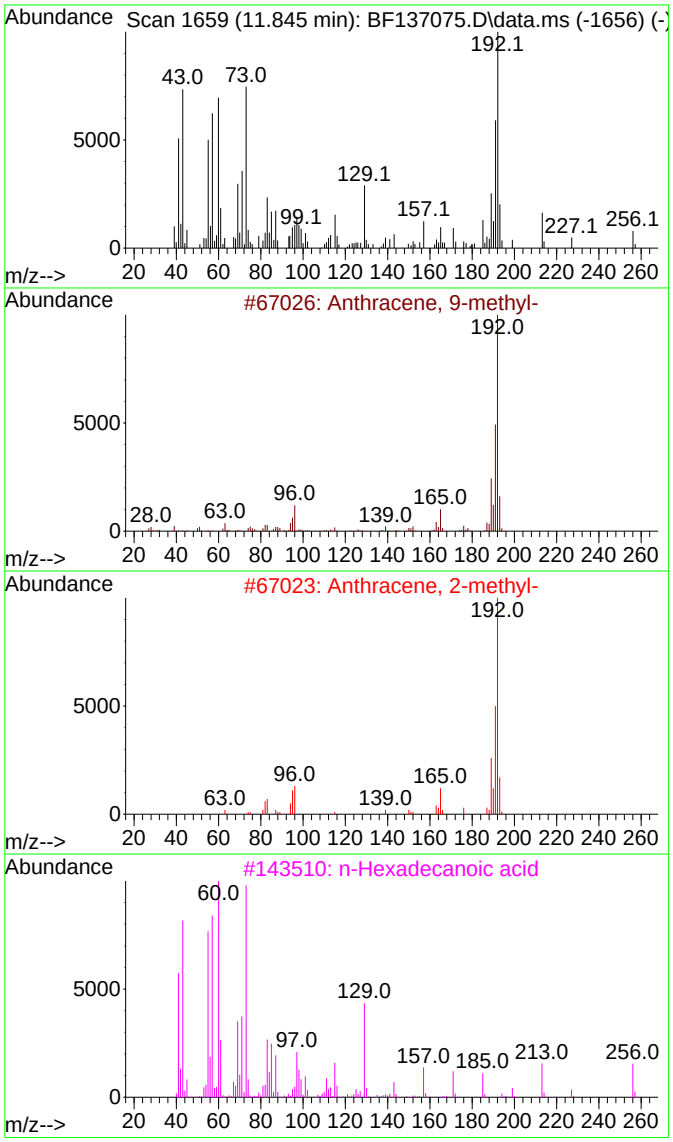
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

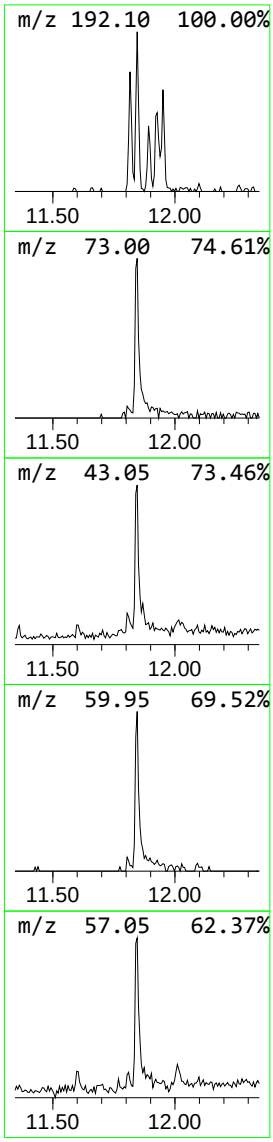
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Anthracene, 9-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	8.34 ng	139744	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137075.D
Acq On : 15 Jan 2024 21:03
Operator : CG\JU
Sample : P1139-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

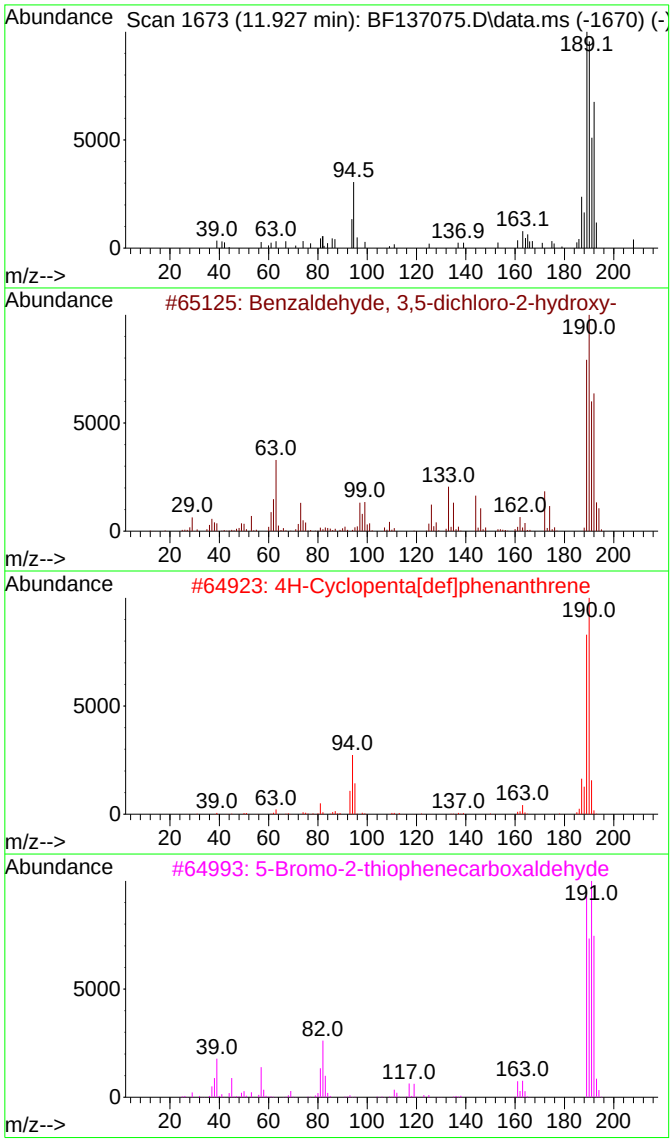
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

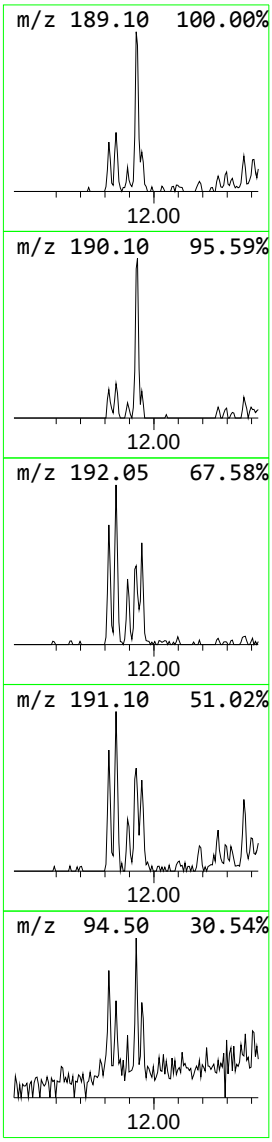
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	2.86 ng	47949	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
3	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	47
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22





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Sample : P1139-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-314-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

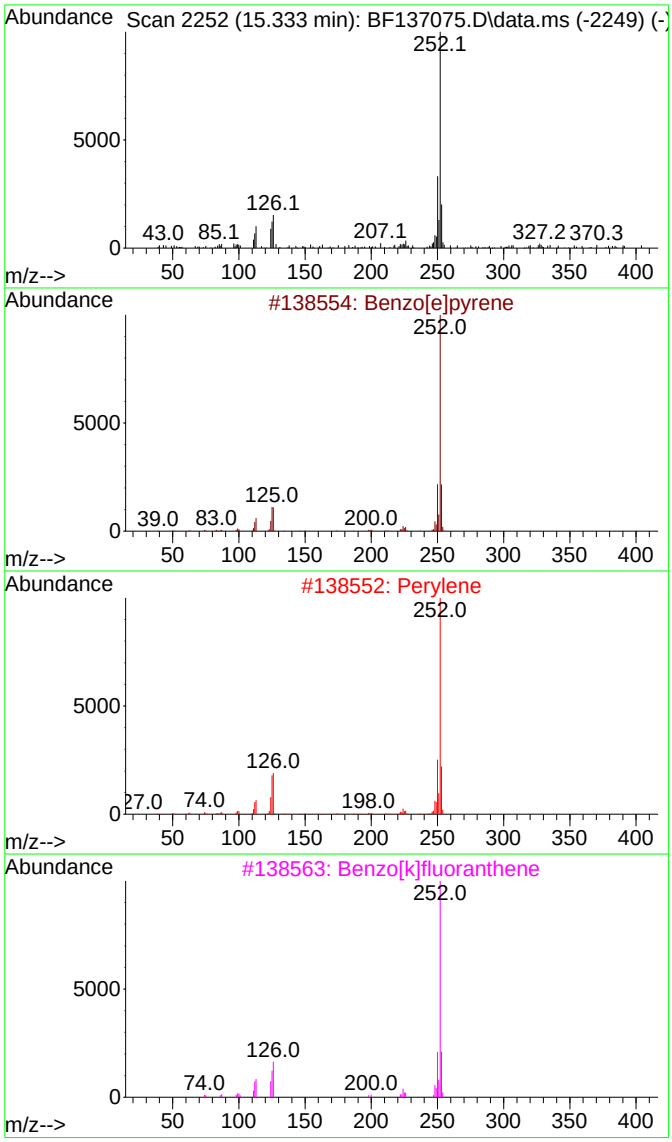
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

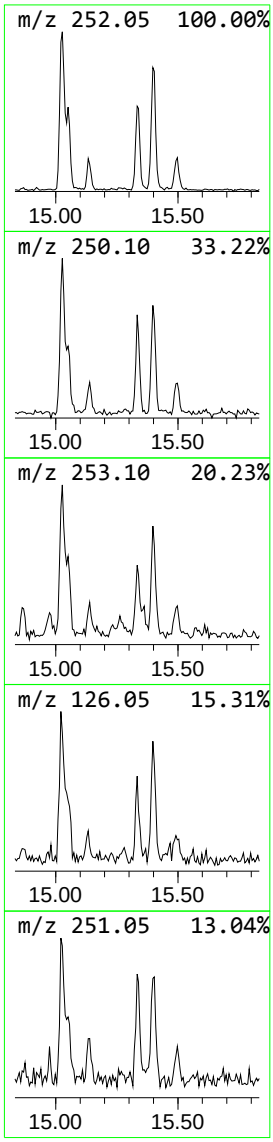
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	3.93 ng	41514	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Perylene	252	C20H12	000198-55-0	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	81





Tentatively Identified Compound (LSC) summary

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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.004	2.6	ng	27434	1	6.787	208736	20.0
Anthracene, 1-m...	11.816	3.6	ng	60040	4	11.310	334922	20.0
Anthracene, 9-m...	11.845	8.3	ng	139744	4	11.310	334922	20.0
Benzaldehyde, 3...	11.927	2.9	ng	47949	4	11.310	334922	20.0
Benzo[e]pyrene	15.333	3.9	ng	41514	6	15.462	211013	20.0