LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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: BF139134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	14	20	rVB	229855	360137	34.20%	3.812%
2	5.104	503	512	518	rBV	17872	24534	2.33%	0.260%
3	5.510	575	581	586	rVB	274256	351327	33.36%	3.718%
4	6.445	736	740	745	rBV2	10890	14025	1.33%	0.148%
5	6.516	746	752	763	rVB	266281	337376	32.04%	3.571%
6	6.898	812	817	822	rVB	448643	535228	50.82%	5.665%
7	7.051	838	843	849	rVB	20000	24563	2.33%	0.260%
8	7.451	906	911	916	rBV	162810	197990	18.80%	2.095%
9	8.181	1030	1035	1040	rBV	487150	591072	56.13%	6.256%
10	8.487	1081	1087	1096	rBV	8972	12474	1.18%	0.132%
11	8.892	1151	1156	1161	rBV4	7802	11006	1.05%	0.116%
12	9.251	1212	1217	1222	rBV	236127	275931	26.20%	2.920%
13	9.934	1328	1333	1337	rBV	458683	558367	53.02%	5.909%
14	9.963	1337	1338	1342	rVB	12602	10574	1.00%	0.112%
15	10.481	1422	1426	1432	rVB	10661	13244	1.26%	0.140%
16	10.716	1461	1466	1471	rVB	135254	161346	15.32%	1.708%
17	11.222	1547	1552	1556	rVB	10162	13591	1.29%	0.144%
18	11.316	1564	1568	1572	rVB	9187	11034	1.05%	0.117%
19	11.422	1581	1586	1588	rBV	420355	595914	56.59%	6.307%
20	11.492	1594	1598	1601	rBV	29354	34739	3.30%	0.368%
21	11.528	1601	1604	1611	rVB3	8974	11958	1.14%	0.127%
22	11.645	1618	1624	1630	rBV	22751	32679	3.10%	0.346%
23	11.851	1650	1659	1665	rBV7	8094	20124	1.91%	0.213%
24	11.945	1665	1675	1680	rBV2	50178	104519	9.92%	1.106%
25	12.033	1686	1690	1698	rVB	44235	76783	7.29%	0.813%
26	12.233	1717	1724	1730	rVB2	51762	90310	8.58%	0.956%
27	12.469	1760	1764	1767	rBV	19731	24907	2.37%	0.264%
28	12.504	1767	1770	1775	rVV4	8508	14279	1.36%	0.151%
29	12.551	1775	1778	1785	rVB2	20939	28208	2.68%	0.299%
30	12.633	1786	1792	1797	rBV	542242	697111	66.20%	7.378%
31	12.780	1815	1817	1822	rVB	15514	19904	1.89%	0.211%
32	12.857	1823	1830	1837	rBV	423194	697111	66.20%	7.378%
33	13.004	1847	1855	1861	rVB	209867	307803	29.23%	3.258%
34	13.074	1861	1867	1871	rBV3	32452	63190	6.00%	0.669%
35	13.186	1878	1886	1890	rBV	48921	87913	8.35%	0.930%
36	13.251	1894	1897	1900	rBV2	31424	37084	3.52%	0.392%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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	13.292	1900	1904	1907	rBV2	32044	44829	4.26%	0.474%
38	13.380	1916	1919	1922	rBV	12235	14541	1.38%	0.154%
39	13.416	1922	1925	1930	rVV3	12326	16303	1.55%	0.173%
40	13.586	1947	1954	1957	rBV8	17150	42703	4.05%	0.452%
41	13.692	1968	1972	1985	rVB	50479	109292	10.38%	1.157%
42	13.804	1986	1991	1994	rBV2	48350	80746	7.67%	0.855%
43	13.833	1994	1996	1998	rBV	14406	16033	1.52%	0.170%
44	13.898	2004	2007	2014	rVB3	57763	88136	8.37%	0.933%
45	14.057	2026	2034	2045	rBV2	483100	1053107	100.00%	11.146%
46	14.163	2049	2052	2055	rVB	21964	25504	2.42%	0.270%
47	14.474	2103	2105	2109	rVB2	25578	29289	2.78%	0.310%
48	14.539	2112	2116	2119	rBV2	41726	64662	6.14%	0.684%
49	15.104	2207	2212	2222	rVB	179858	400289	38.01%	4.236%
50	15.198	2224	2228	2237	rVB3	49629	120253	11.42%	1.273%
51	15.410	2259	2264	2269	rVB	86969	132598	12.59%	1.403%
52	15.468	2270	2274	2280	rBV	105759	154261	14.65%	1.633%
53	15.533	2280	2285	2290	rBV	218696	342334	32.51%	3.623%
54	16.033	2366	2370	2375	rBV	35097	58495	5.55%	0.619%
55	17.015	2531	2537	2548	rVB2	52401	125042	11.87%	1.323%
56	17.462	2608	2613	2622	rVB	39559	81876	7.77%	0.867%

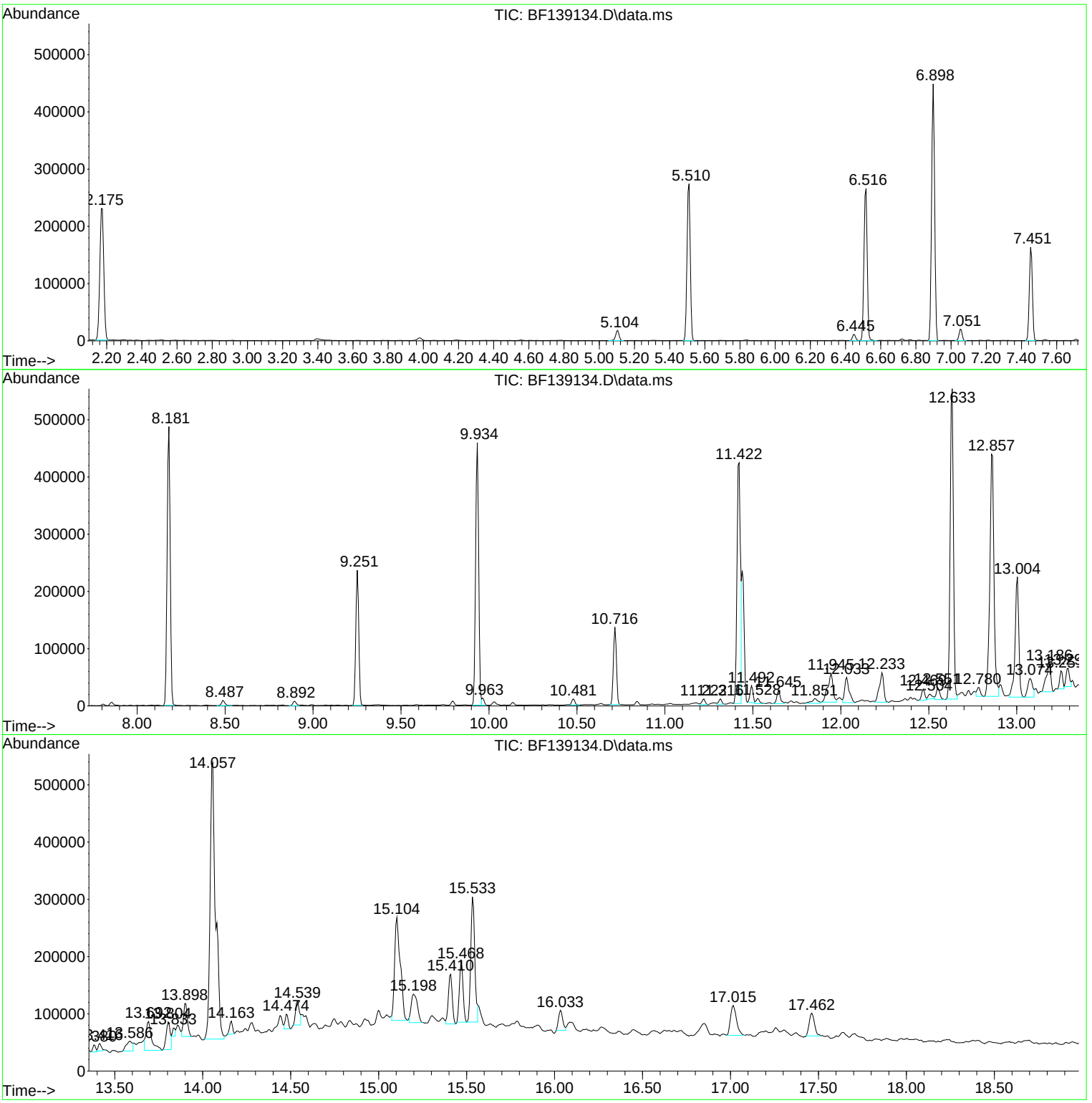
Sum of corrected areas: 9448648

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
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Instrument :
BNA_F
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S-910-K1-0-0.5-081524

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

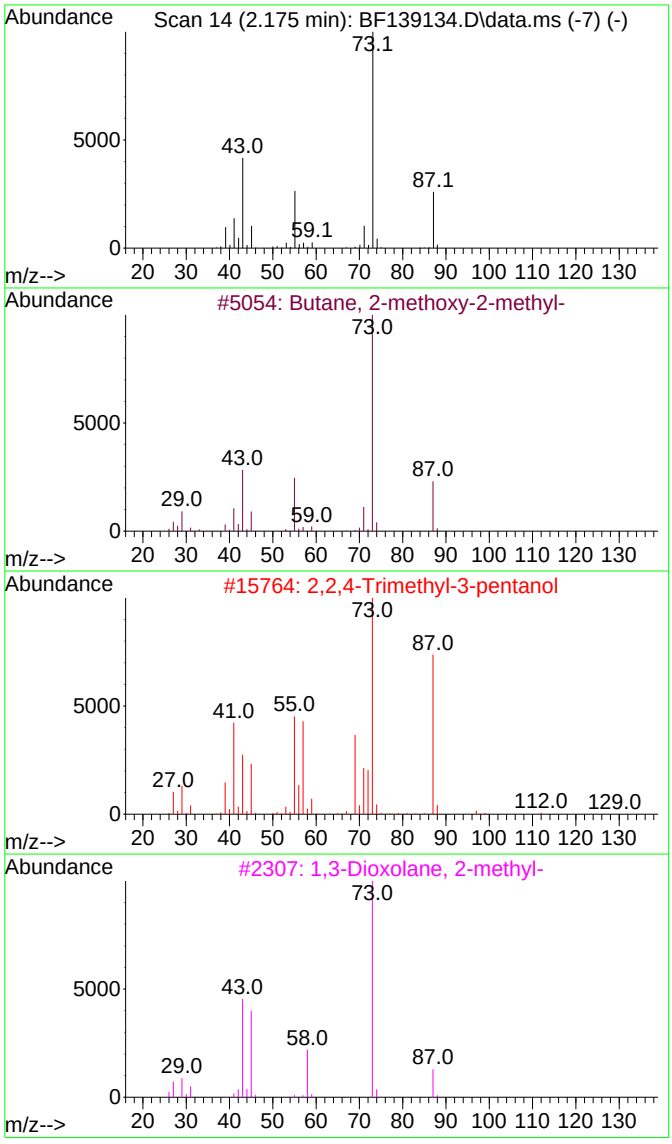
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

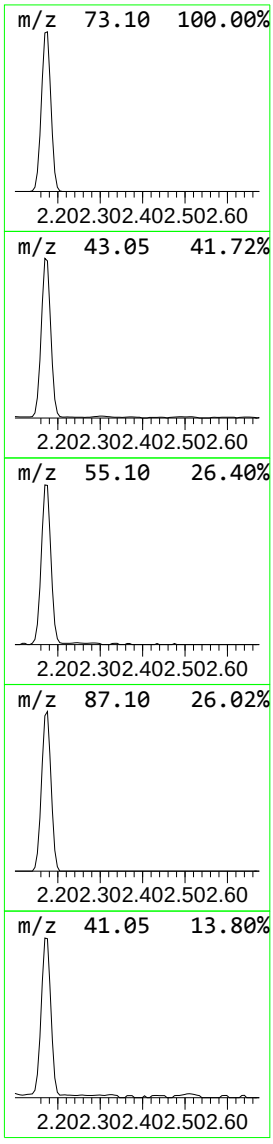
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	13.46 ng	360137	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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

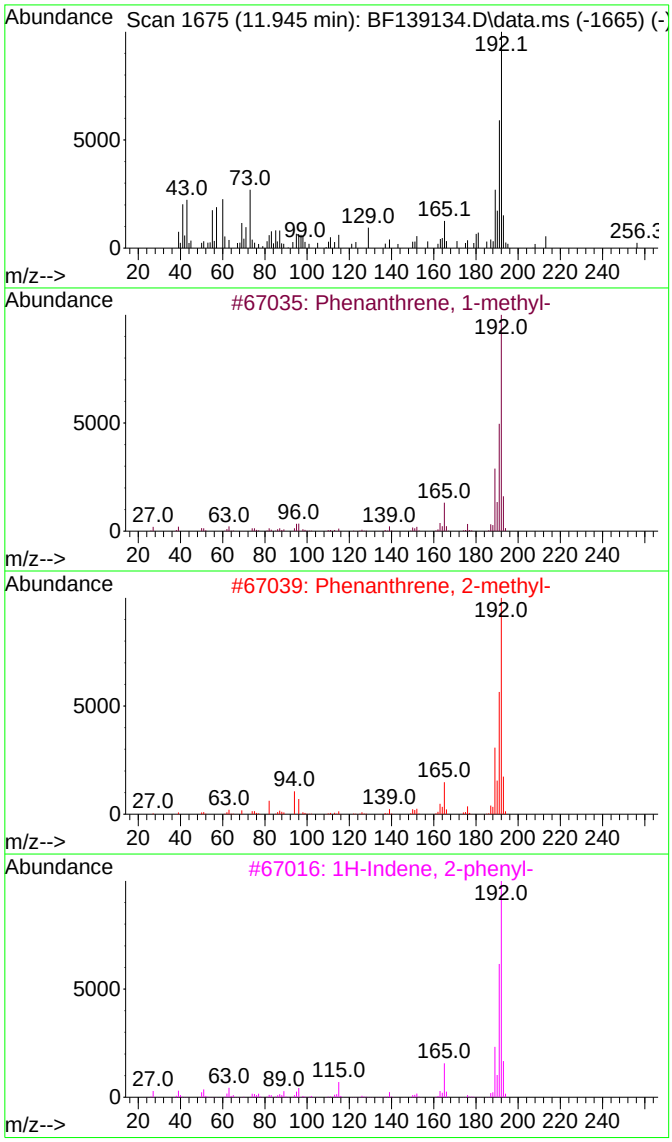
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

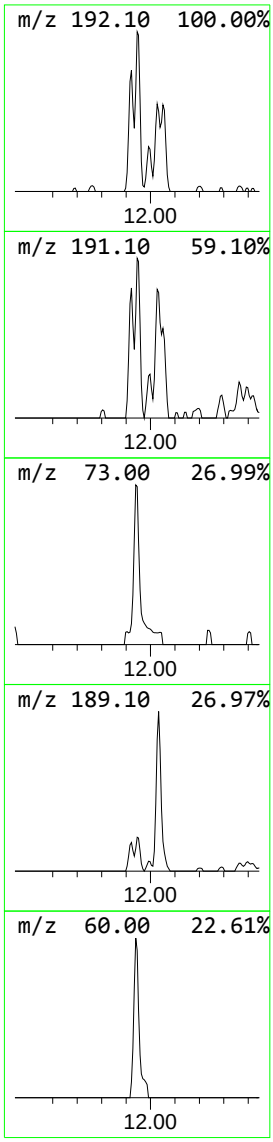
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.51 ng	104519	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

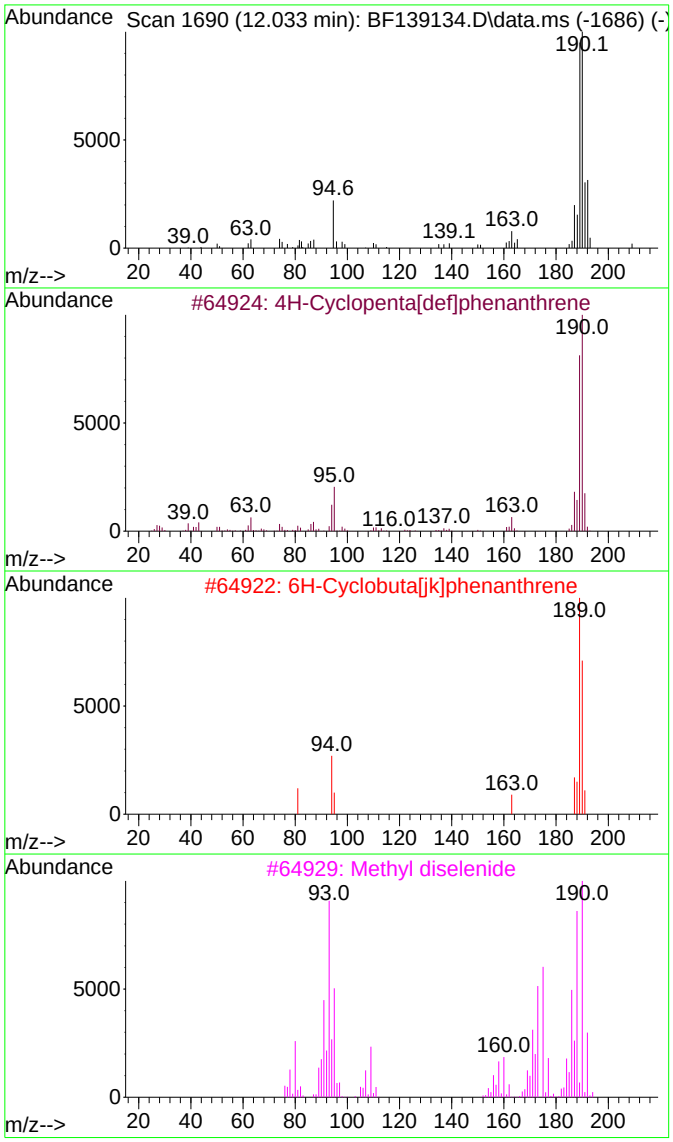
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

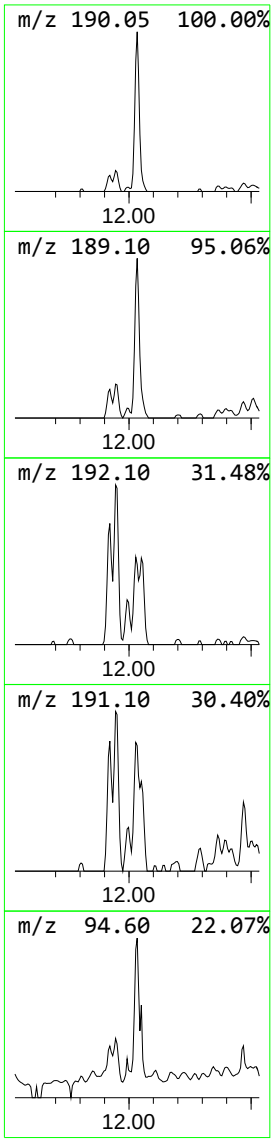
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.58 ng	76783	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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

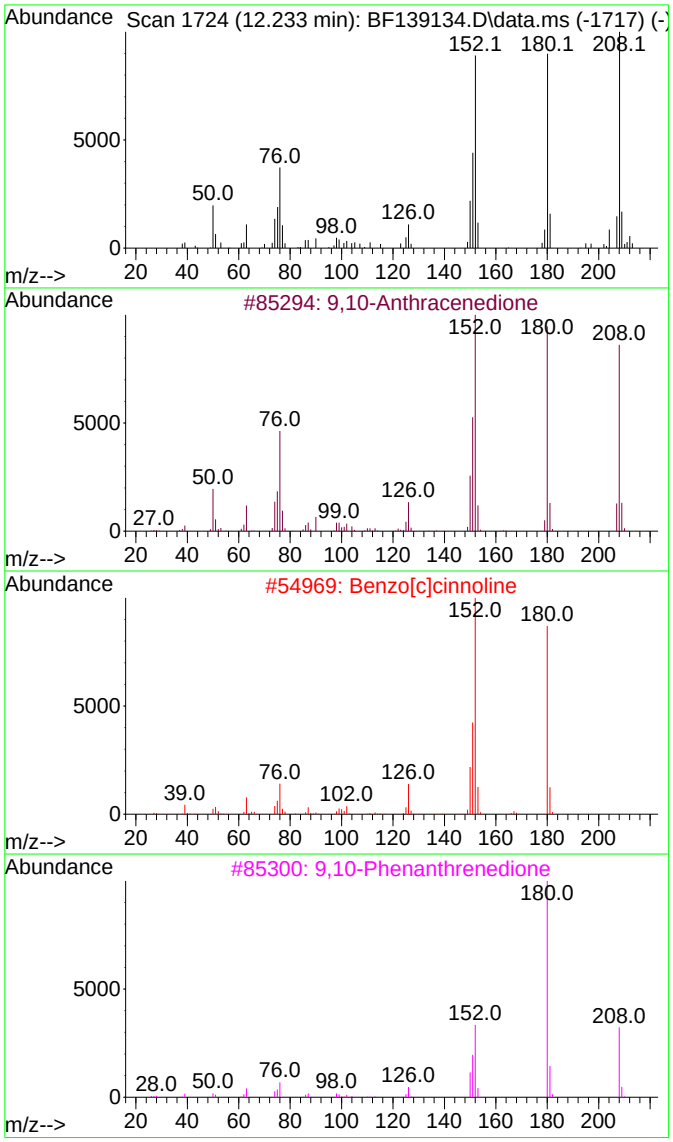
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

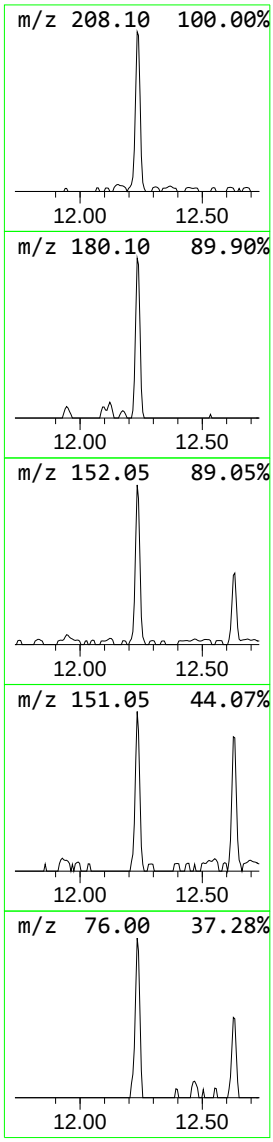
****

Peak Number 4 9,10-Anthracenedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	3.03 ng	90310	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	92
3	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	60
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
5	9H-Fluoren-9-one	180	C13H8O	000486-25-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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

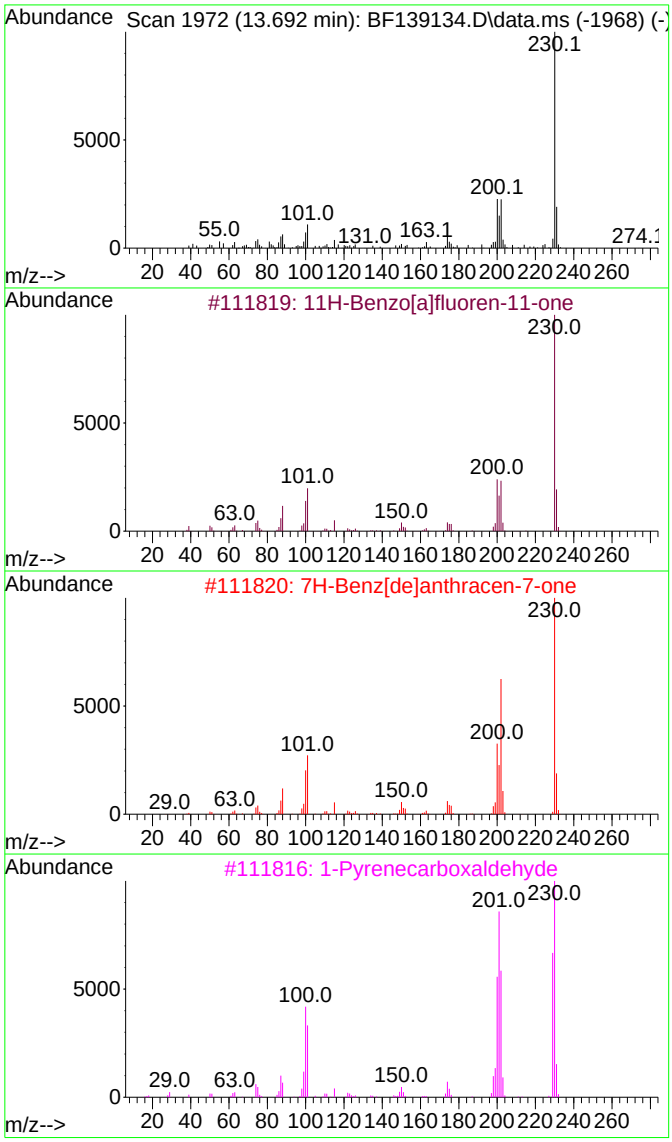
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

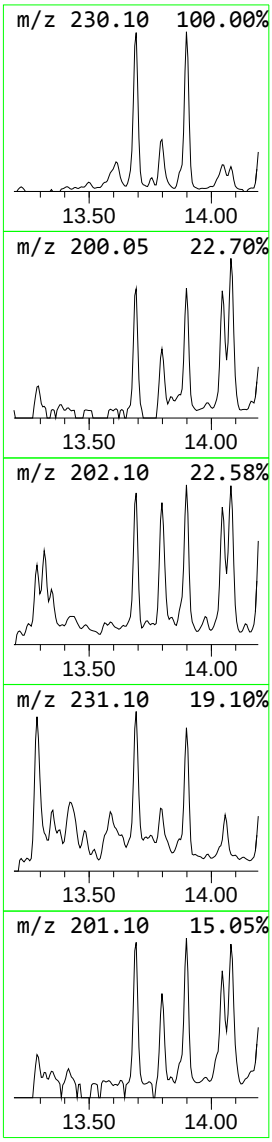
****

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.692	2.08 ng	109292	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	94
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	87
3	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	83
4	.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	76
5	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	72





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Instrument :
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ClientSampleId :
S-910-K1-0-0.5-081524

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

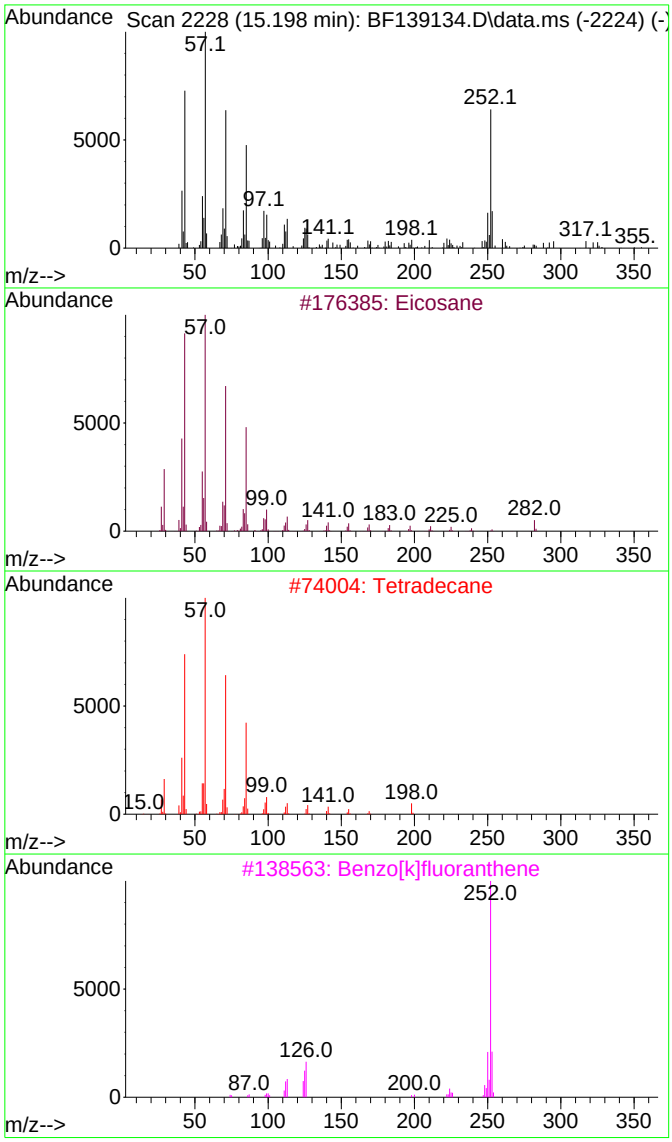
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

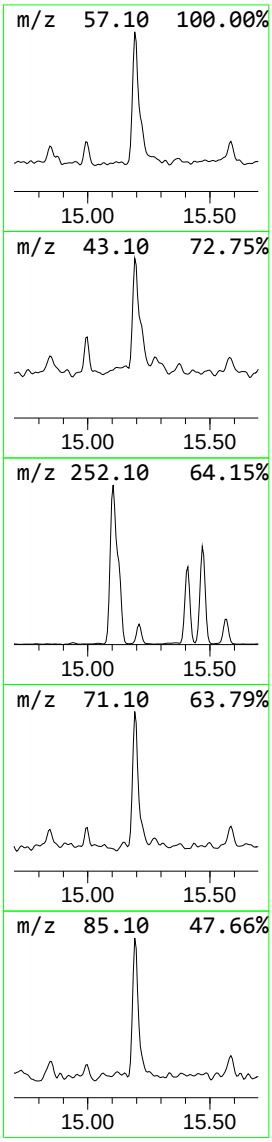
****

Peak Number 6 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	7.03 ng	120253	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	84
2	Tetradecane	198	C14H30	000629-59-4	83
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	83
4	Benzo[a]pyrene	252	C20H12	000050-32-8	70
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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

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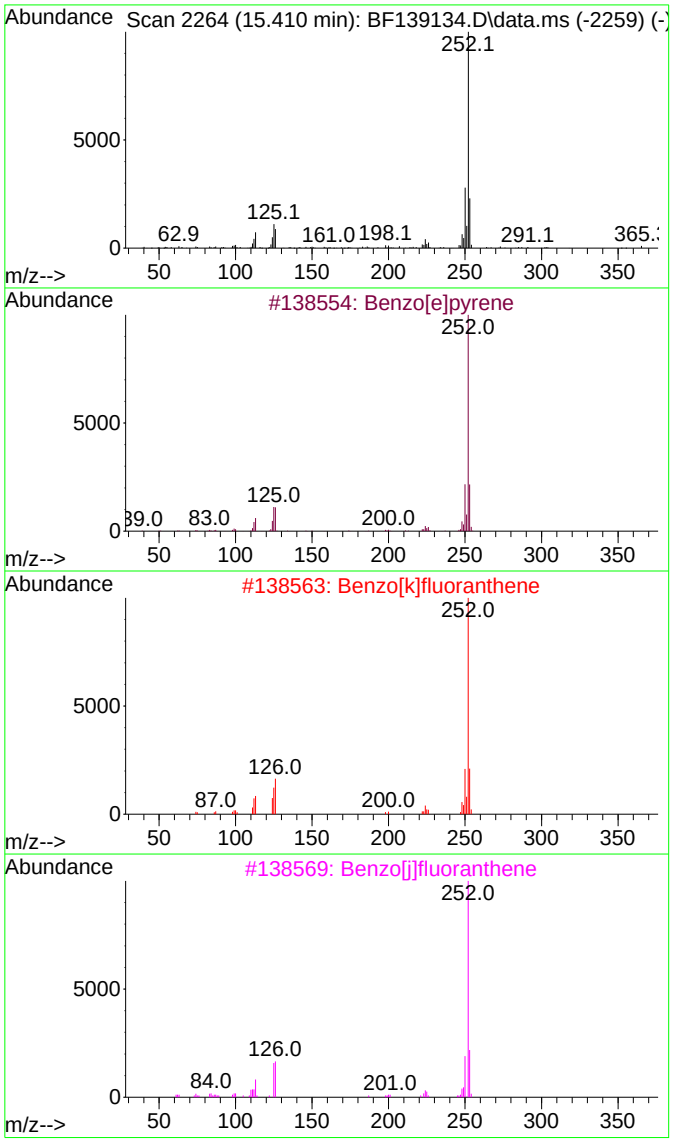
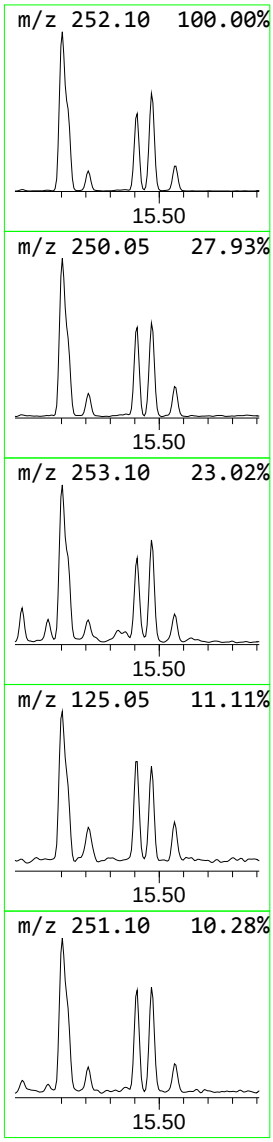
Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	7.75 ng	132598	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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

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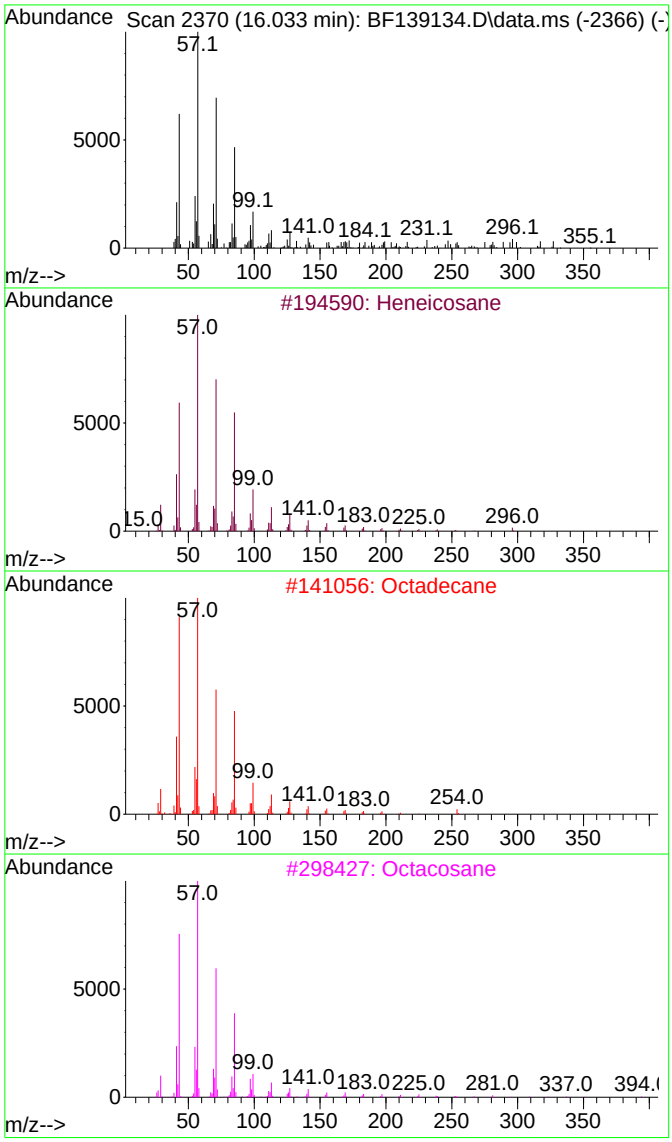
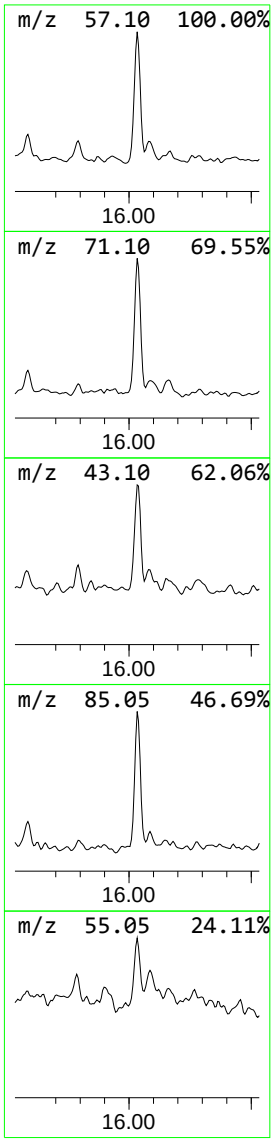
Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	3.42 ng	58495	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Octadecane	254	C18H38	000593-45-3	95
3	Octacosane	394	C28H58	000630-02-4	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5	Hexacosane	366	C26H54	000630-01-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139134.D
Acq On : 22 Aug 2024 20:50
Operator : RC/JU
Sample : P3641-07 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0-0.5-081524

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...	2.175	13.5	ng	360137	1	6.898	535228	20.0
Phenanthrene, 1...	11.945	3.5	ng	104519	4	11.422	595914	20.0
4H-Cyclopenta[d...	12.033	2.6	ng	76783	4	11.422	595914	20.0
9,10-Anthracene...	12.233	3.0	ng	90310	4	11.422	595914	20.0
11H-Benzo[a]flu...	13.692	2.1	ng	109292	5	14.057	1053110	20.0
Eicosane	15.198	7.0	ng	120253	6	15.533	342334	20.0
Benzo[e]pyrene	15.410	7.8	ng	132598	6	15.533	342334	20.0
Heneicosane	16.033	3.4	ng	58495	6	15.533	342334	20.0