LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139111.D
Acq On : 21 Aug 2024 19:49
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	14	24	31	rVB	688179	1132124	54.40%	6.666%
2	5.122	506	515	522	rBV	81225	134167	6.45%	0.790%
3	5.516	576	582	587	rBV	1554872	2079855	99.94%	12.247%
4	6.516	745	752	765	rBV	1514479	2081097	100.00%	12.254%
5	6.898	812	817	822	rVB	393538	490832	23.59%	2.890%
6	7.457	905	912	917	rBV	952118	1247647	59.95%	7.346%
7	8.175	1029	1034	1039	rBV	461582	580787	27.91%	3.420%
8	8.487	1082	1087	1096	rBV	26824	33848	1.63%	0.199%
9	9.251	1211	1217	1222	rBV	1462695	1791136	86.07%	10.547%
10	9.928	1327	1332	1337	rBV	420041	531597	25.54%	3.130%
11	10.028	1344	1349	1354	rVB	21391	31354	1.51%	0.185%
12	10.716	1460	1466	1471	rBV	758661	944164	45.37%	5.559%
13	11.416	1580	1585	1588	rBV	384704	556406	26.74%	3.276%
14	11.492	1594	1598	1601	rBV	20535	24581	1.18%	0.145%
15	11.939	1671	1674	1679	rVB2	50016	68341	3.28%	0.402%
16	12.028	1685	1689	1698	rVB2	41139	64518	3.10%	0.380%
17	12.233	1717	1724	1728	rBV2	23828	46585	2.24%	0.274%
18	12.627	1786	1791	1796	rBV	447094	554991	26.67%	3.268%
19	12.727	1804	1808	1814	rBV5	16336	29744	1.43%	0.175%
20	12.857	1822	1830	1836	rBV	357693	593698	28.53%	3.496%
21	12.904	1836	1838	1843	rVB2	27260	32337	1.55%	0.190%
22	13.004	1846	1855	1860	rBV	1100154	1393787	66.97%	8.207%
23	13.075	1860	1867	1871	rBV2	16714	32799	1.58%	0.193%
24	13.186	1875	1886	1890	rBV	52054	96714	4.65%	0.569%
25	13.251	1893	1897	1900	rBV	52540	65260	3.14%	0.384%
26	13.804	1985	1991	1994	rBV	50769	87862	4.22%	0.517%
27	13.898	2003	2007	2014	rVB5	54410	99254	4.77%	0.584%
28	13.969	2014	2019	2022	rBV2	50937	69266	3.33%	0.408%
29	14.010	2022	2026	2028	rBV	19695	27043	1.30%	0.159%
30	14.051	2028	2033	2037	rBV2	450189	758079	36.43%	4.464%
31	14.157	2047	2051	2055	rBV	33335	45518	2.19%	0.268%
32	14.533	2112	2115	2118	rBV3	24275	33732	1.62%	0.199%
33	14.586	2121	2124	2129	rVB2	39541	55039	2.64%	0.324%
34	15.098	2206	2211	2222	rVB	144732	324362	15.59%	1.910%
35	15.198	2223	2228	2236	rVB4	40546	73414	3.53%	0.432%
36	15.404	2258	2263	2268	rVV	68148	98679	4.74%	0.581%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139111.D
Acq On : 21 Aug 2024 19:49
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.463	2269	2273	2279	rVV	82901	123811	5.95%	0.729%
38	15.533	2279	2285	2298	rVB	198548	358465	17.22%	2.111%
39	16.033	2366	2370	2375	rBV	19093	31561	1.52%	0.186%
40	17.004	2530	2535	2544	rVB2	43141	95678	4.60%	0.563%
41	17.451	2605	2611	2618	rBV	30233	63042	3.03%	0.371%

Sum of corrected areas: 16983174

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
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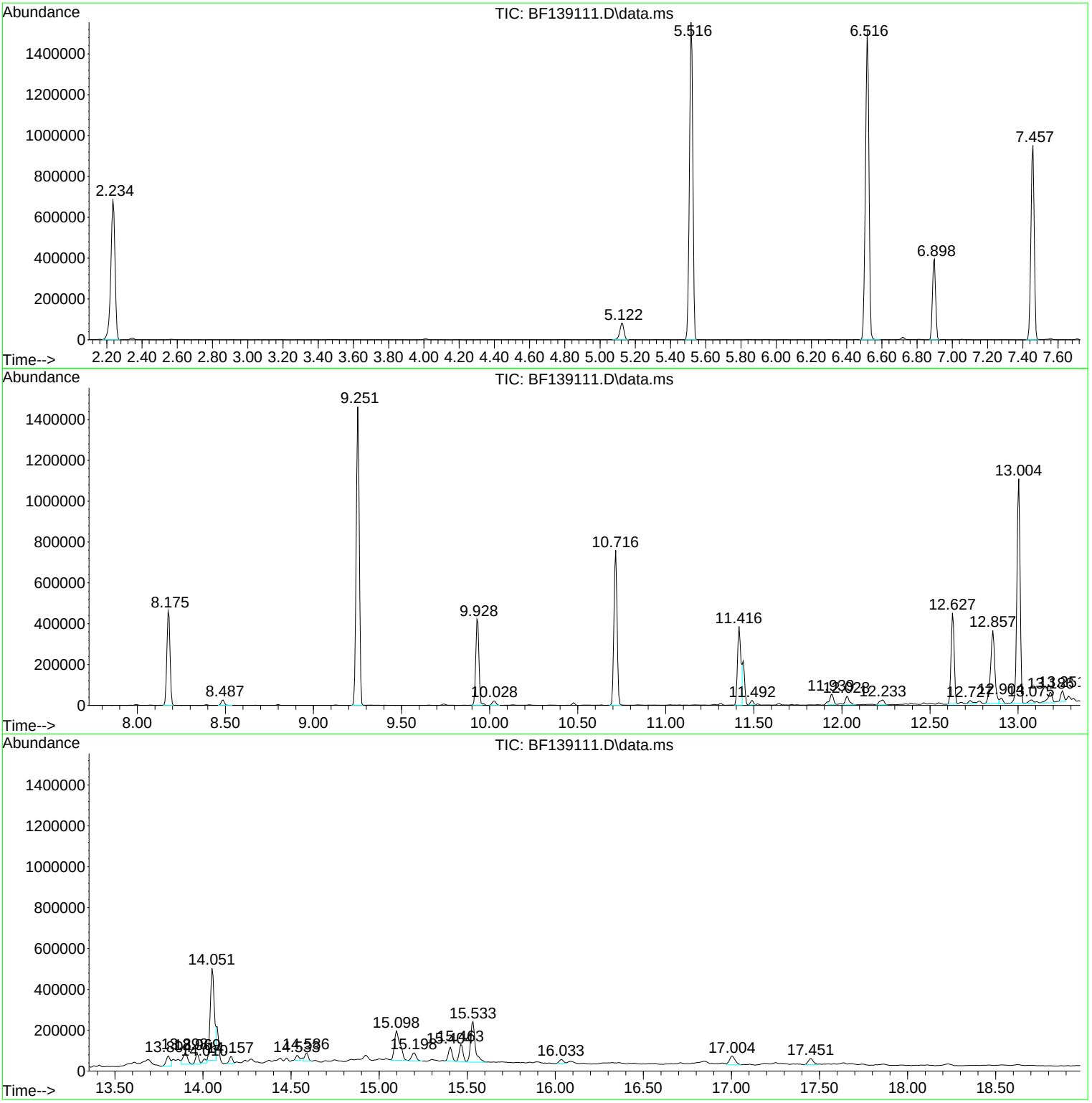
Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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\BF082124\
Data File : BF139111.D
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Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

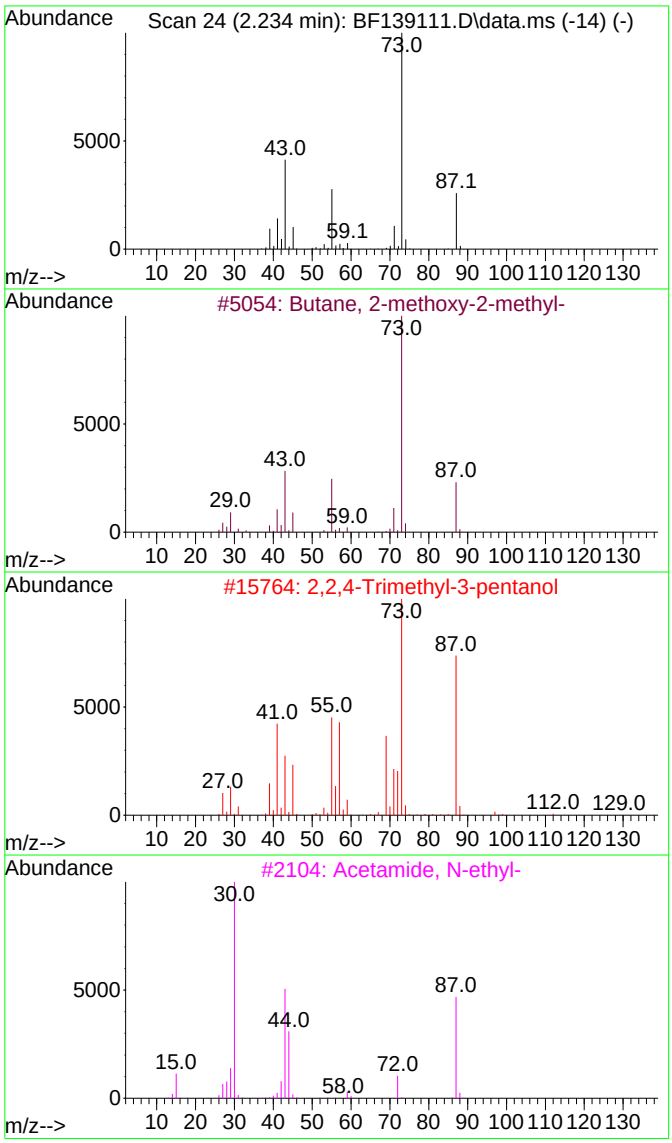
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

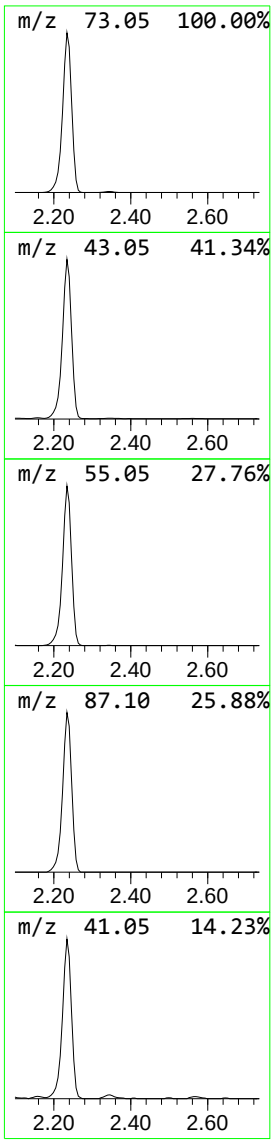
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	46.13 ng	1132120	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

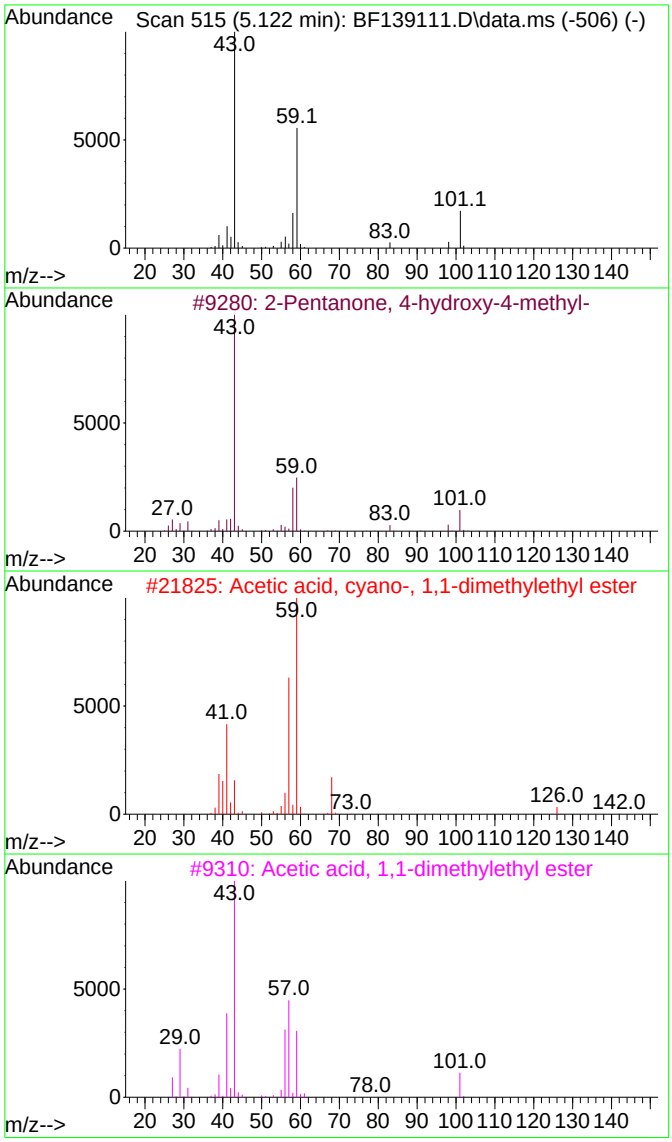
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

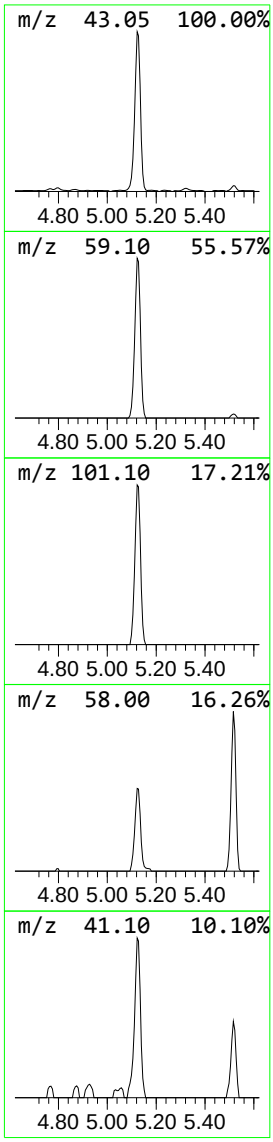
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	5.47 ng	134167	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Acetone	58	C3H6O	000067-64-1	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139111.D
Acq On : 21 Aug 2024 19:49
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

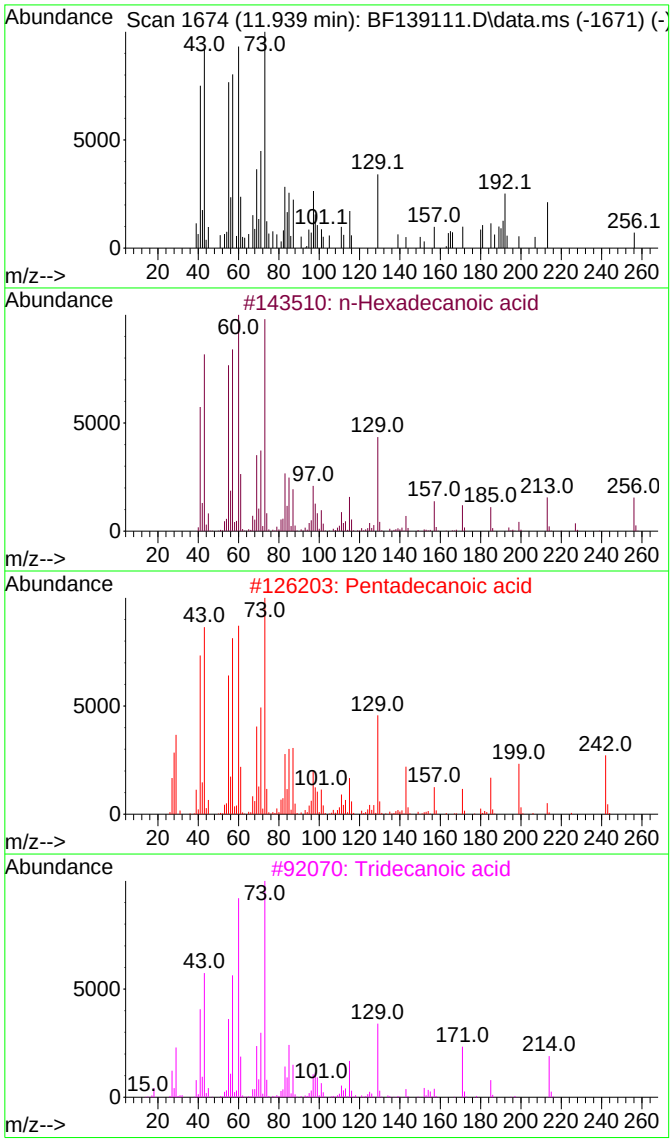
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

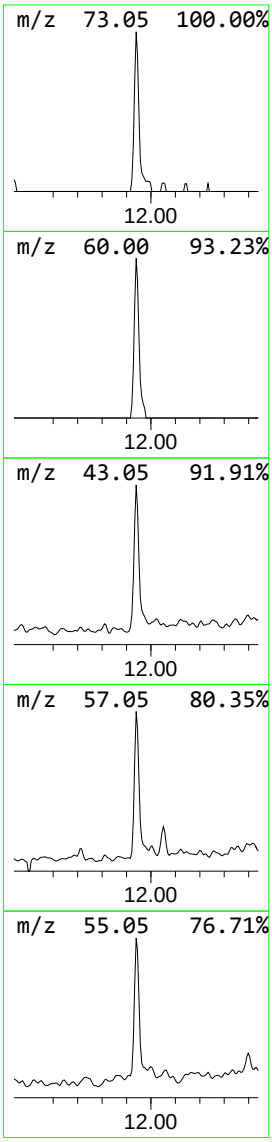
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.46 ng	68341	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
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Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

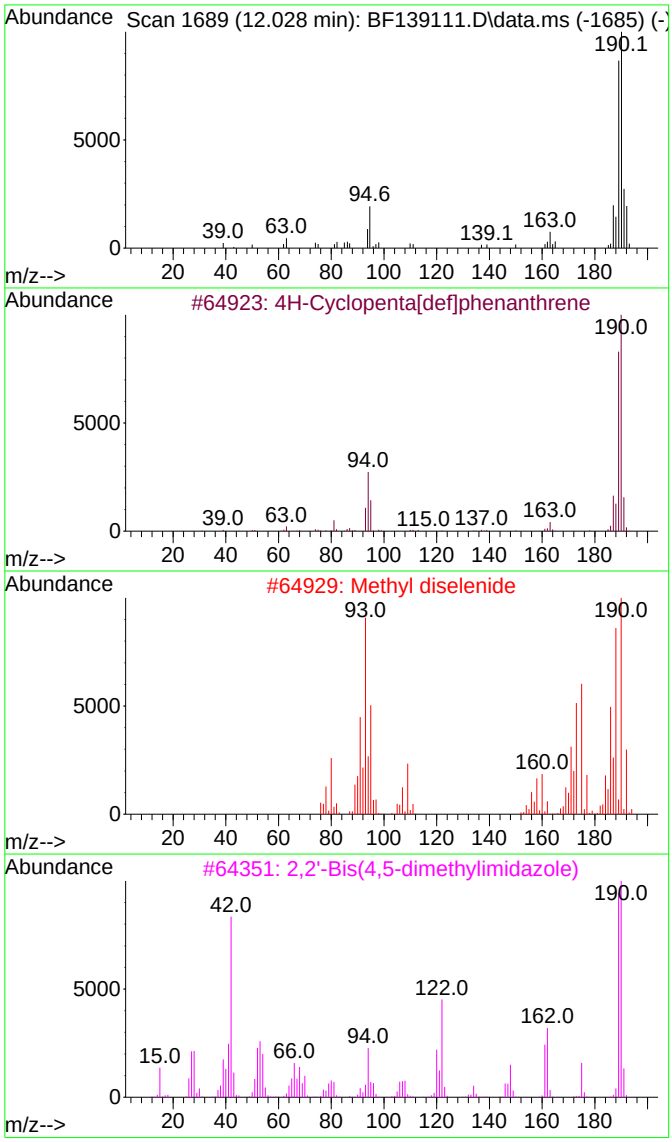
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

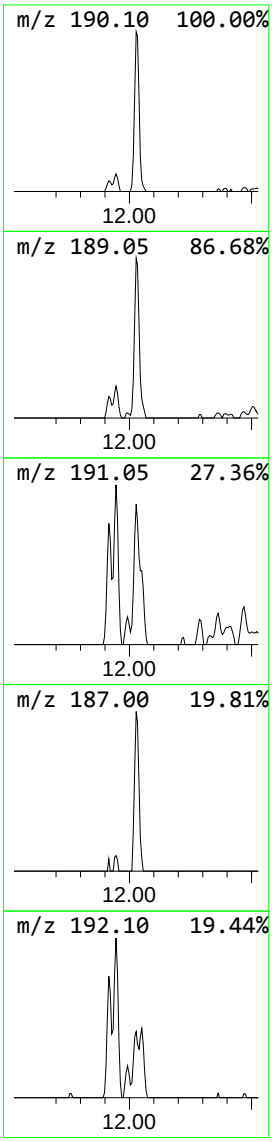
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	2.32 ng	64518	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Methyl diselenide	190	C2H6Se2	007101-31-7	49
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	36
5	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
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Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

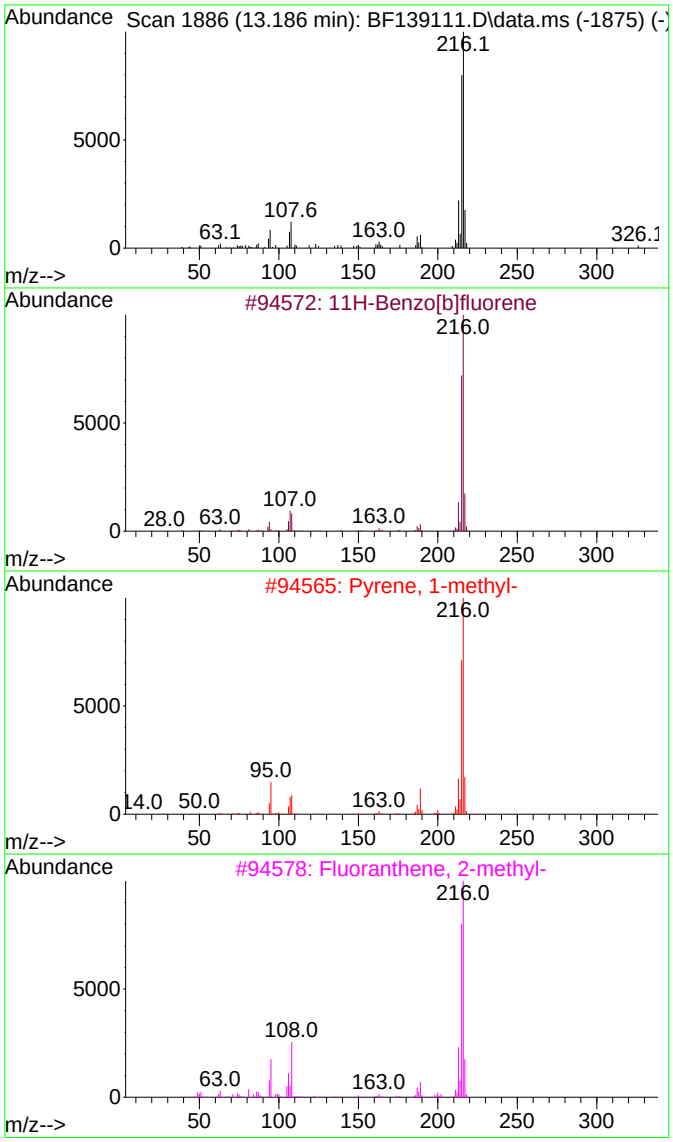
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

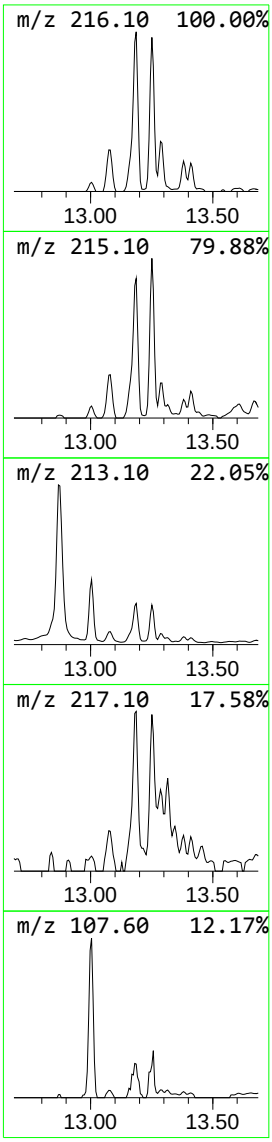
****

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.186	2.55 ng	96714	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	97
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91





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Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

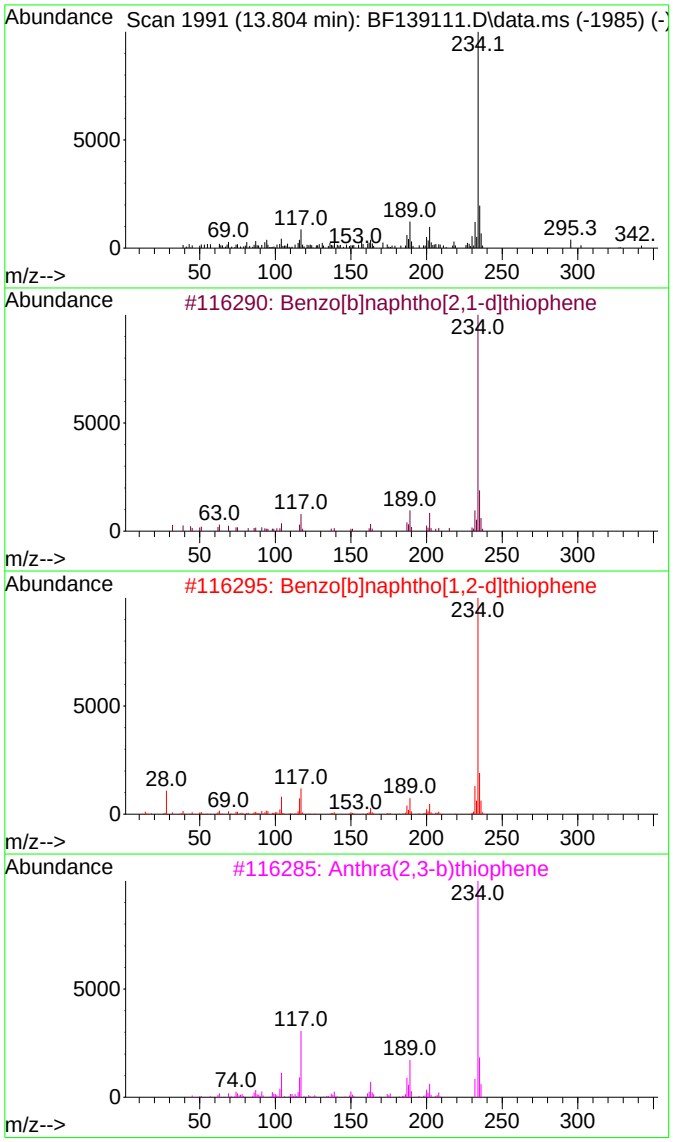
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

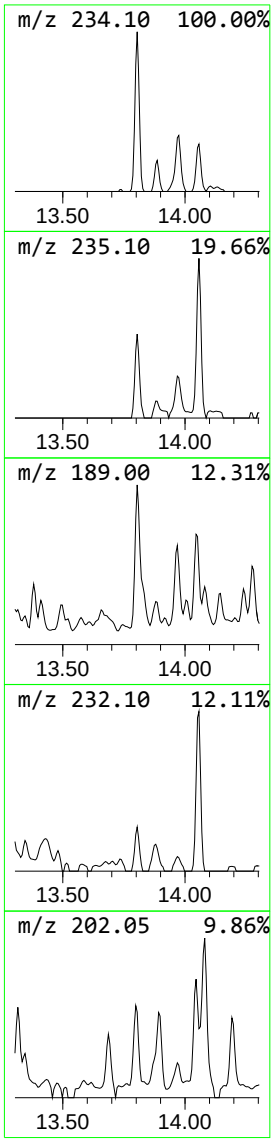
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	2.32 ng	87862	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	97
2	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	95
3	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	94
4	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	93
5	Phenanthro[4,3-b]thiophene	234	C16H10S	000195-68-6	81





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

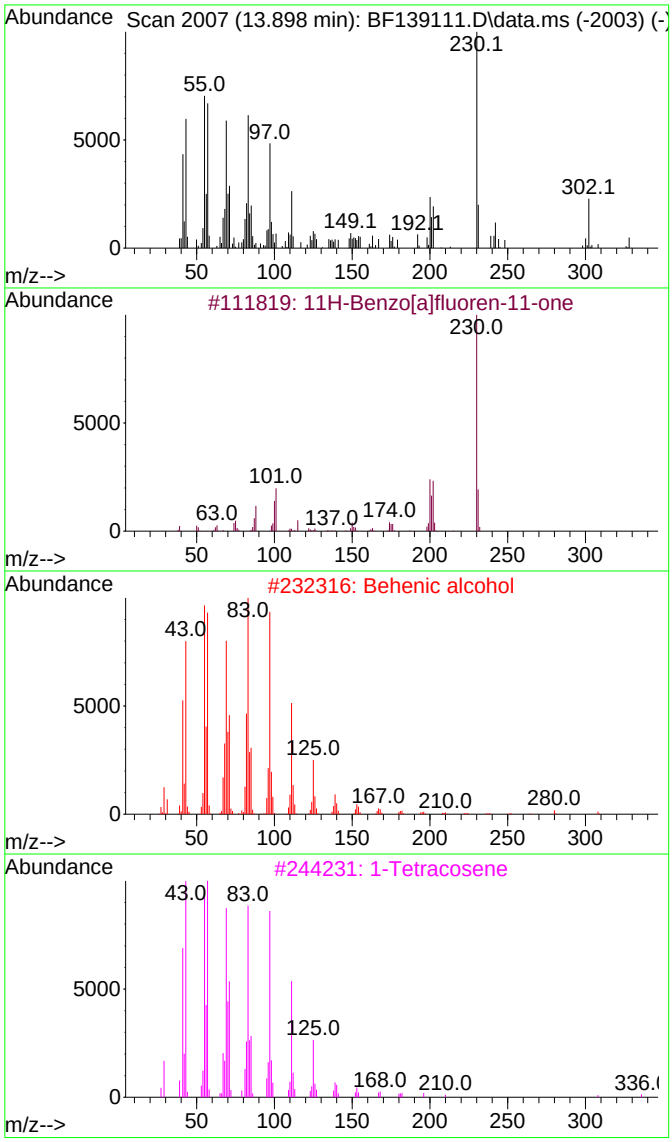
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

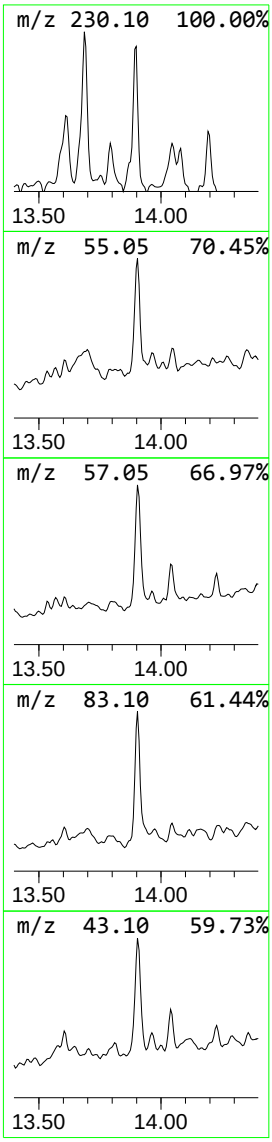
****

Peak Number 7 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.62 ng	99254	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	45
2	Behenic alcohol	326	C22H46O	000661-19-8	42
3	1-Tetracosene	336	C24H48	010192-32-2	42
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	42
5	1-Hexacosene	364	C26H52	018835-33-1	42





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Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

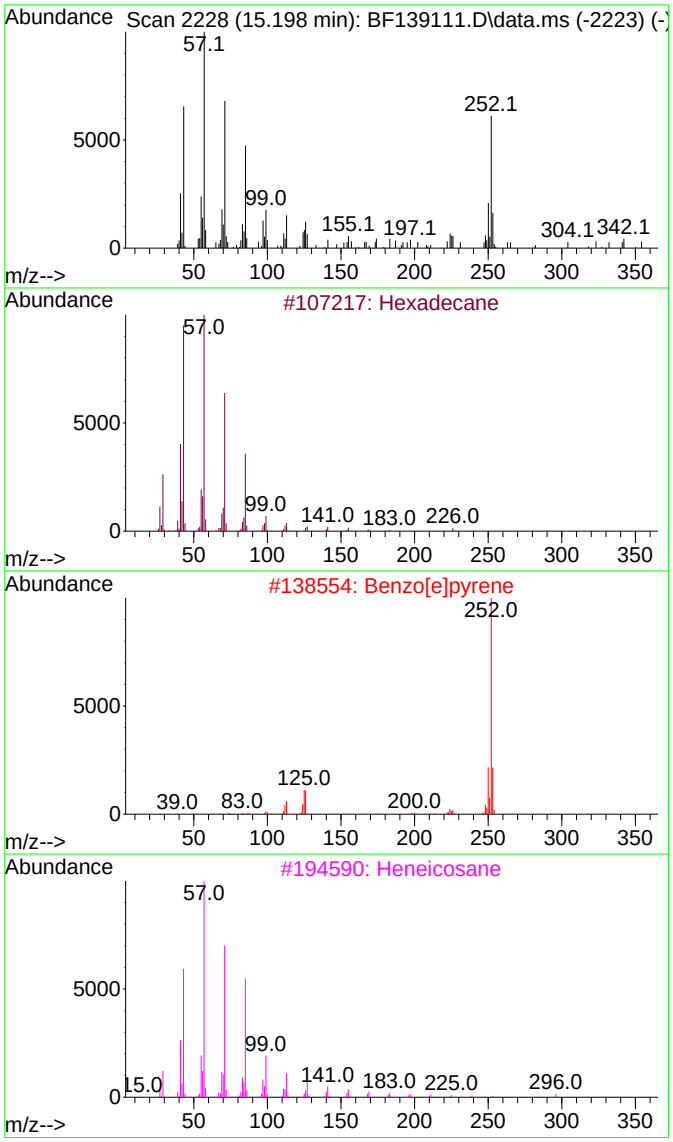
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

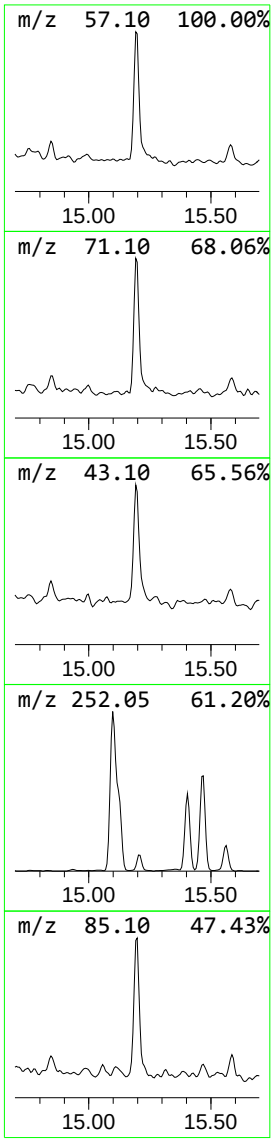
****

Peak Number 8 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	4.10 ng	73414	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Benzo[e]pyrene	252	C20H12	000192-97-2	50
3	Heneicosane	296	C21H44	000629-94-7	46
4	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	46
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	46





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Data File : BF139111.D
Acq On : 21 Aug 2024 19:49
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

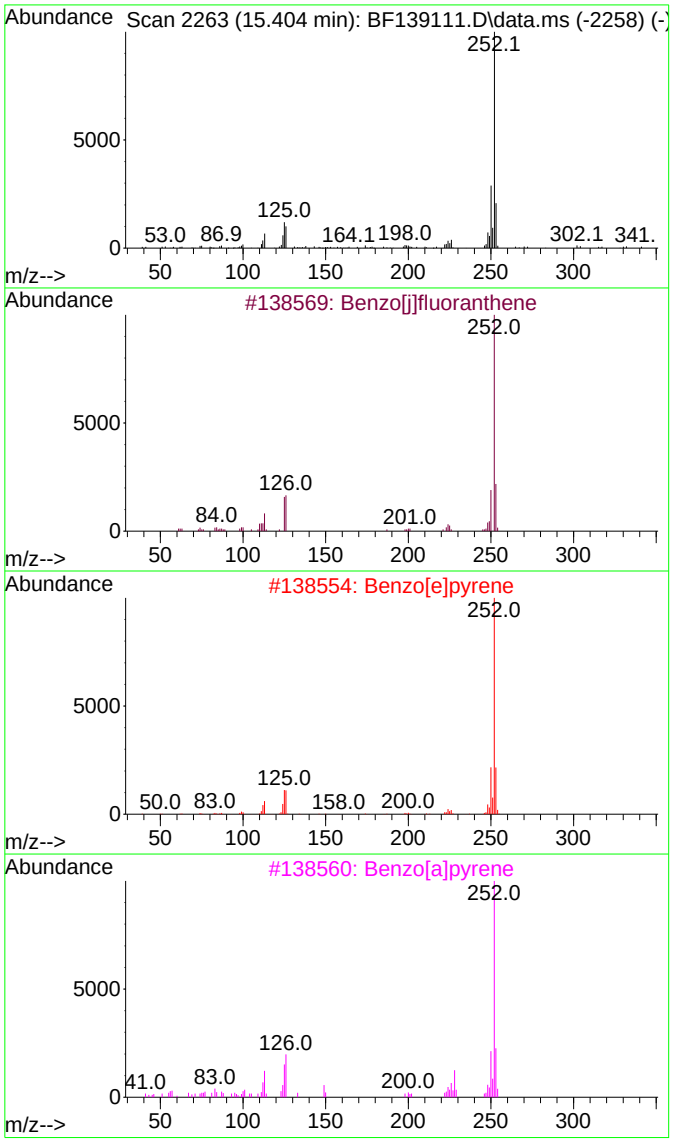
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

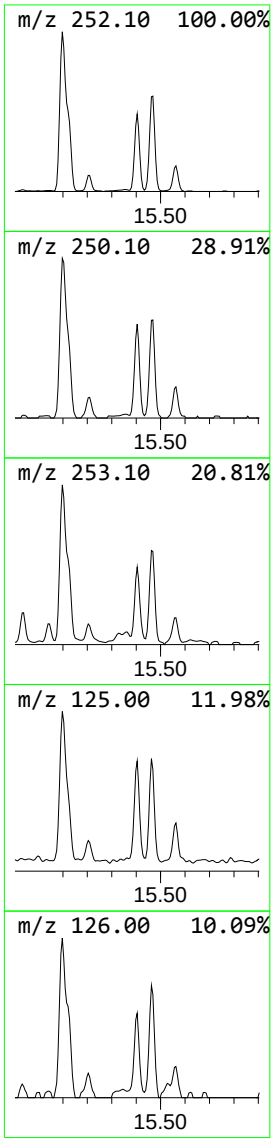
****

Peak Number 9 Benzo[j]fluoranthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	5.51 ng	98679	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	90
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139111.D
Acq On : 21 Aug 2024 19:49
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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
Butane, 2-metho...	2.234	46.1	ng	1132120	1	6.898	490832	20.0
2-Pentanone, 4-...	5.122	5.5	ng	134167	1	6.898	490832	20.0
n-Hexadecanoic ...	11.939	2.5	ng	68341	4	11.416	556406	20.0
4H-Cyclopenta[d...	12.028	2.3	ng	64518	4	11.416	556406	20.0
11H-Benzo[b]flu...	13.186	2.5	ng	96714	5	14.057	758079	20.0
Benzo[b]naphtho...	13.804	2.3	ng	87862	5	14.057	758079	20.0
11H-Benzo[a]flu...	13.898	2.6	ng	99254	5	14.057	758079	20.0
Hexadecane	15.198	4.1	ng	73414	6	15.533	358465	20.0
Benzo[j]fluoran...	15.404	5.5	ng	98679	6	15.533	358465	20.0