LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 289

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: BF135206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	491	494	500	rBV	43608	50954	2.51%	0.281%
2	5.392	558	562	565	rBV	1935635	1759443	86.80%	9.712%
3	6.398	729	733	746	rBV	1780027	1852816	91.40%	10.227%
4	6.598	765	767	773	rBV	22043	31983	1.58%	0.177%
5	6.763	791	795	798	rBV	999290	795610	39.25%	4.392%
6	7.322	886	890	894	rBV	1213797	1179449	58.19%	6.510%
7	8.039	1008	1012	1016	rBV	1269703	1043627	51.49%	5.761%
8	9.122	1191	1196	1199	rBV	2260476	2027049	100.00%	11.189%
9	9.239	1211	1216	1220	rVB	33146	31607	1.56%	0.174%
10	9.798	1307	1311	1314	rBV	1365889	1110245	54.77%	6.128%
11	9.827	1314	1316	1321	rVB	44104	35280	1.74%	0.195%
12	10.004	1341	1346	1352	rBV	20797	22756	1.12%	0.126%
13	10.345	1401	1404	1409	rVB	37108	29027	1.43%	0.160%
14	10.586	1441	1445	1455	rBV	1285364	1171981	57.82%	6.469%
15	10.716	1463	1467	1471	rVB4	17409	25362	1.25%	0.140%
16	11.186	1545	1547	1551	rVB2	25594	23832	1.18%	0.132%
17	11.286	1561	1564	1567	rBV	1166139	1096060	54.07%	6.050%
18	11.310	1567	1568	1572	rVV	305006	204639	10.10%	1.130%
19	11.363	1572	1577	1581	rVB	81103	80669	3.98%	0.445%
20	11.527	1599	1605	1611	rBV2	24184	43088	2.13%	0.238%
21	11.692	1628	1633	1639	rVB8	13299	22123	1.09%	0.122%
22	11.792	1647	1650	1652	rBV	33445	26511	1.31%	0.146%
23	11.827	1652	1656	1660	rBV	232158	232876	11.49%	1.285%
24	11.904	1666	1669	1672	rBV	52927	55624	2.74%	0.307%
25	12.345	1741	1744	1747	rBV2	24719	25545	1.26%	0.141%
26	12.386	1748	1751	1756	rVV5	43858	52598	2.59%	0.290%
27	12.433	1756	1759	1762	rVB	25364	24892	1.23%	0.137%
28	12.504	1768	1771	1775	rBV	369432	335076	16.53%	1.850%
29	12.616	1787	1790	1795	rBV3	41438	51276	2.53%	0.283%
30	12.733	1805	1810	1814	rBV	303611	324548	16.01%	1.791%
31	12.886	1832	1836	1839	rBV	1607671	1410849	69.60%	7.788%
32	13.068	1860	1867	1871	rVB2	49972	73979	3.65%	0.408%
33	13.133	1875	1878	1881	rVV4	36301	35723	1.76%	0.197%
34	13.168	1881	1884	1887	rVV2	32911	37589	1.85%	0.207%
35	13.204	1887	1890	1897	rVV2	85764	99703	4.92%	0.550%
36	13.316	1907	1909	1912	rBV	69154	68517	3.38%	0.378%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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	13.357	1912	1916	1925	rVB7	54339	106700	5.26%	0.589%
38	13.580	1952	1954	1958	rVB2	20128	22067	1.09%	0.122%
39	13.827	1993	1996	2002	rBV4	45350	81371	4.01%	0.449%
40	13.945	2011	2016	2018	rBV2	686701	771466	38.06%	4.258%
41	13.968	2018	2020	2025	rVB	136181	116818	5.76%	0.645%
42	14.045	2031	2033	2036	rVB	26425	24053	1.19%	0.133%
43	14.427	2095	2098	2100	rBV2	26778	23126	1.14%	0.128%
44	14.457	2101	2103	2105	rBV3	25844	29433	1.45%	0.162%
45	14.586	2122	2125	2129	rVB2	36152	40909	2.02%	0.226%
46	14.874	2171	2174	2178	rVB	82805	83881	4.14%	0.463%
47	14.980	2188	2192	2195	rBV	114282	163291	8.06%	0.901%
48	15.133	2216	2218	2219	rBV2	27479	23697	1.17%	0.131%
49	15.280	2240	2243	2249	rVB	70155	89044	4.39%	0.492%
50	15.345	2250	2254	2259	rBV	93416	115615	5.70%	0.638%
51	15.409	2260	2265	2269	rBV	571235	705605	34.81%	3.895%
52	15.886	2343	2346	2351	rBV	50174	76147	3.76%	0.420%
53	16.874	2510	2514	2521	rBV4	40017	79803	3.94%	0.440%
54	17.321	2586	2590	2599	rVB3	33749	70733	3.49%	0.390%

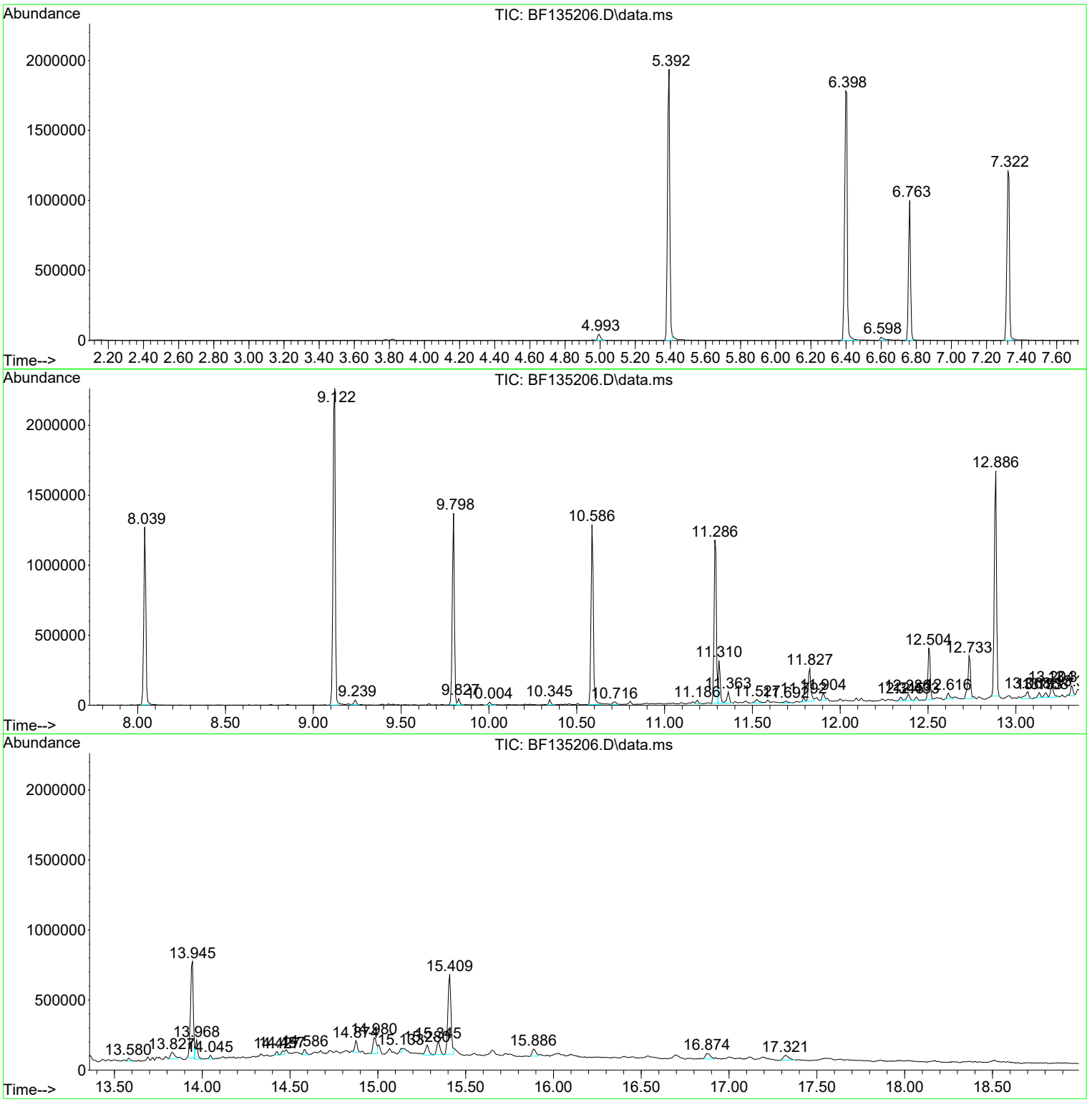
Sum of corrected areas: 18116665

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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

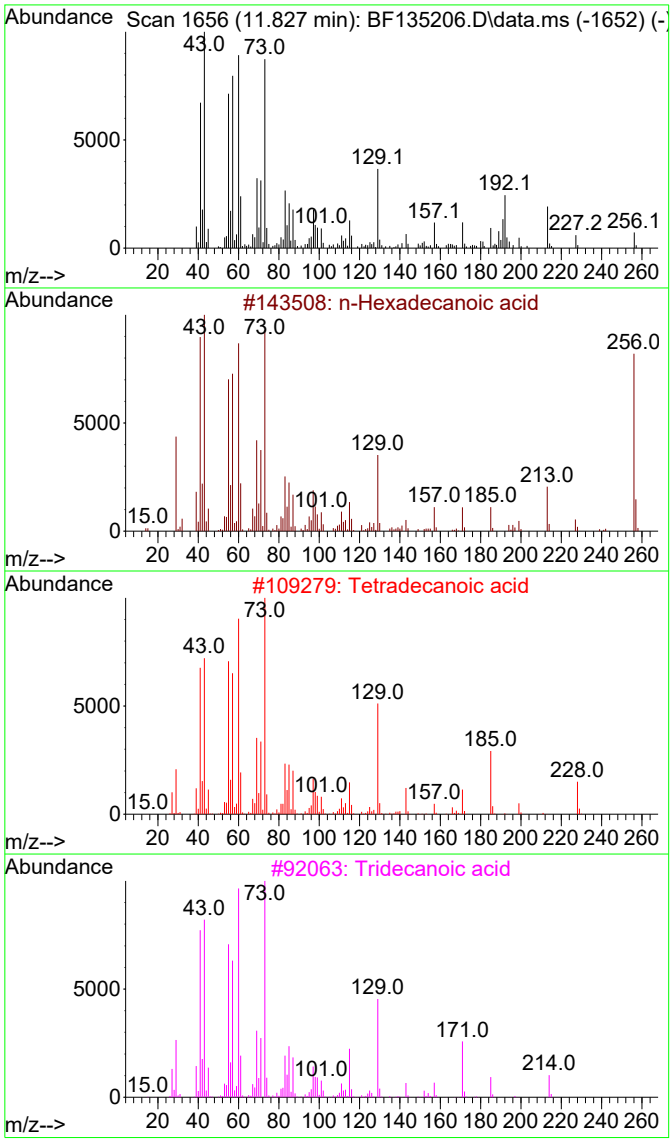
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

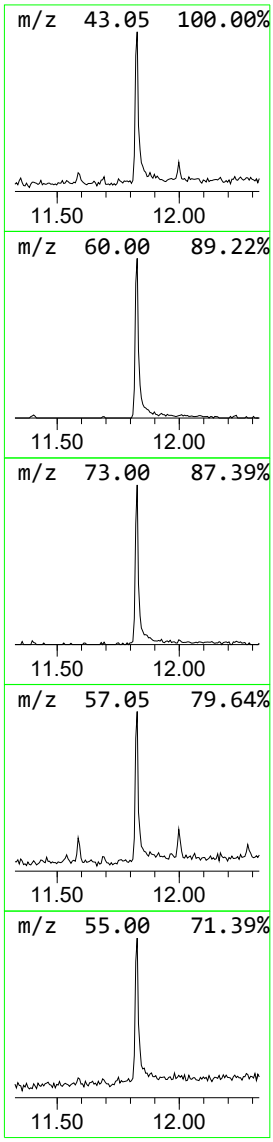
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	4.25 ng	232876	Phenanthrene-d10	11.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

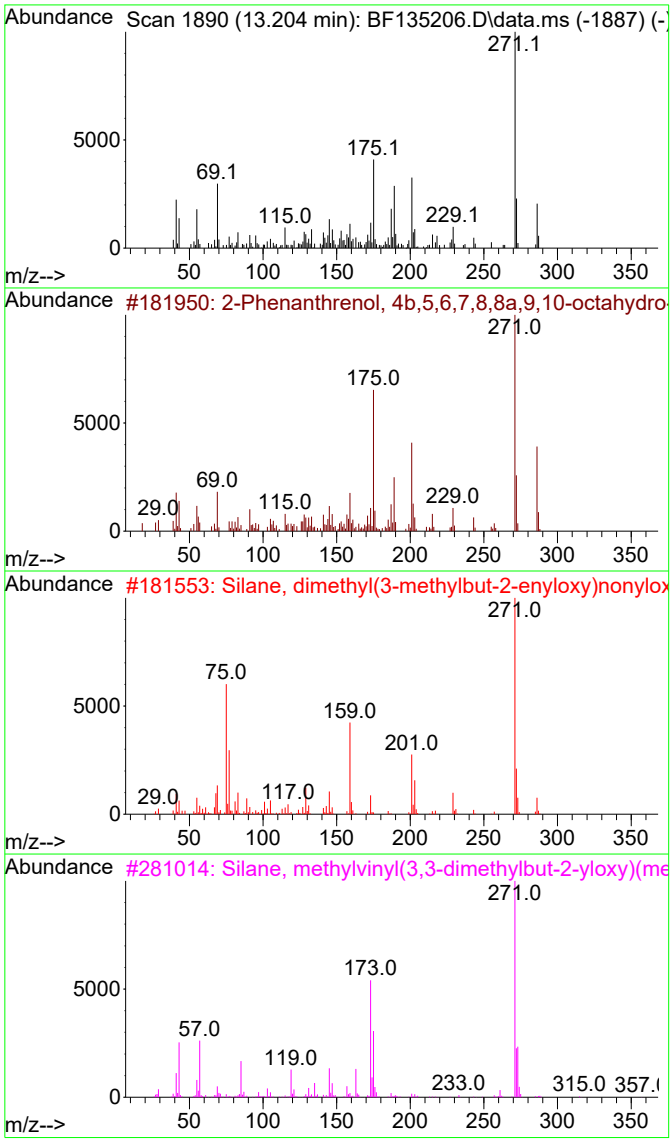
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

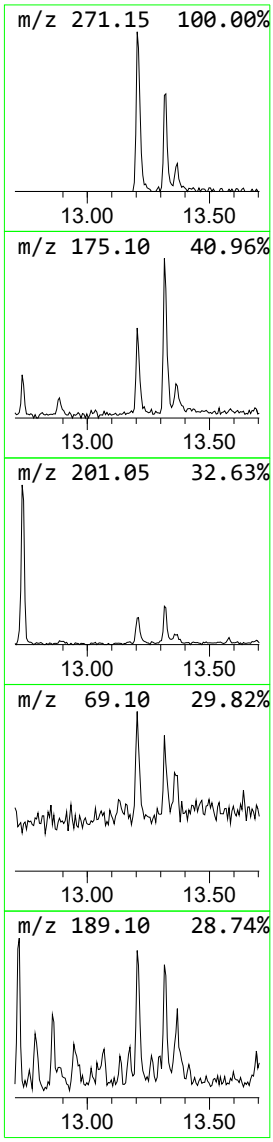
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	2.58 ng	99703	Chrysene-d12	13.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	70
2	Silane, dimethyl(3-methylbut-2-e...	286	C16H34O2Si	1000347-96-9	47
3	Silane, methylvinyl(3,3-dimethyl...	372	C19H40O3Si2	1000421-66-5	38
4	2-(1H-1,2,4-triazol-5-yl)-1H-iso...	286	C13H14N4O2Si	1000472-32-7	37
5	3-Methyl-1-phenyl-4-azafluorenone	271	C19H13NO	062578-46-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

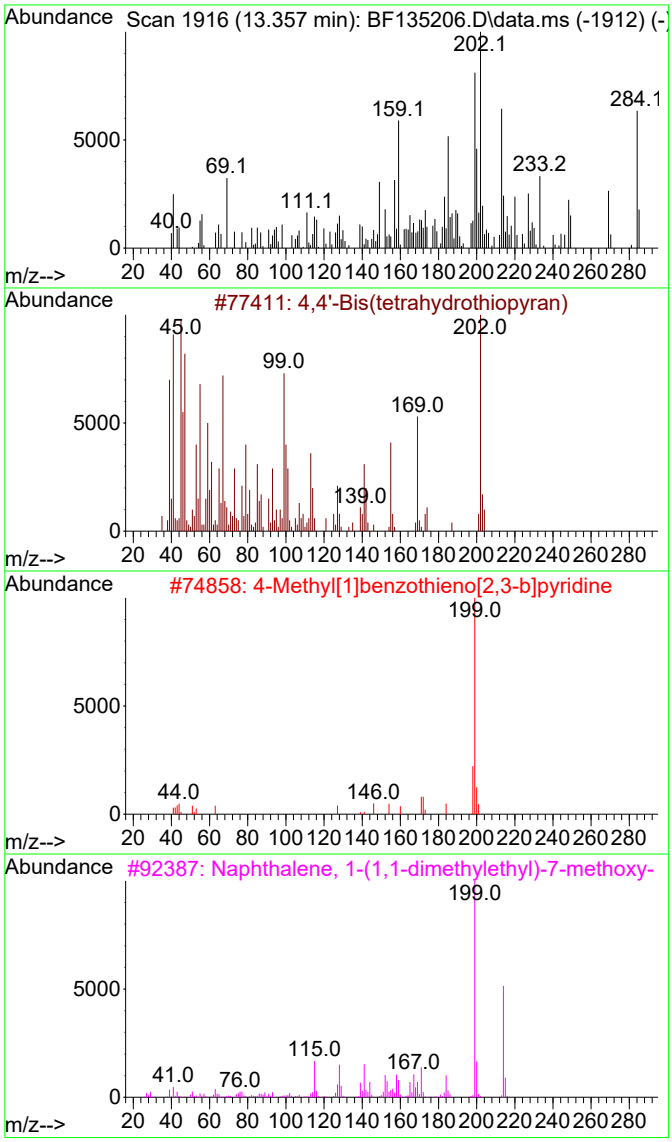
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

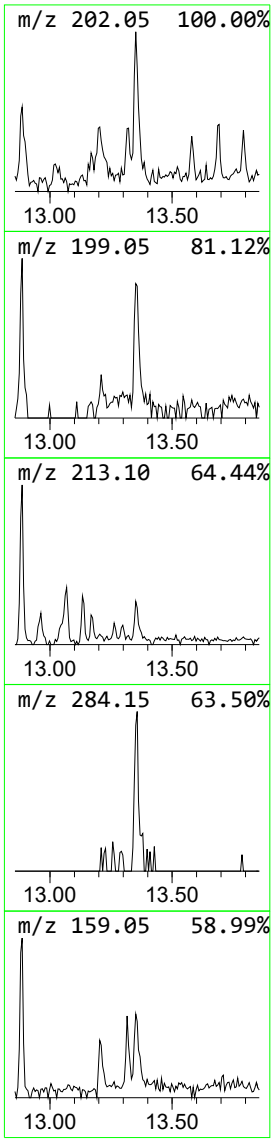
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	2.77 ng	106700	Chrysene-d12	13.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	56
2	4-Methyl[1]benzothieno[2,3-b]pyr...	199	C12H9NS	003573-95-3	25
3	Naphthalene, 1-(1,1-dimethylethy...	214	C15H18O	060683-42-3	25
4	5-Hydroxy-3-methyl-1-phenylpyraz...	202	C11H10N2O2	060484-29-9	18
5	8.alpha.-Estra-1,3,5(10)-trien-1...	284	C19H24O2	013865-88-8	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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

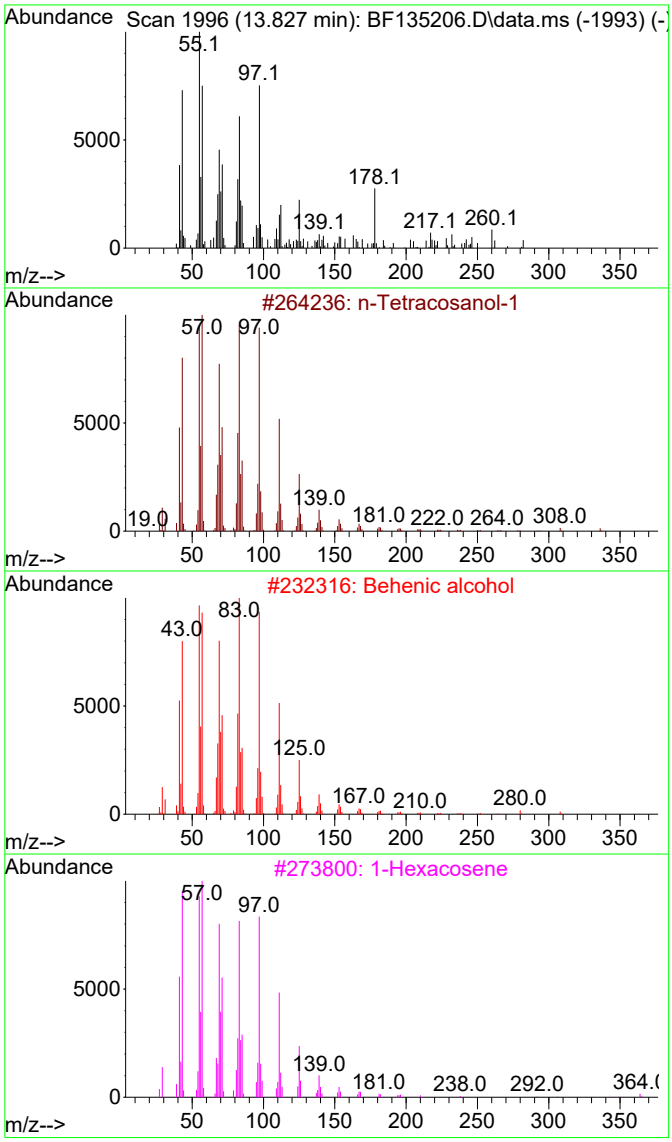
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

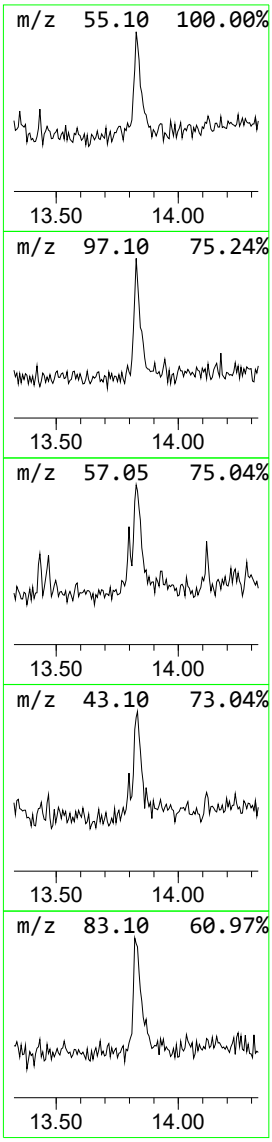
****

Peak Number 4 n-Tetracosanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	2.11 ng	81371	Chrysene-d12	13.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	72
2	Behenic alcohol	326	C22H46O	000661-19-8	58
3	1-Hexacosene	364	C26H52	018835-33-1	52
4	1-Octene, 6-methyl-	126	C9H18	013151-10-5	49
5	1-Eicosanol	298	C20H42O	000629-96-9	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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

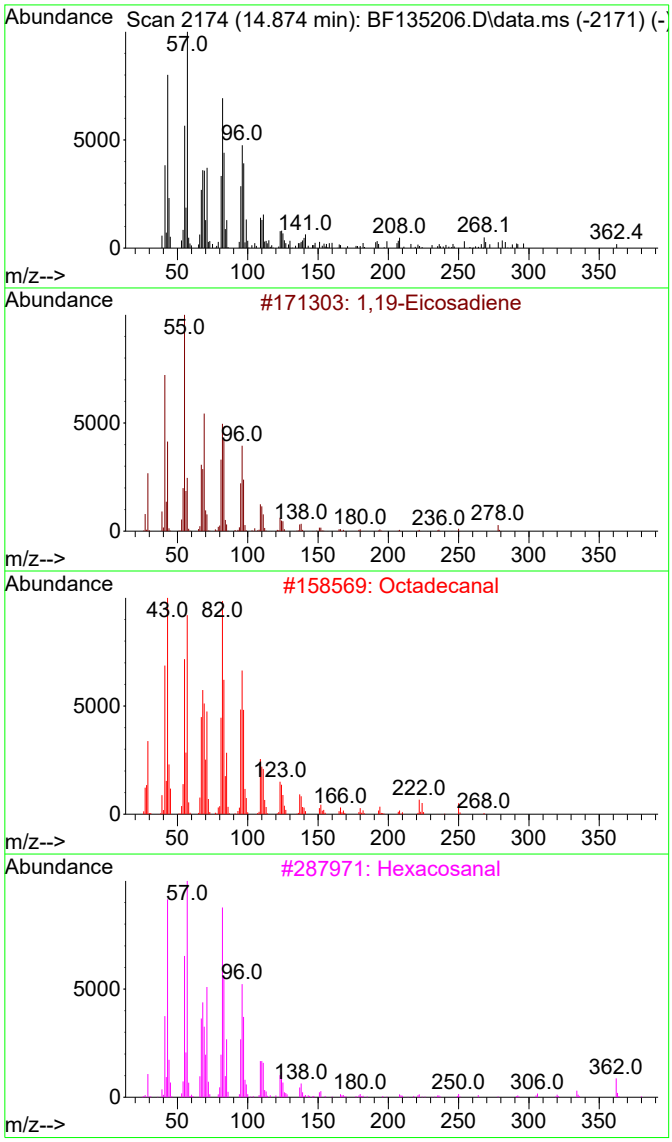
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

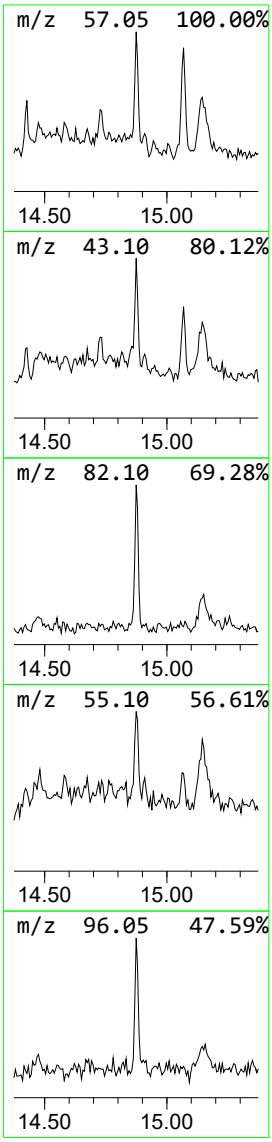
****

Peak Number 5 1,19-Eicosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	2.38 ng	83881	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	93
2	Octadecanal	268	C18H36O	000638-66-4	87
3	Hexacosanal	380	C26H52O	026627-85-0	86
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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

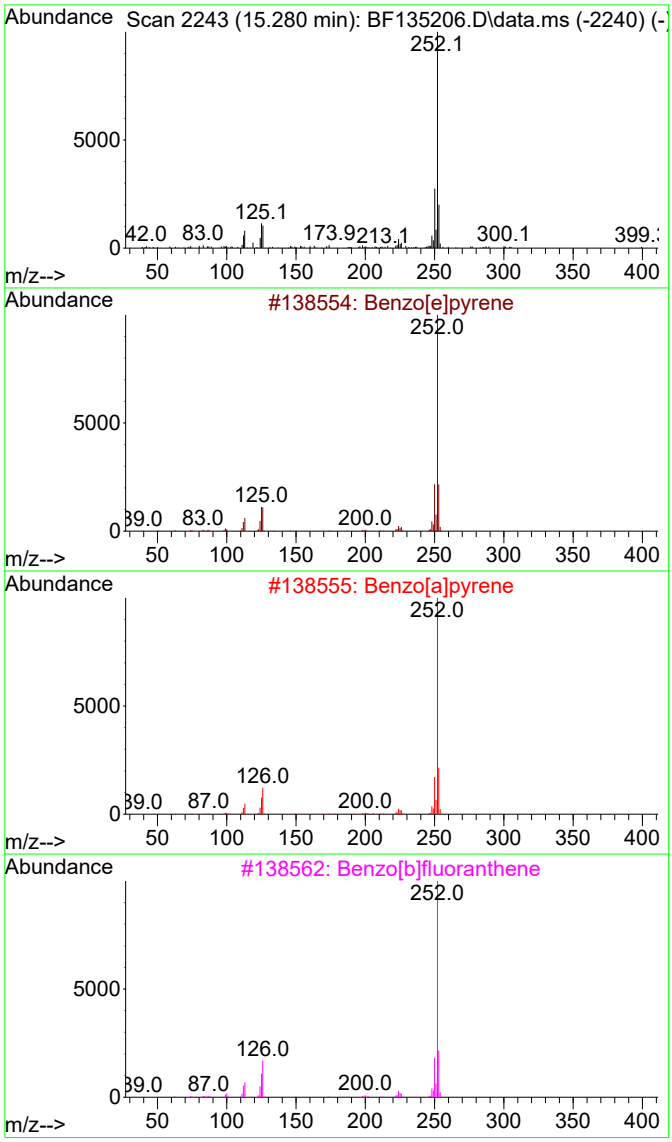
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

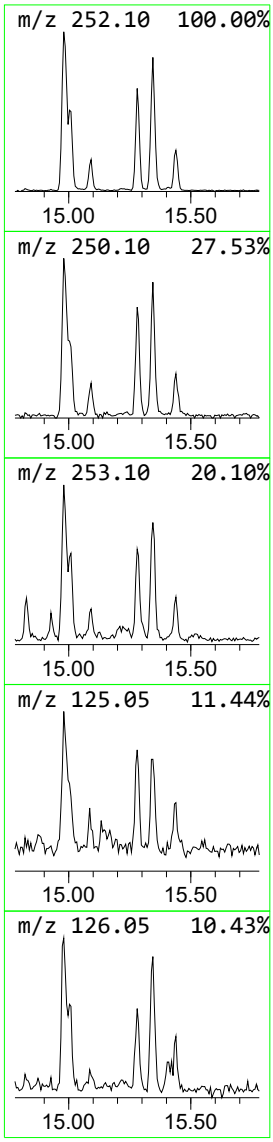
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	2.52 ng	89044	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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

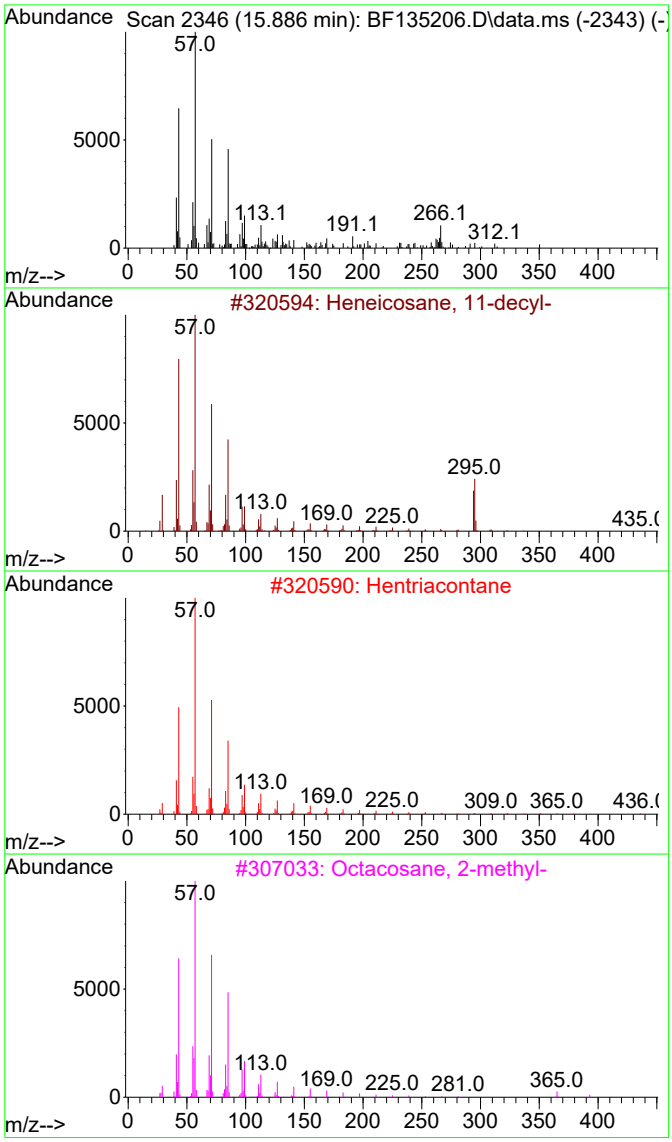
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

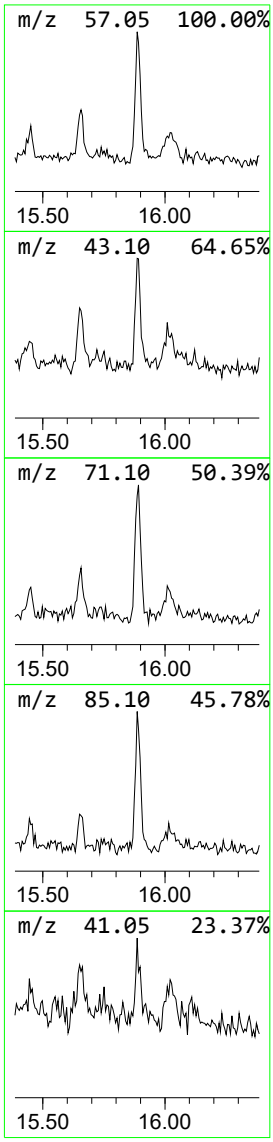
****

Peak Number 7 Heneicosane, 11-decyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	2.16 ng	76147	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	81
2	Hentriacontane	437	C31H64	000630-04-6	74
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	74
4	Octacosane	394	C28H58	000630-02-4	74
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135206.D
Acq On : 13 Sep 2023 05:00
Operator : CG\JU
Sample : 04371-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

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
n-Hexadecanoic ...	11.827	4.3	ng	232876	4	11.286	1096060	20.0
2-Phenanthrenol...	13.204	2.6	ng	99703	5	13.945	771466	20.0
4,4'-Bis(tetrah...	13.357	2.8	ng	106700	5	13.945	771466	20.0
n-Tetracosanol-1	13.827	2.1	ng	81371	5	13.945	771466	20.0
1,19-Eicosadiene	14.874	2.4	ng	83881	6	15.410	705605	20.0
Benzo[e]pyrene	15.280	2.5	ng	89044	6	15.410	705605	20.0
Heneicosane, 11...	15.886	2.2	ng	76147	6	15.410	705605	20.0