LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-345

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: BF136701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	16	rVB3	9554	16129	1.23%	0.155%
2	5.010	494	497	507	rVB	34243	37074	2.84%	0.356%
3	5.422	563	567	570	rBV	1262364	1085497	83.02%	10.429%
4	6.428	734	738	741	rBV	1331528	1123092	85.90%	10.790%
5	6.780	795	798	802	rVB	512558	392170	29.99%	3.768%
6	7.339	889	893	896	rBV	742862	673457	51.51%	6.470%
7	8.057	1011	1015	1018	rBV	609971	476415	36.44%	4.577%
8	8.380	1067	1070	1079	rBV	7651	14868	1.14%	0.143%
9	9.133	1194	1198	1202	rBV	1475199	1307467	100.00%	12.561%
10	9.674	1286	1290	1294	rVB	23115	19537	1.49%	0.188%
11	9.816	1310	1314	1317	rBV	530344	430938	32.96%	4.140%
12	9.845	1317	1319	1323	rVB	22996	18543	1.42%	0.178%
13	9.916	1328	1331	1335	rVB4	10792	14075	1.08%	0.135%
14	10.016	1345	1348	1353	rBV	15647	16330	1.25%	0.157%
15	10.363	1404	1407	1413	rBV2	21142	19092	1.46%	0.183%
16	10.604	1445	1448	1452	rBV	757571	665140	50.87%	6.390%
17	10.733	1465	1470	1476	rVB4	17616	22952	1.76%	0.221%
18	11.115	1531	1535	1539	rBV3	21961	25059	1.92%	0.241%
19	11.304	1563	1567	1569	rBV	456681	363863	27.83%	3.496%
20	11.327	1569	1571	1575	rVV	135578	104923	8.02%	1.008%
21	11.380	1578	1580	1583	rVB	34982	26824	2.05%	0.258%
22	11.539	1602	1607	1612	rBV2	11052	14900	1.14%	0.143%
23	11.839	1655	1658	1664	rBV	204392	201959	15.45%	1.940%
24	11.921	1669	1672	1674	rVV2	29433	34068	2.61%	0.327%
25	11.945	1674	1676	1680	rVB	15802	14807	1.13%	0.142%
26	12.104	1698	1703	1705	rBV2	15232	17699	1.35%	0.170%
27	12.133	1705	1708	1713	rVB2	27155	26593	2.03%	0.255%
28	12.257	1723	1729	1732	rBV8	11980	22373	1.71%	0.215%
29	12.292	1732	1735	1740	rVV6	11558	21137	1.62%	0.203%
30	12.357	1742	1746	1749	rVV2	70080	78985	6.04%	0.759%
31	12.521	1770	1774	1777	rBV	181802	178964	13.69%	1.719%
32	12.551	1777	1779	1788	rVB5	61432	124173	9.50%	1.193%
33	12.627	1789	1792	1796	rBV2	70282	75585	5.78%	0.726%
34	12.751	1805	1813	1819	rVB	160013	189498	14.49%	1.821%
35	12.804	1819	1822	1827	rBV6	14406	21458	1.64%	0.206%
36	12.868	1830	1833	1835	rBV3	17296	23777	1.82%	0.228%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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	12.904	1835	1839	1842	rVB	1143989	1093341	83.62%	10.504%
38	12.968	1848	1850	1854	rVB3	13191	17048	1.30%	0.164%
39	13.080	1867	1869	1872	rVB2	25387	24835	1.90%	0.239%
40	13.221	1890	1893	1897	rBV6	22148	35406	2.71%	0.340%
41	13.286	1900	1904	1912	rVV3	78797	155950	11.93%	1.498%
42	13.445	1929	1931	1933	rBV	24215	19166	1.47%	0.184%
43	13.474	1934	1936	1944	rVB8	23746	38202	2.92%	0.367%
44	13.845	1995	1999	2010	rBV8	48796	127866	9.78%	1.228%
45	13.956	2014	2018	2021	rVV2	440471	482650	36.91%	4.637%
46	13.986	2021	2023	2025	rVB	71513	54400	4.16%	0.523%
47	14.598	2124	2127	2132	rVB	55479	57236	4.38%	0.550%
48	15.003	2193	2196	2199	rBV	94852	123563	9.45%	1.187%
49	15.439	2266	2270	2274	rBV	234674	279512	21.38%	2.685%

Sum of corrected areas: 10408596

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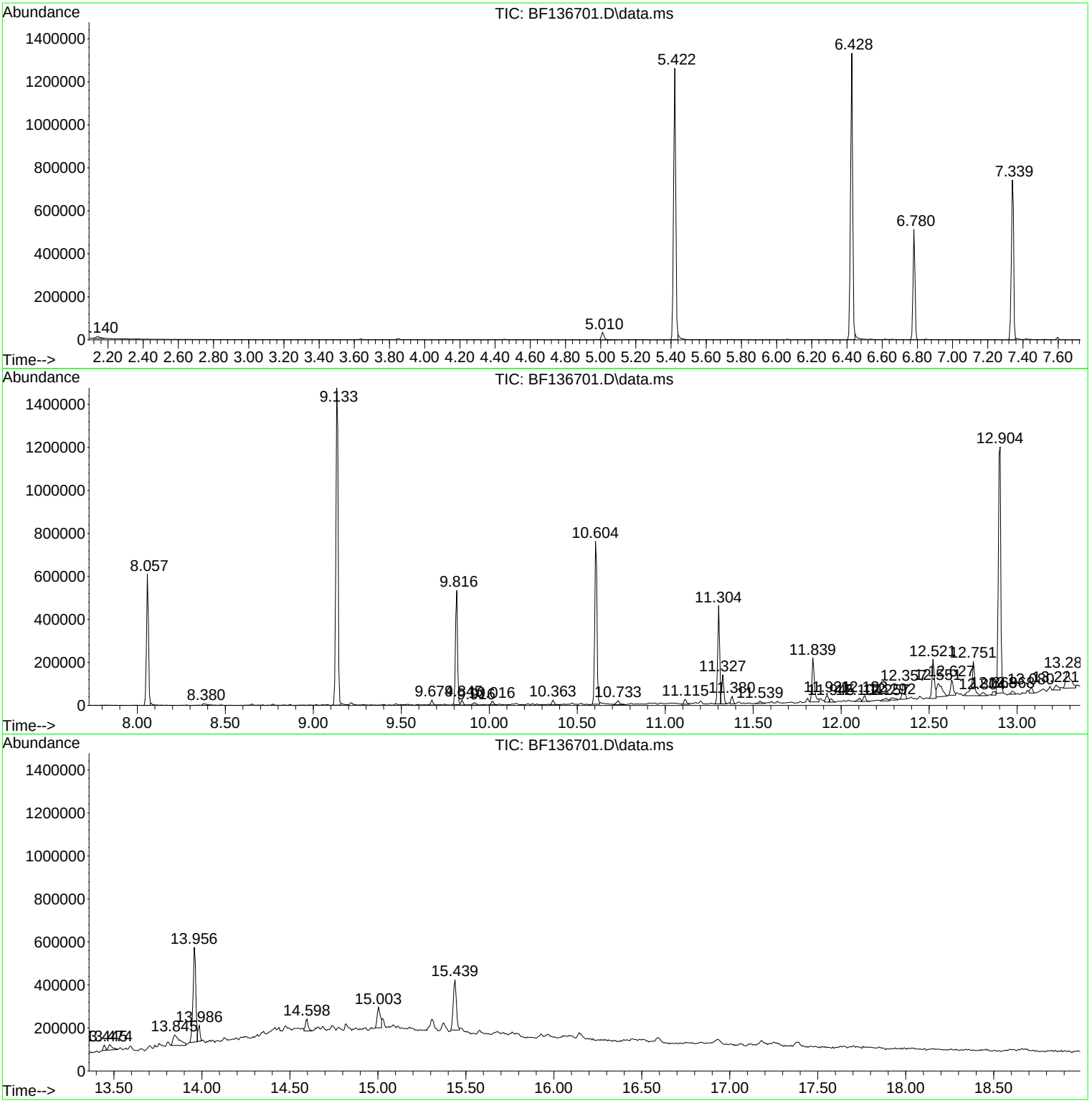
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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

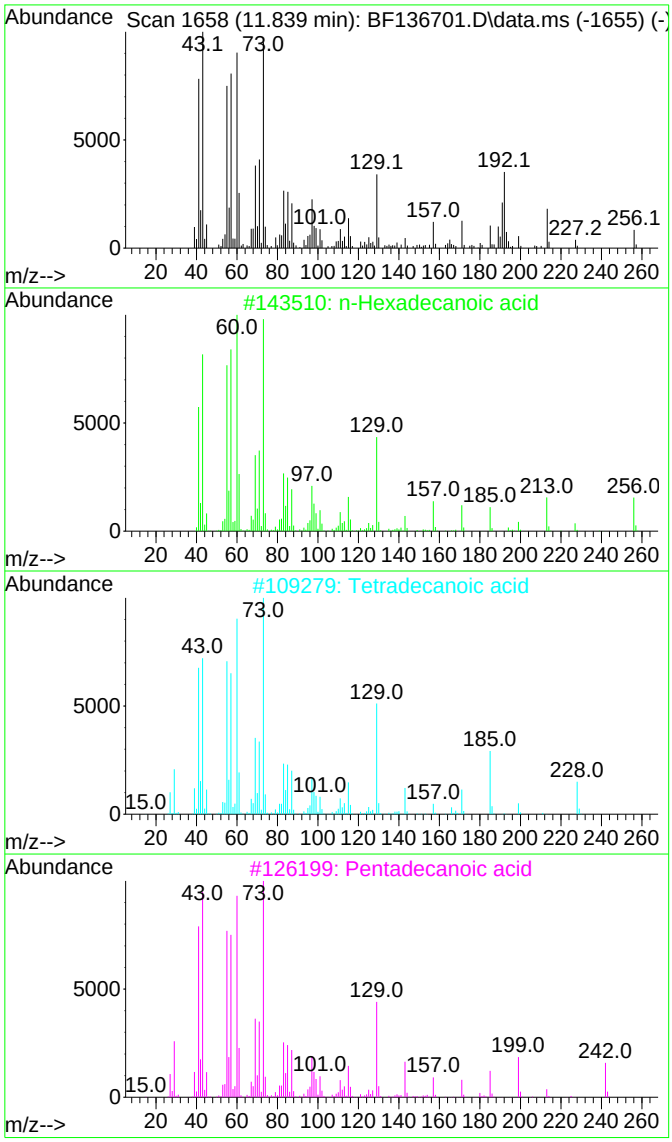
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

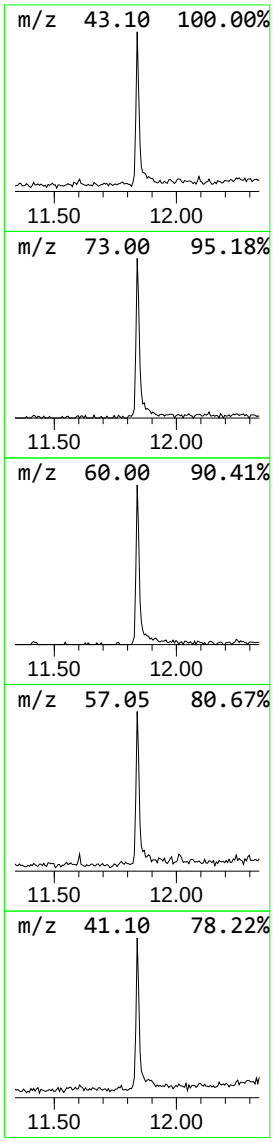
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	11.10 ng	201959	Phenanthrene-d10	11.304

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

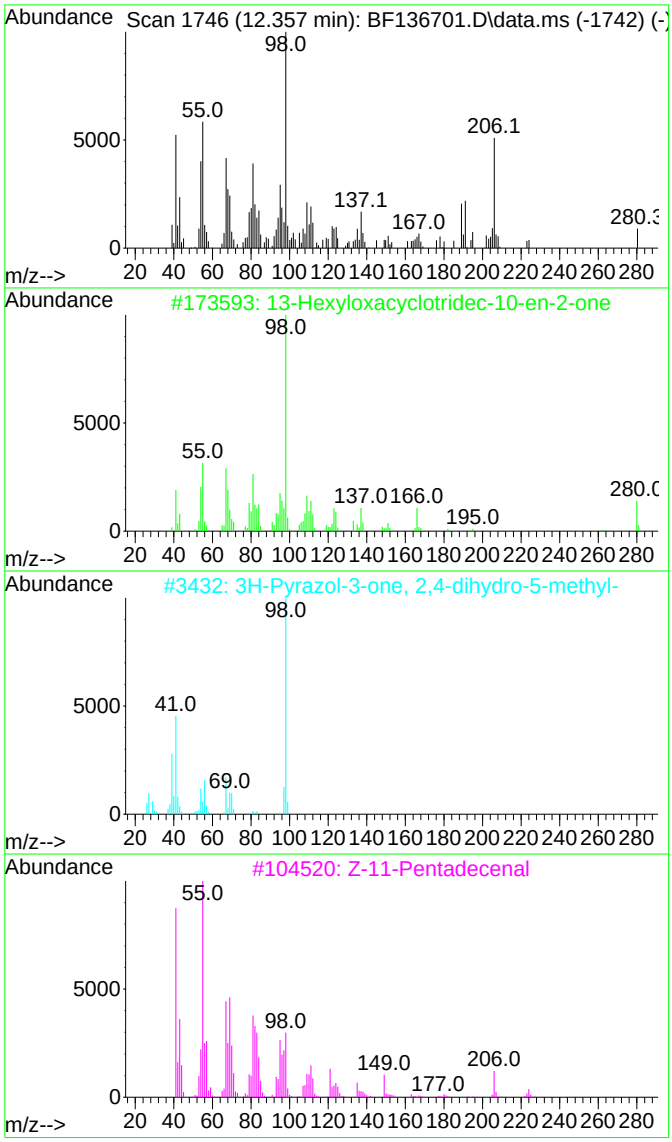
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

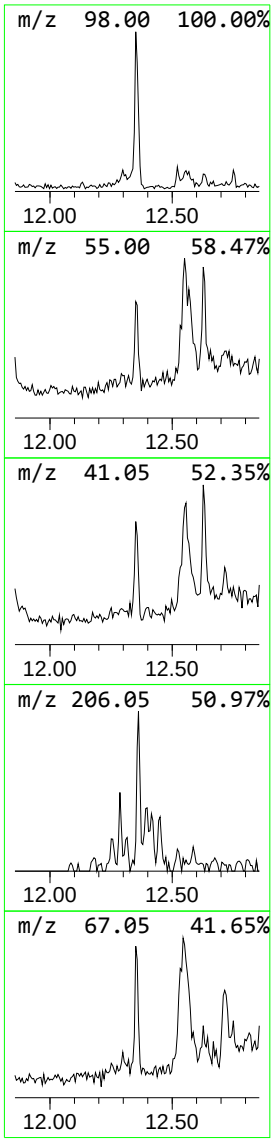
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 13-Hexyloxacyclotridec-10-e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	4.34 ng	78985	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Hexyloxacyclotridec-10-en-2-one	280	C18H32O2	127062-51-5	91
2	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	38
3	Z-11-Pentadecenal	224	C15H28O	1010130-84-6	25
4	Z-1,6-Tridecadiene	180	C13H24	1000130-98-3	25
5	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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

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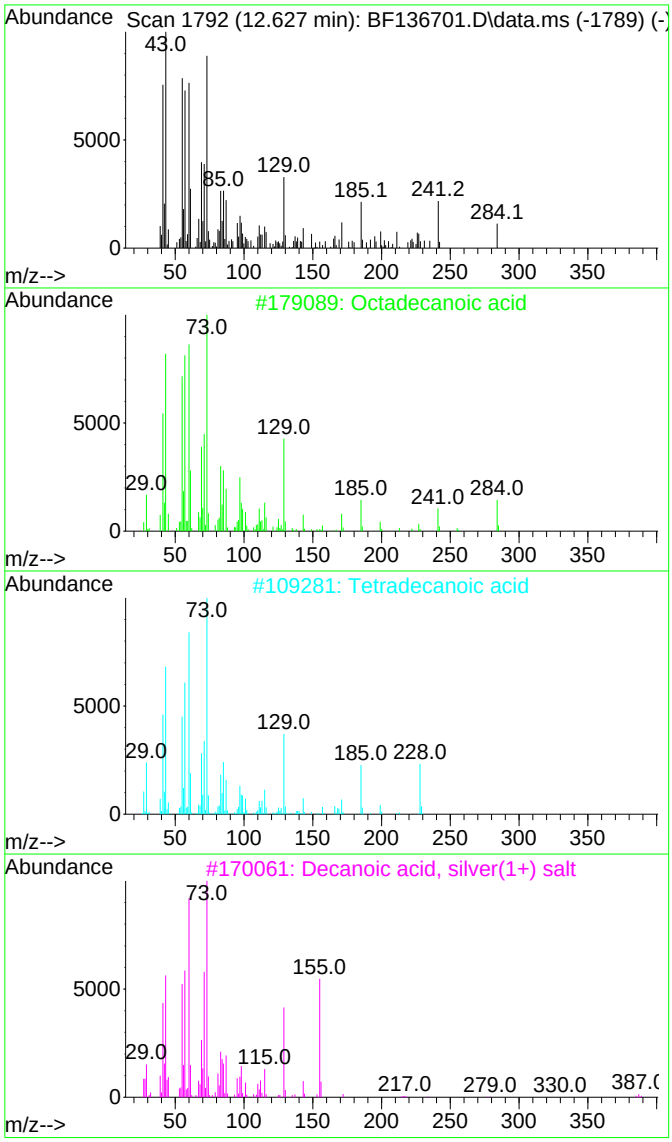
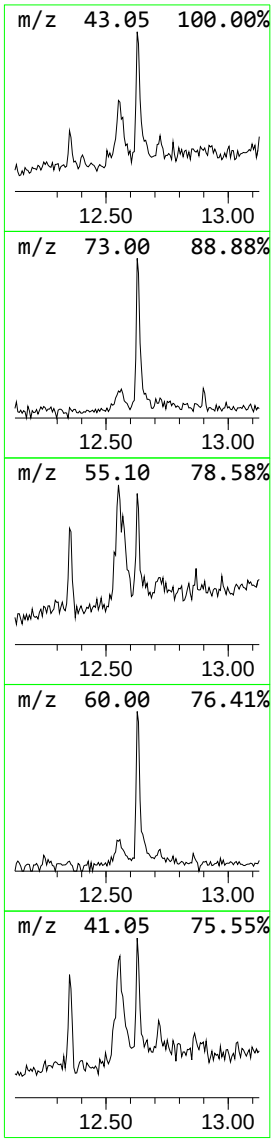
Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	4.15 ng	75585	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Hexadecane	226	C16H34	000544-76-3	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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

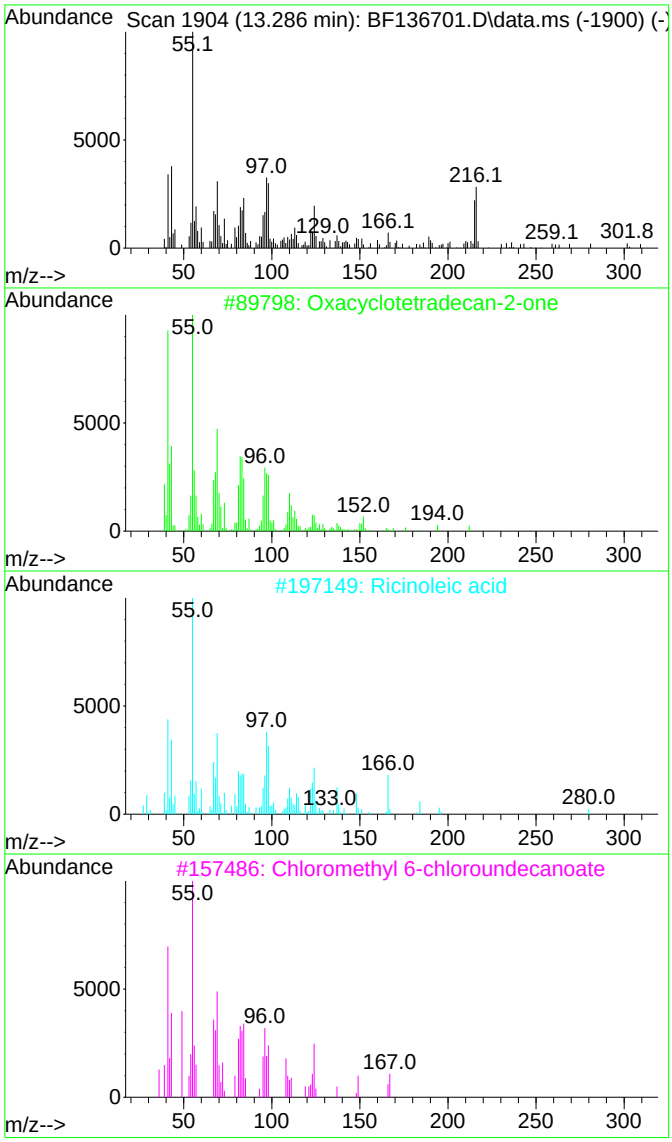
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

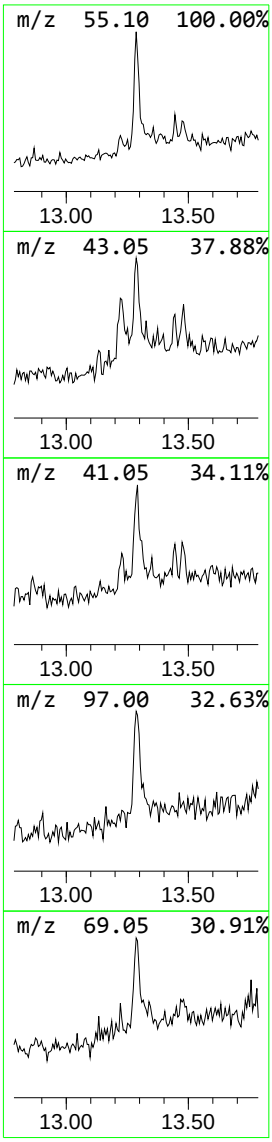
****

Peak Number 4 unknown13.286 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	6.46 ng	155950	Chrysene-d12	13.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxacyclotetradecan-2-one	212	C13H24O2	001725-04-8	43
2	Ricinoleic acid	298	C18H34O3	000141-22-0	35
3	Chloromethyl 6-chloroundecanoate	268	C12H22Cl2O2	080418-92-4	22
4	Myristoleic acid	226	C14H26O2	000544-64-9	22
5	Undecylenic acid	184	C11H20O2	000112-38-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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

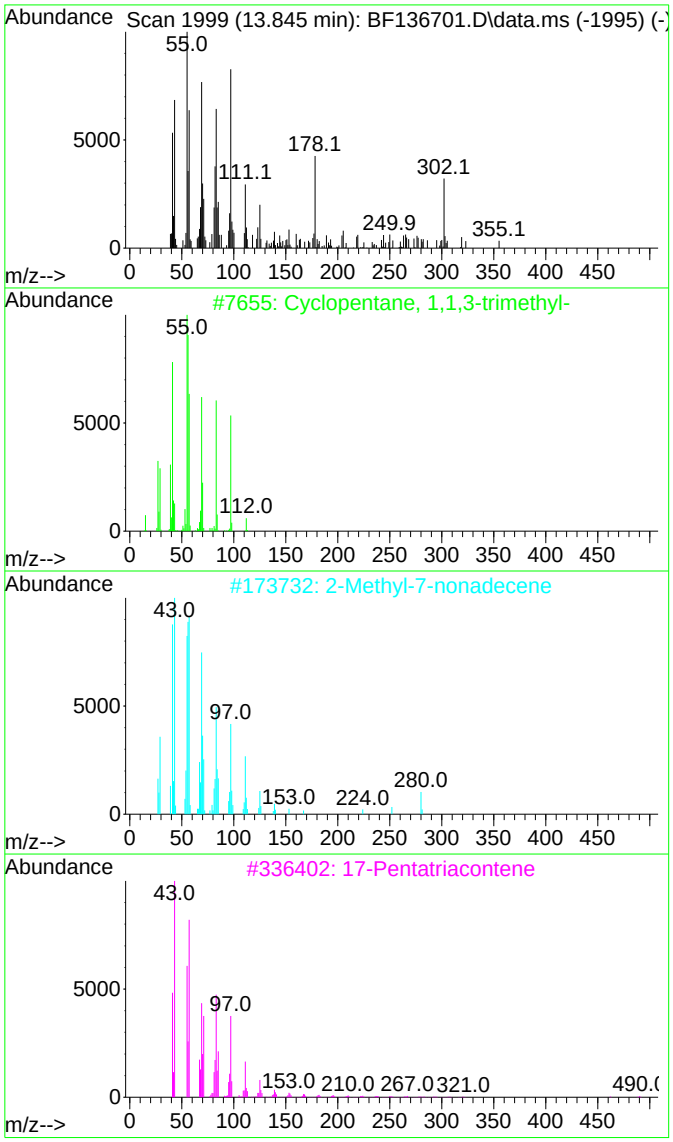
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

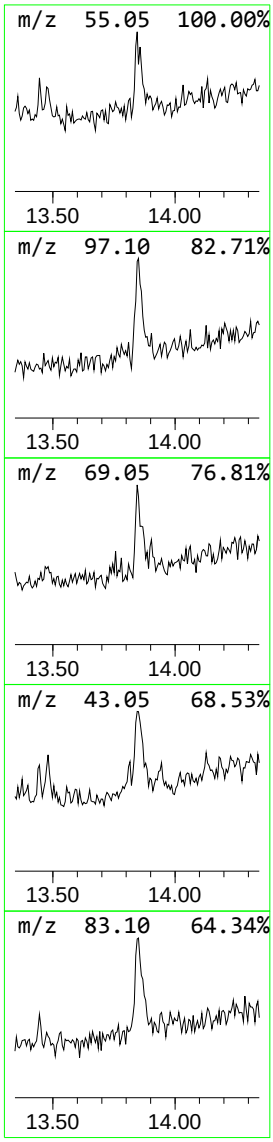
****

Peak Number 5 unknown13.845 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.30 ng	127866	Chrysene-d12	13.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	49
2	2-Methyl-7-nonadecene	280	C20H40	219750-68-2	49
3	17-Pentatriacontene	491	C35H70	006971-40-0	46
4	Triacontan-15-ol	438	C30H62O	031849-26-0	43
5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
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Operator : CG\JU
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

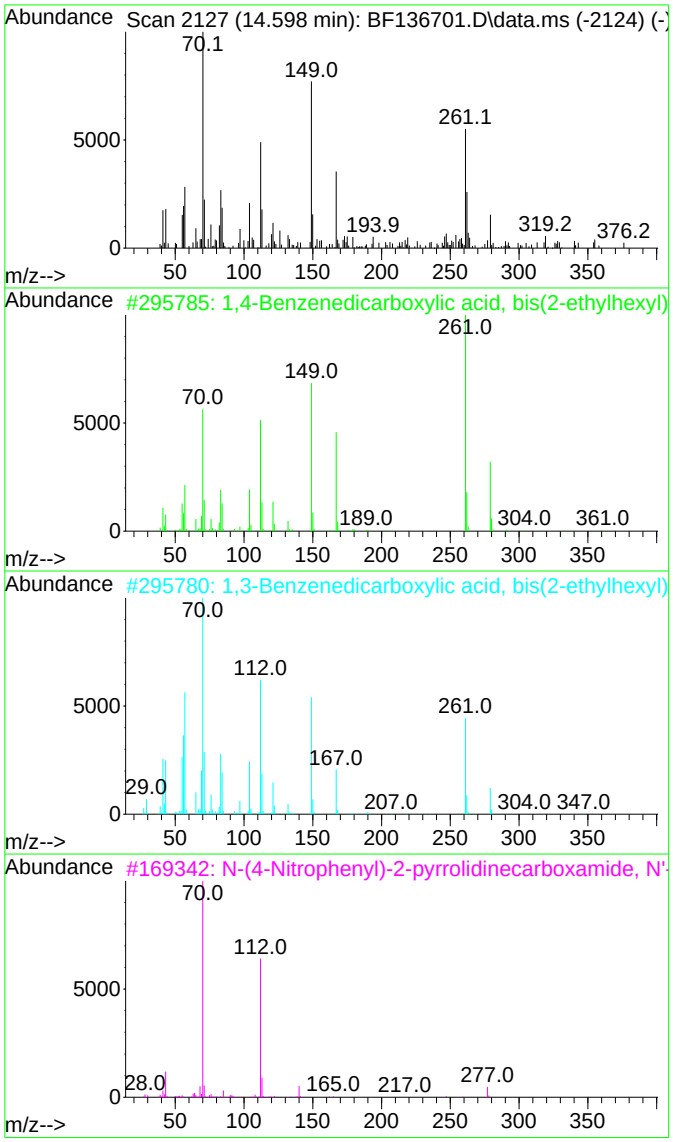
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

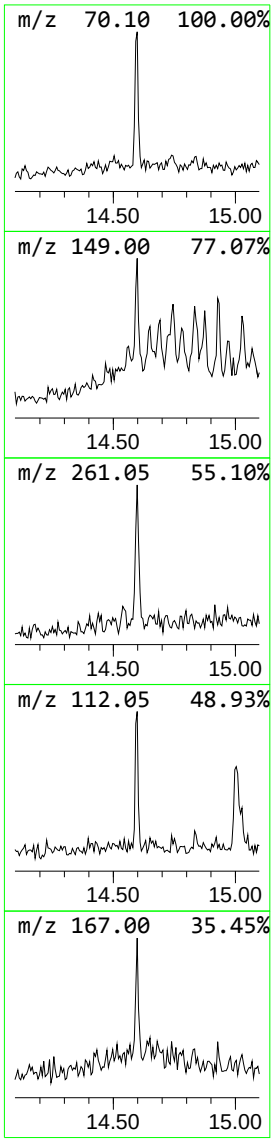
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	2.37 ng	57236	Chrysene-d12	13.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
3	N-(4-Nitrophenyl)-2-pyrrolidinec...	277	C13H15N3O4	1286682-74-3	22
4	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	18
5	Furane-2-carboxaldehyde, 5-(2-be...	261	C12H7NO2S2	039689-07-1	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136701.D
Acq On : 22 Dec 2023 23:29
Operator : CG\JU
Sample : 05969-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

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
n-Hexadecanoic ...	11.839	11.1	ng	201959	4	11.304	363863	20.0
13-Hexyloxacycl...	12.357	4.3	ng	78985	4	11.304	363863	20.0
Octadecanoic acid	12.627	4.2	ng	75585	4	11.304	363863	20.0
unknown13.286	13.286	6.5	ng	155950	5	13.956	482650	20.0
unknown13.845	13.845	5.3	ng	127866	5	13.956	482650	20.0
1,4-Benzenedica...	14.598	2.4	ng	57236	5	13.956	482650	20.0