LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
Data File : BF135455.D
Acq On : 26 Sep 2023 16:25
Operator : CG\JU
Sample : 04531-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-A

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.998	491	495	503	rVB	34624	50638	1.25%	0.151%
2	5.393	558	562	582	rBV	3934072	3948007	97.26%	11.749%
3	6.404	729	734	748	rBV	3759958	4059407	100.00%	12.081%
4	6.593	760	766	780	rBV	74785	156290	3.85%	0.465%
5	6.751	790	793	800	rBV	1228460	1076725	26.52%	3.204%
6	7.322	885	890	893	rBV	2451754	2569973	63.31%	7.648%
7	8.034	1007	1011	1014	rBV	1550339	1364869	33.62%	4.062%
8	9.110	1189	1194	1197	rBV	4123249	3844557	94.71%	11.441%
9	9.234	1209	1215	1226	rVB	1518984	1657161	40.82%	4.932%
10	9.381	1236	1240	1245	rVB2	37783	40969	1.01%	0.122%
11	9.786	1302	1309	1313	rBV	1611101	1442680	35.54%	4.293%
12	9.822	1313	1315	1320	rVB	76004	67119	1.65%	0.200%
13	9.998	1339	1345	1349	rBV	58054	65873	1.62%	0.196%
14	10.339	1399	1403	1407	rBV	66607	59680	1.47%	0.178%
15	10.581	1440	1444	1461	rBV	2144470	2166126	53.36%	6.446%
16	10.792	1475	1480	1487	rBV4	20874	55821	1.38%	0.166%
17	10.886	1490	1496	1500	rBV3	38367	71439	1.76%	0.213%
18	11.280	1559	1563	1565	rBV	1536967	1293681	31.87%	3.850%
19	11.304	1565	1567	1571	rVV	461783	357591	8.81%	1.064%
20	11.357	1571	1576	1579	rVB	146501	142894	3.52%	0.425%
21	11.680	1627	1631	1638	rVB2	43597	42031	1.04%	0.125%
22	11.816	1651	1654	1660	rBV	378206	372621	9.18%	1.109%
23	11.898	1664	1668	1671	rBV	80518	81705	2.01%	0.243%
24	12.386	1745	1751	1756	rBV4	95983	131626	3.24%	0.392%
25	12.498	1767	1770	1774	rBV	535084	449158	11.06%	1.337%
26	12.533	1774	1776	1780	rVB2	75302	67089	1.65%	0.200%
27	12.604	1785	1788	1794	rBV4	45228	78673	1.94%	0.234%
28	12.727	1803	1809	1812	rBV	448103	480642	11.84%	1.430%
29	12.780	1815	1818	1824	rVB3	33032	41212	1.02%	0.123%
30	12.874	1830	1834	1838	rBV	2693808	2562128	63.12%	7.625%
31	12.951	1843	1847	1851	rBV2	25910	43236	1.07%	0.129%
32	13.063	1863	1866	1870	rVB	70758	73672	1.81%	0.219%
33	13.169	1880	1884	1887	rBV2	43676	50763	1.25%	0.151%
34	13.451	1929	1932	1936	rBV4	44653	53928	1.33%	0.160%
35	13.857	1996	2001	2007	rBV5	62146	167691	4.13%	0.499%
36	13.939	2010	2015	2018	rVV2	1043333	1217989	30.00%	3.625%

LSC Area Percent Report

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Operator : CG\JU
Sample : 04531-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-A

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.963	2018	2019	2022	rVB	219796	137256	3.38%	0.408%
38	14.045	2030	2033	2036	rVB	46179	43852	1.08%	0.131%
39	14.327	2079	2081	2084	rVB	55136	47568	1.17%	0.142%
40	14.410	2093	2095	2100	rVB3	46149	56814	1.40%	0.169%
41	14.698	2141	2144	2155	rVB2	151329	212151	5.23%	0.631%
42	14.786	2156	2159	2163	rVB	166710	163731	4.03%	0.487%
43	14.821	2163	2165	2169	rBV2	34590	40892	1.01%	0.122%
44	14.980	2188	2192	2195	rBV	338719	468205	11.53%	1.393%
45	15.051	2202	2204	2207	rVB3	50024	46259	1.14%	0.138%
46	15.086	2208	2210	2214	rVB	62005	64430	1.59%	0.192%
47	15.280	2239	2243	2249	rVB	190035	242667	5.98%	0.722%
48	15.339	2250	2253	2259	rVB	263030	319139	7.86%	0.950%
49	15.404	2259	2264	2268	rBV	789416	1031378	25.41%	3.069%
50	16.886	2511	2516	2523	rVB2	97611	197830	4.87%	0.589%
51	17.333	2588	2592	2599	rVB2	61972	124640	3.07%	0.371%

Sum of corrected areas: 33602476

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Instrument :
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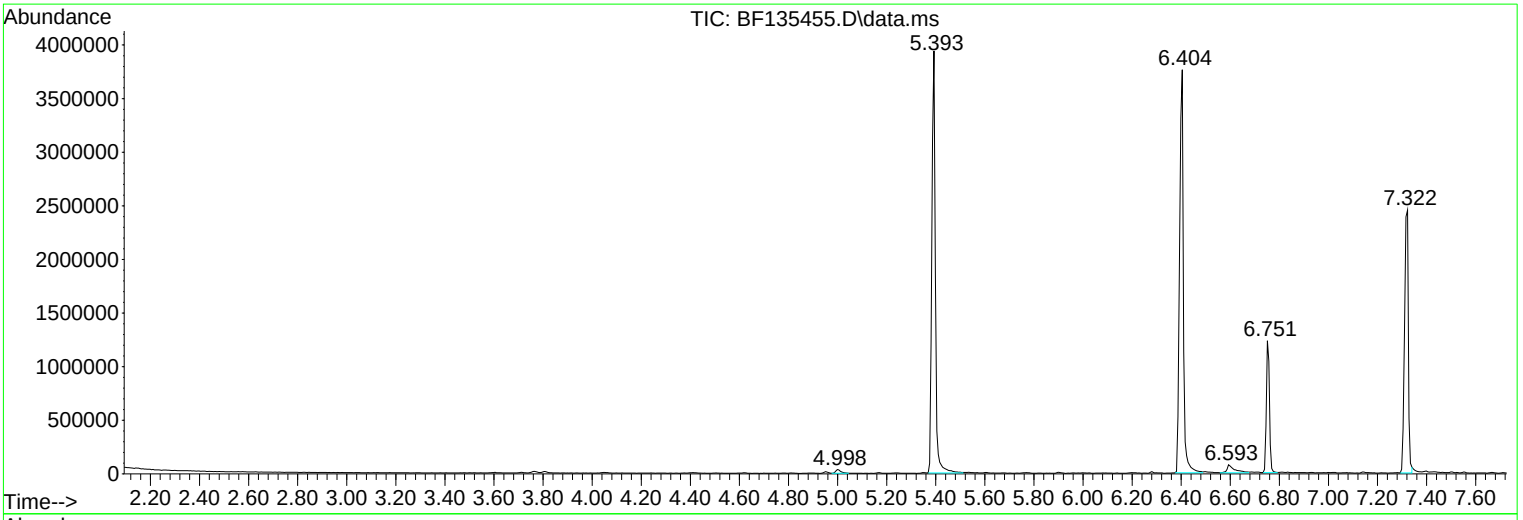
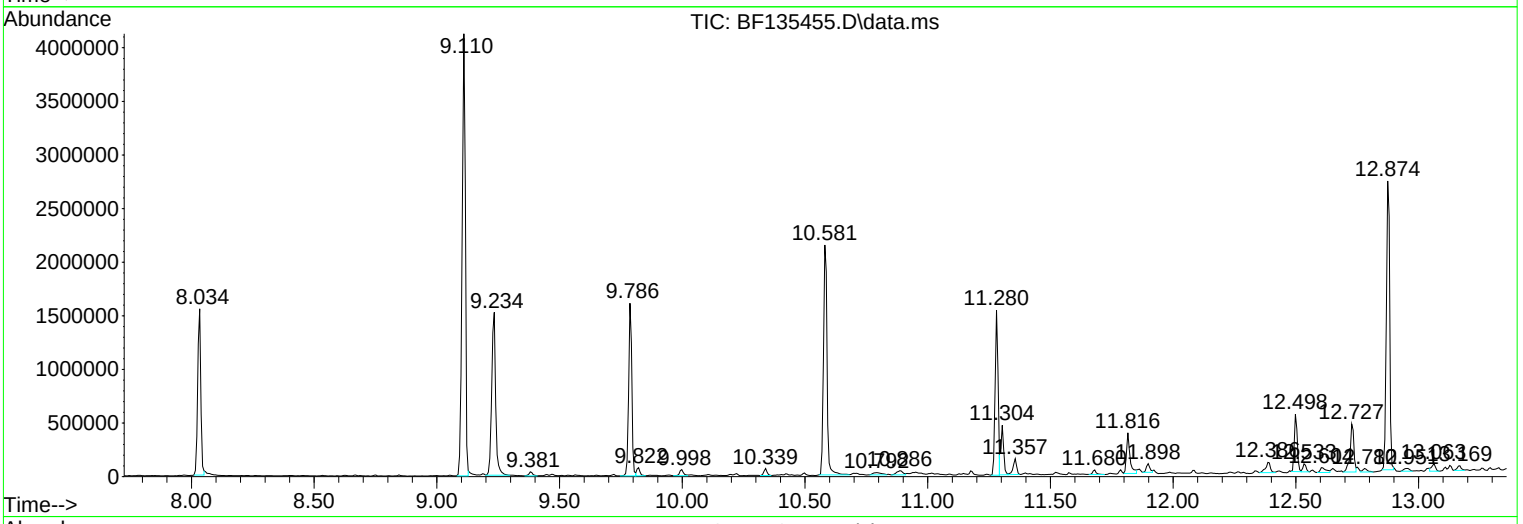
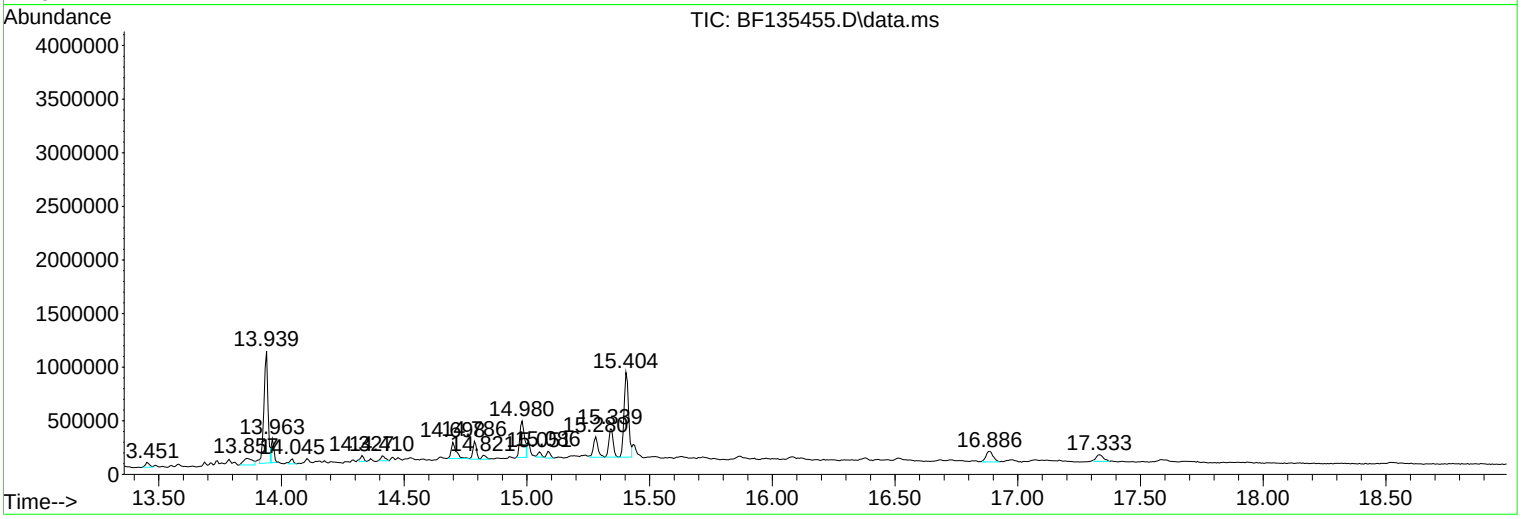
TP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

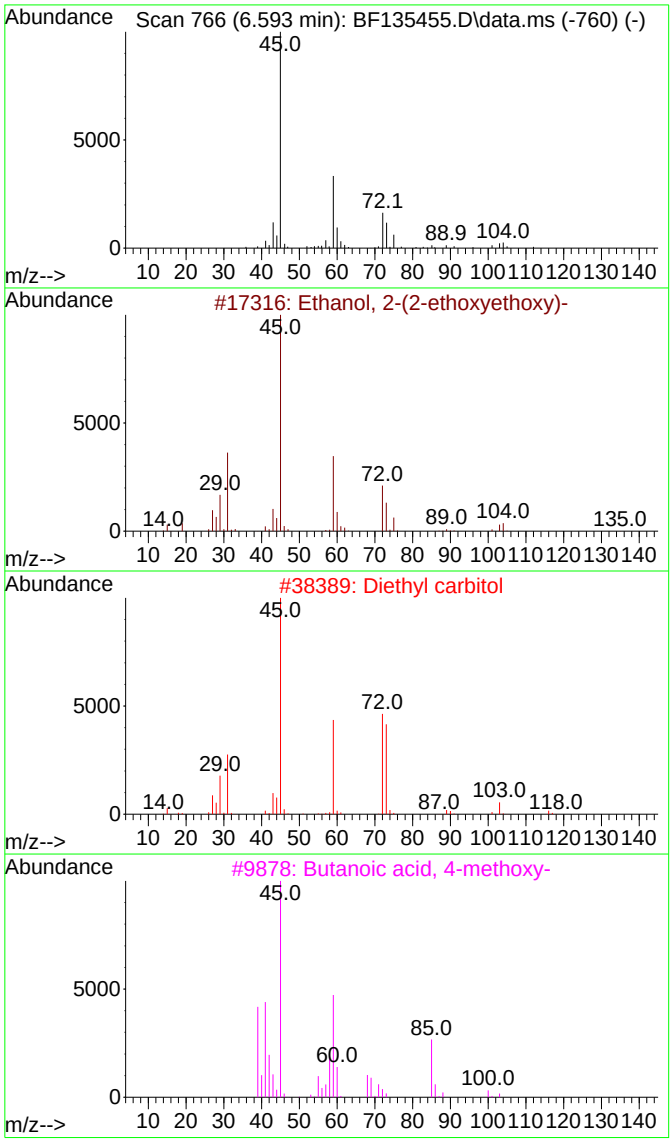
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

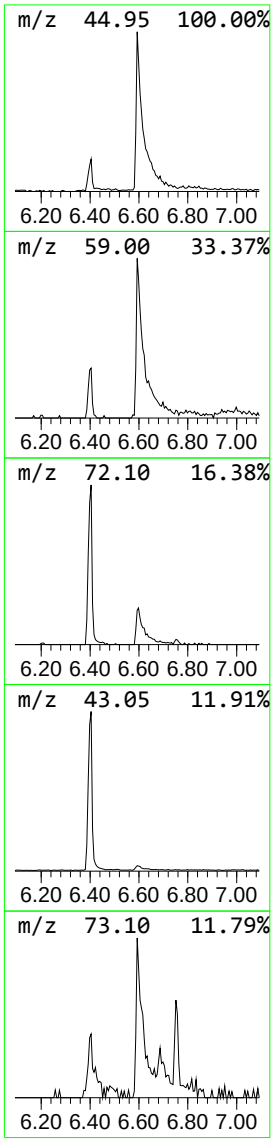
****

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.593	2.90 ng	156290	1,4-Dichlorobenzene-d4	6.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	56
3	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	40
4	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	40
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39





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Operator : CG\JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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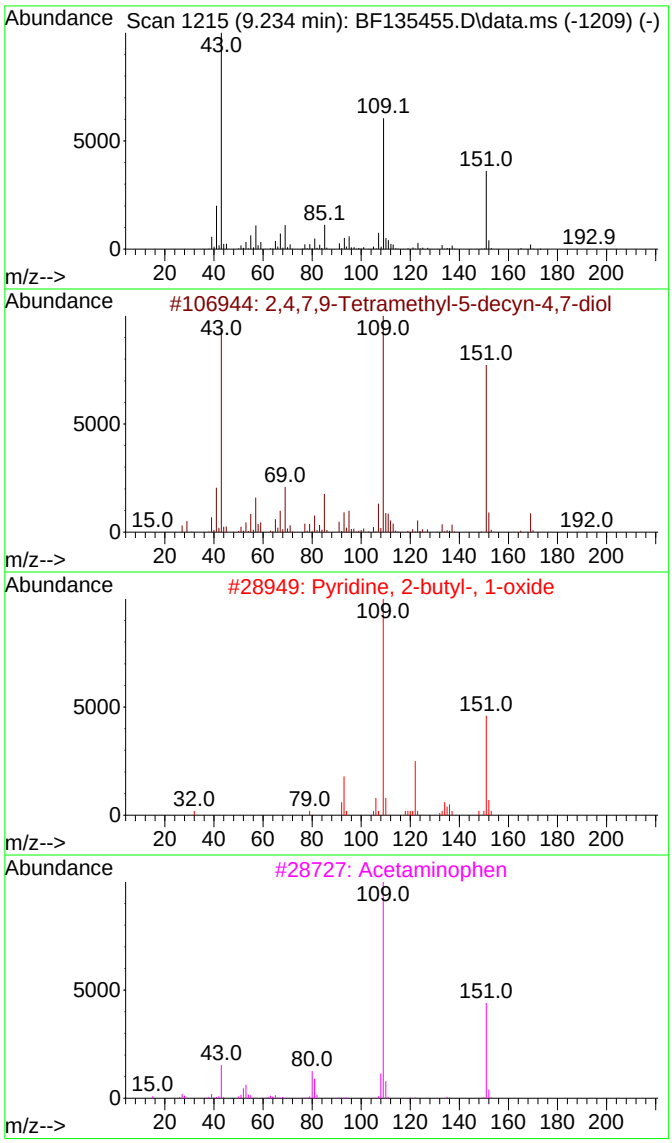
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

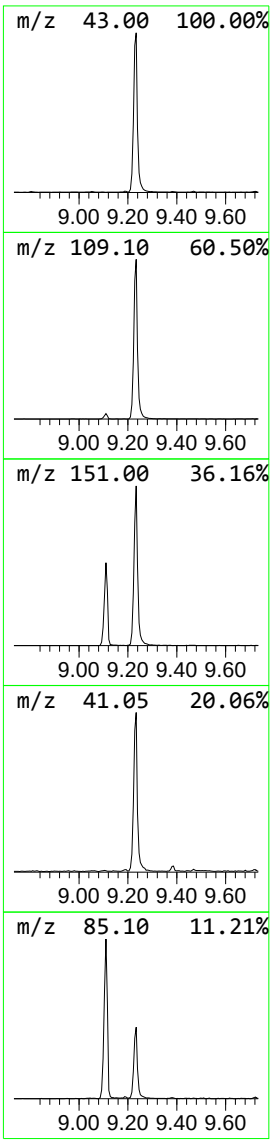
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.234	22.97 ng	1657160	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	47
4	Metacetamol	151	C8H9NO2	000621-42-1	47
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	38





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Sample : 04531-04
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

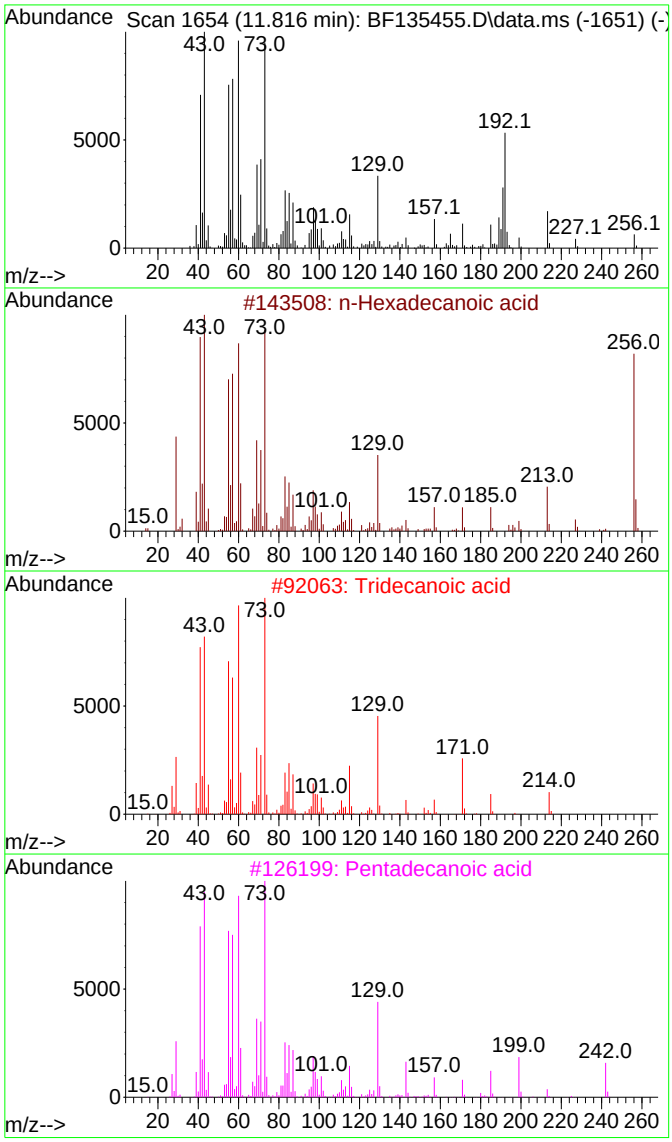
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

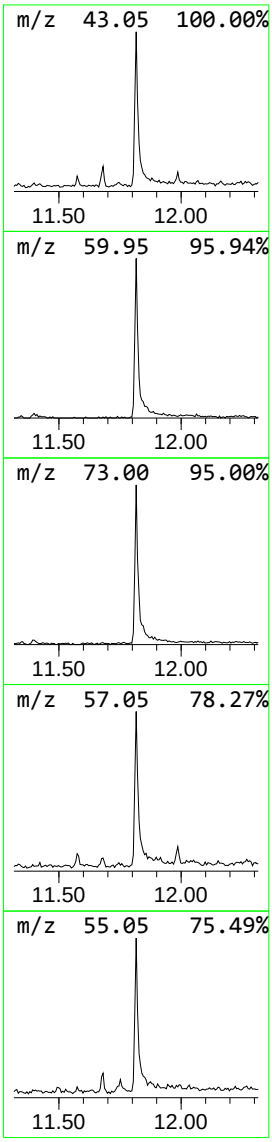
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	5.76 ng	372621	Phenanthrene-d10	11.281

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	56
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
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Sample : 04531-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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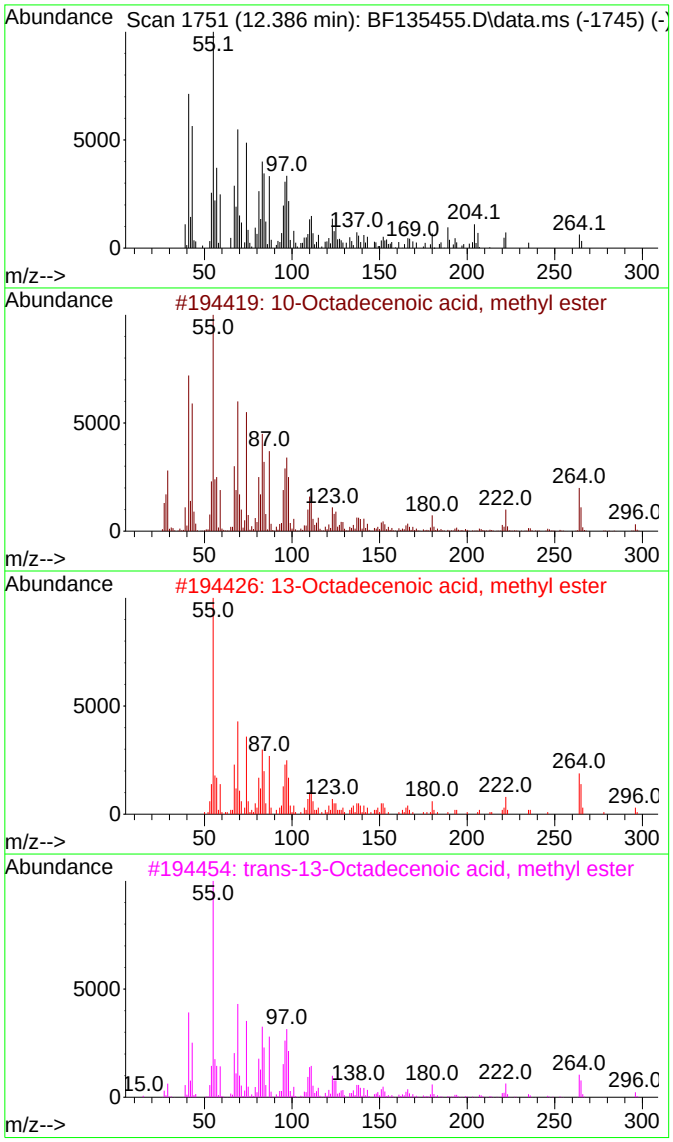
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

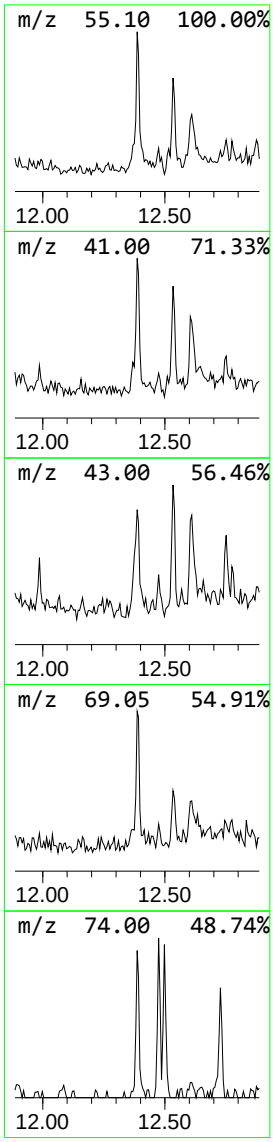
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.386	2.03 ng	131626	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	87
5	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	87





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

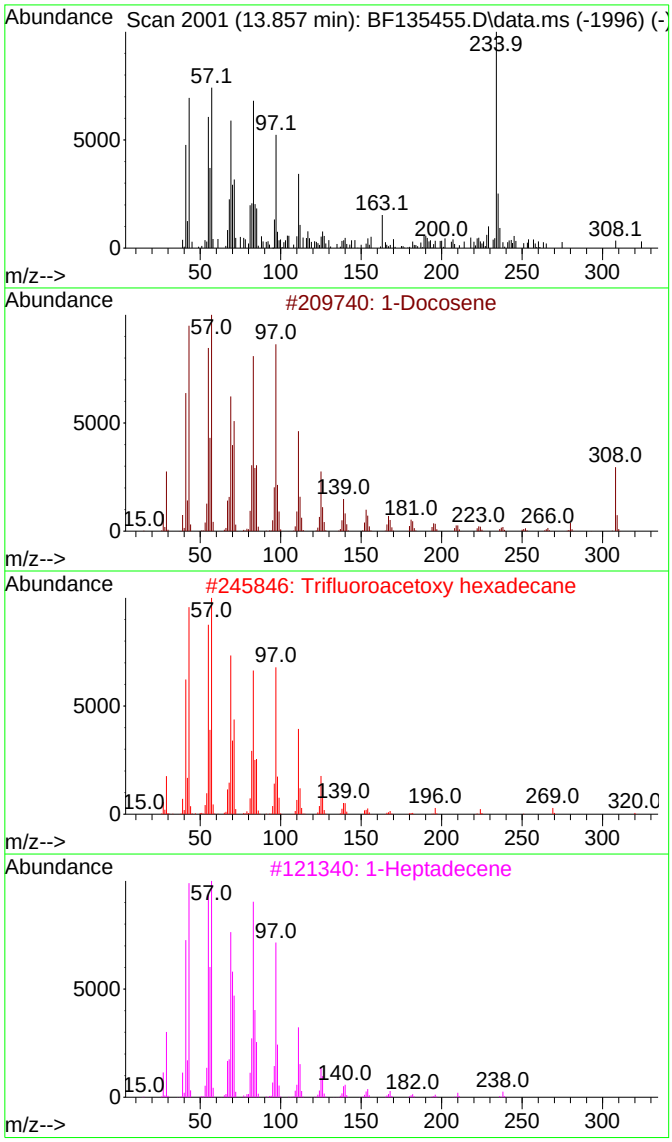
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

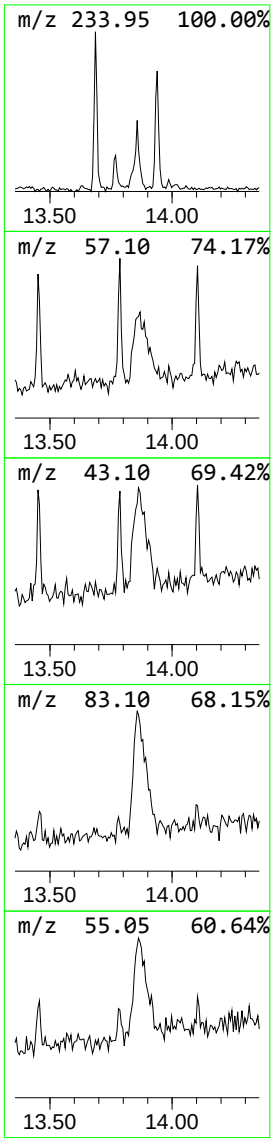
****

Peak Number 6 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.75 ng	167691	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	87
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62
3	1-Heptadecene	238	C17H34	006765-39-5	60
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	60
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	55





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

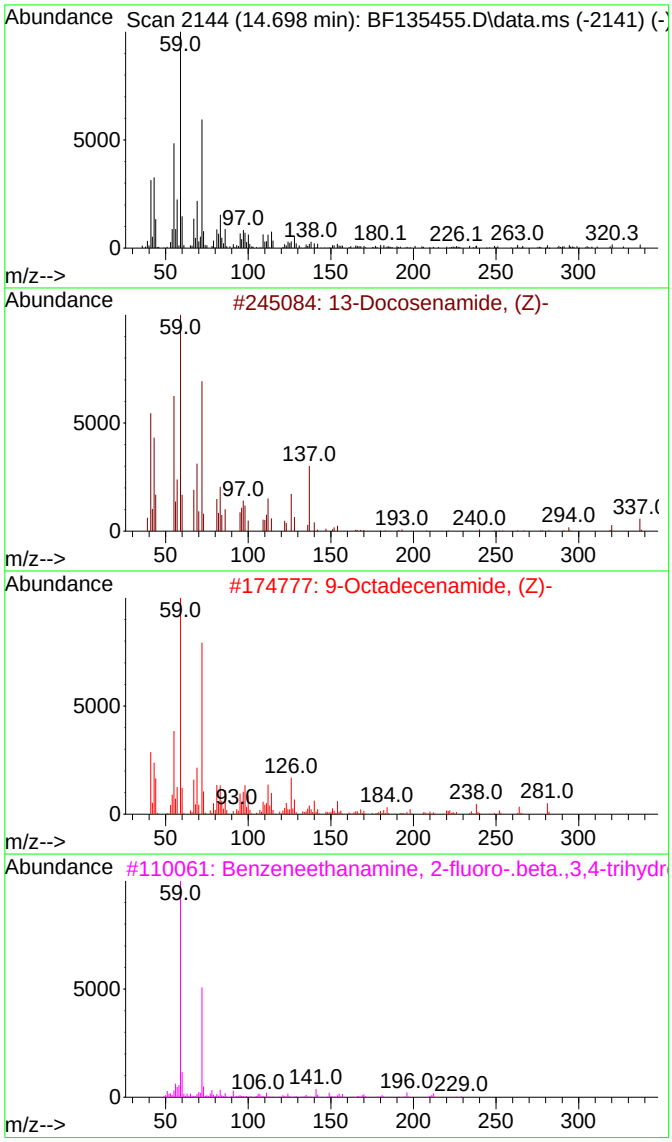
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

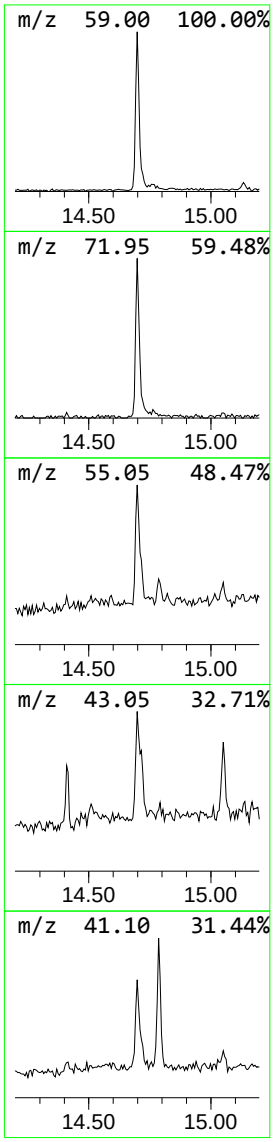
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	4.11 ng	212151	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
4	Hexadecanamide	255	C16H33NO	000629-54-9	59
5	Nonanamide	157	C9H19NO	001120-07-6	53





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Sample : 04531-04
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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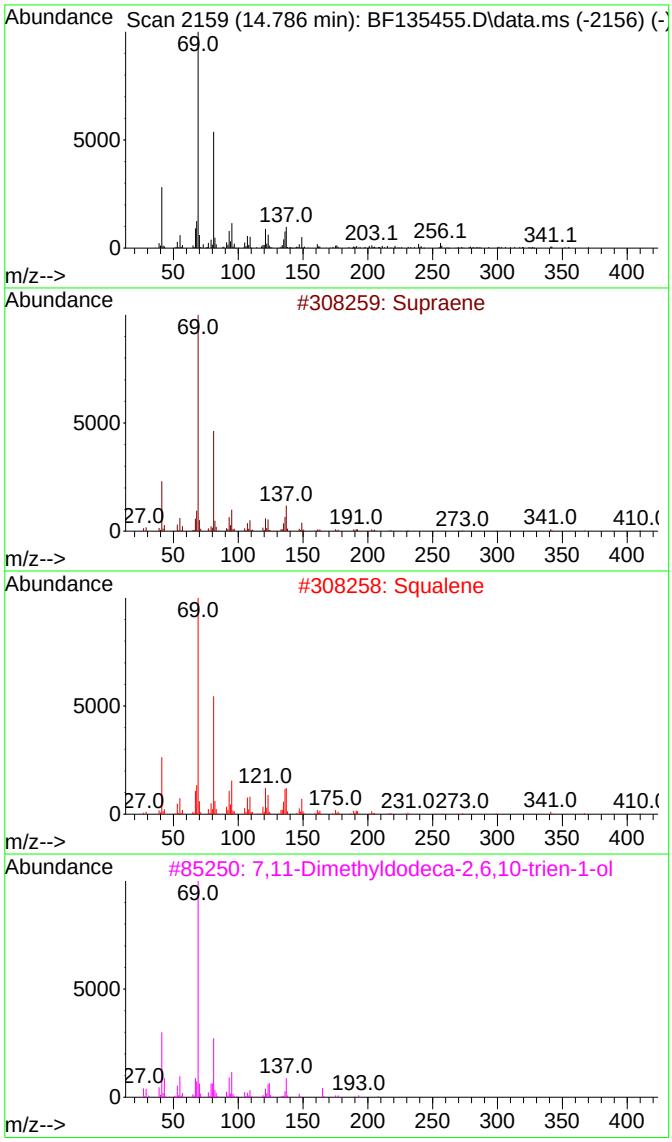
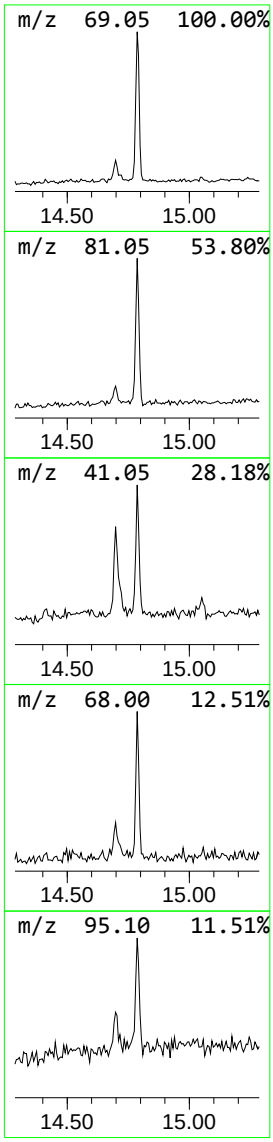
Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	3.17 ng	163731	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
Data File : BF135455.D
Acq On : 26 Sep 2023 16:25
Operator : CG\JU
Sample : 04531-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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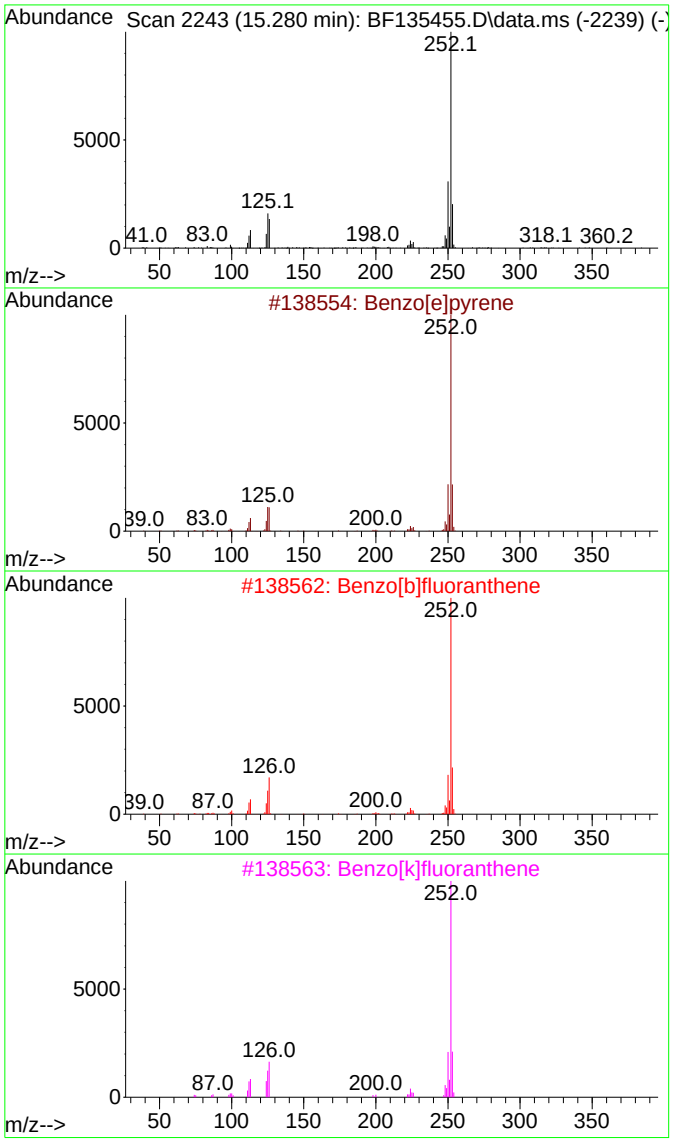
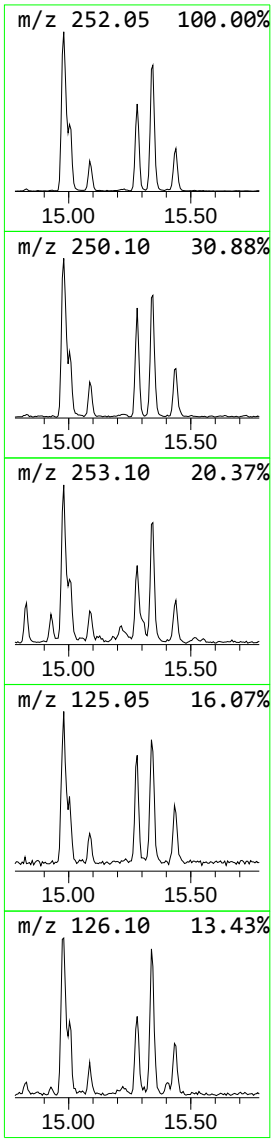
Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	4.71 ng	242667	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
Data File : BF135455.D
Acq On : 26 Sep 2023 16:25
Operator : CG\JU
Sample : 04531-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
Ethanol, 2-(2-e...	6.593	2.9	ng	156290	1	6.751	1076730	20.0
2,4,7,9-Tetrame...	9.234	23.0	ng	1657160	3	9.786	1442680	20.0
n-Hexadecanoic ...	11.816	5.8	ng	372621	4	11.281	1293680	20.0
10-Octadecenoic...	12.386	2.0	ng	131626	4	11.281	1293680	20.0
1-Docosene	13.857	2.8	ng	167691	5	13.939	1217990	20.0
13-Docosenamide...	14.698	4.1	ng	212151	6	15.404	1031380	20.0
Supraene	14.786	3.2	ng	163731	6	15.404	1031380	20.0
Benzo[e]pyrene	15.280	4.7	ng	242667	6	15.404	1031380	20.0