LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042823\
Data File : BF133122.D
Acq On : 28 Apr 2023 14:26
Operator : CG\JU
Sample : 02495-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-01

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	549	553	557	rBV	2103491	1963969	37.94%	6.544%
2	6.363	724	727	739	rVB	1334940	1205803	23.29%	4.018%
3	6.734	786	790	793	rBV	1320290	983560	19.00%	3.277%
4	7.298	881	886	889	rBV	3056492	3010385	58.16%	10.031%
5	8.016	1005	1008	1011	rBV	1732837	1319433	25.49%	4.396%
6	9.098	1187	1192	1195	rBV	5746331	5176386	100.00%	17.248%
7	9.769	1302	1306	1309	rBV	1916621	1477972	28.55%	4.925%
8	10.481	1424	1427	1430	rBV	225257	171254	3.31%	0.571%
9	10.557	1435	1440	1443	rBV	3264379	2916030	56.33%	9.716%
10	11.251	1554	1558	1561	rBV	1750858	1485350	28.69%	4.949%
11	11.716	1633	1637	1640	rBV	80479	98517	1.90%	0.328%
12	11.792	1645	1650	1660	rVV	1302316	1256657	24.28%	4.187%
13	12.574	1779	1783	1796	rBV	1342333	1496932	28.92%	4.988%
14	12.839	1823	1828	1831	rBV	4837512	4553770	87.97%	15.173%
15	13.880	2001	2005	2009	rBV	1092076	1049232	20.27%	3.496%
16	14.480	2103	2107	2113	rBV	418150	457347	8.84%	1.524%
17	14.739	2147	2151	2155	rBV	130259	130169	2.51%	0.434%
18	15.304	2242	2247	2252	rBV	869881	969551	18.73%	3.231%
19	15.651	2302	2306	2316	rBV2	94887	170176	3.29%	0.567%
20	16.233	2401	2405	2410	rBV3	81573	119791	2.31%	0.399%

Sum of corrected areas: 30012284

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042823\
Data File : BF133122.D
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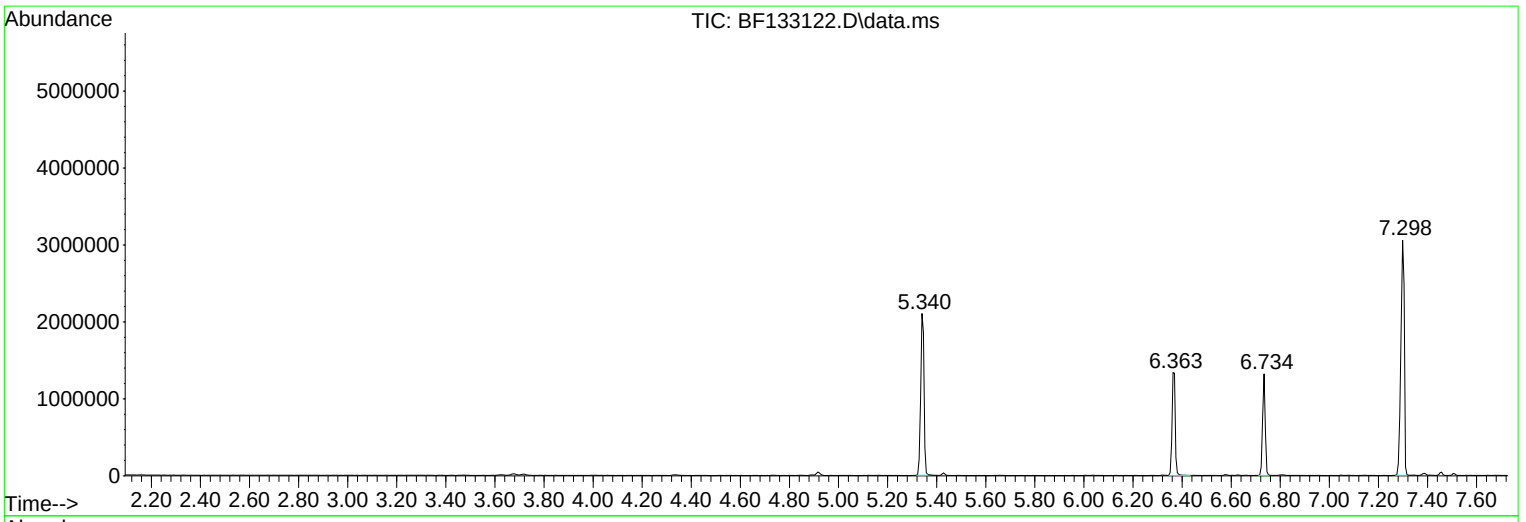
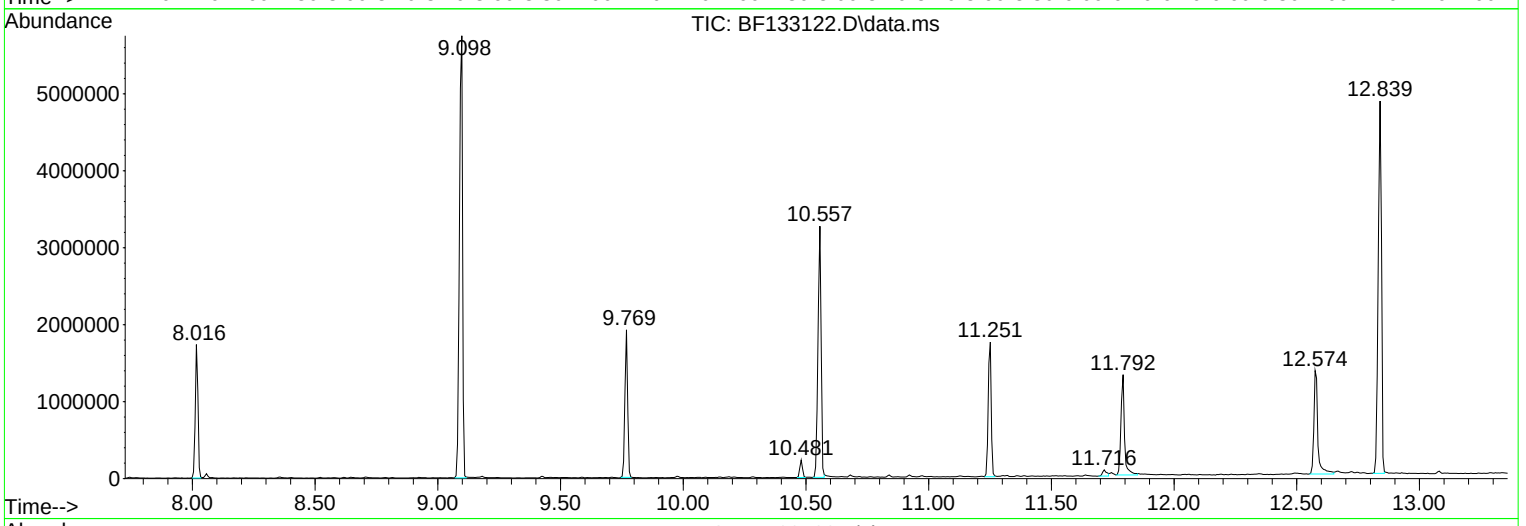
Misc :
ALS Vial : 11 Sample Multiplier: 1

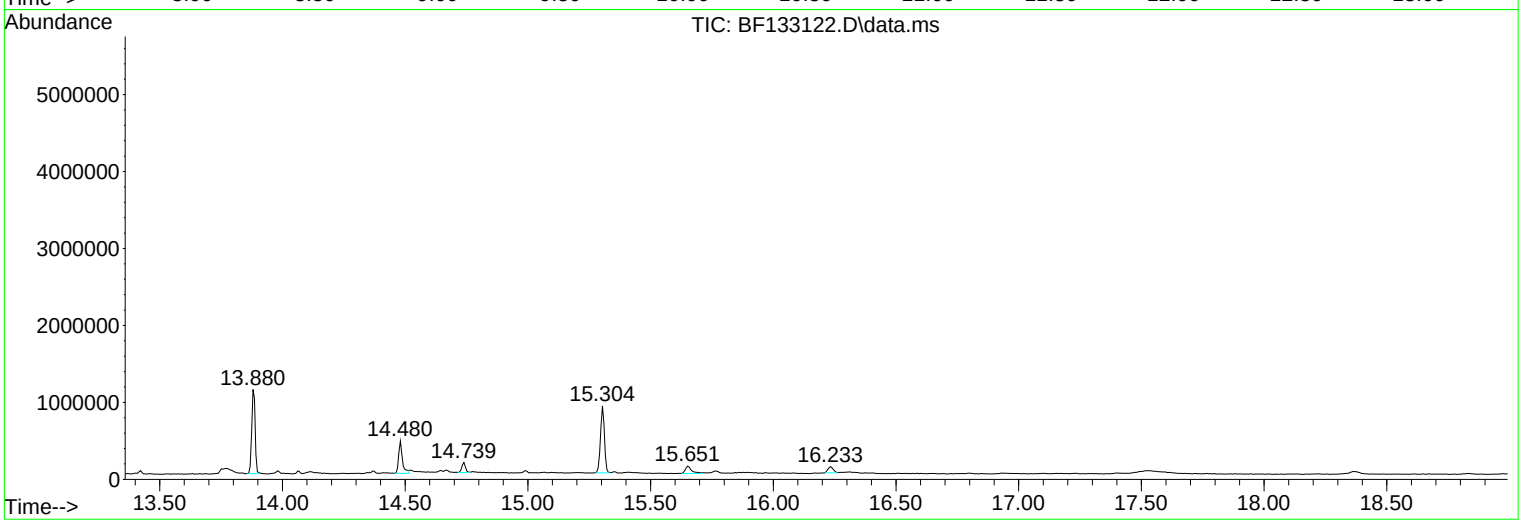
Instrument :
BNA_F
ClientSampleId :
PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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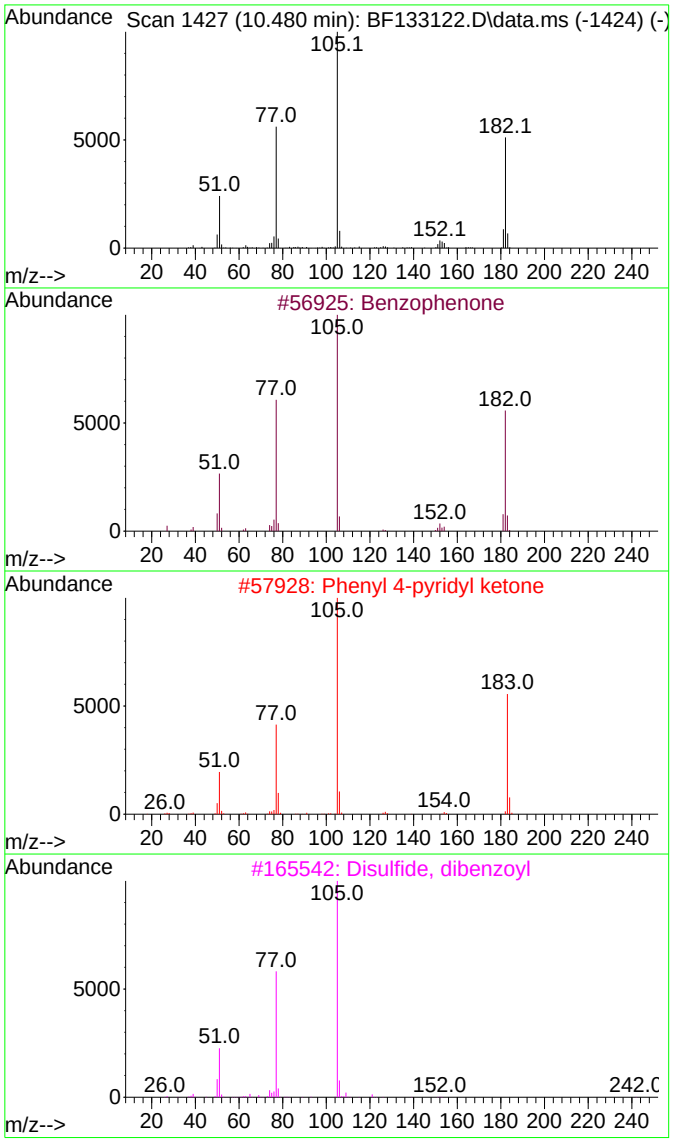
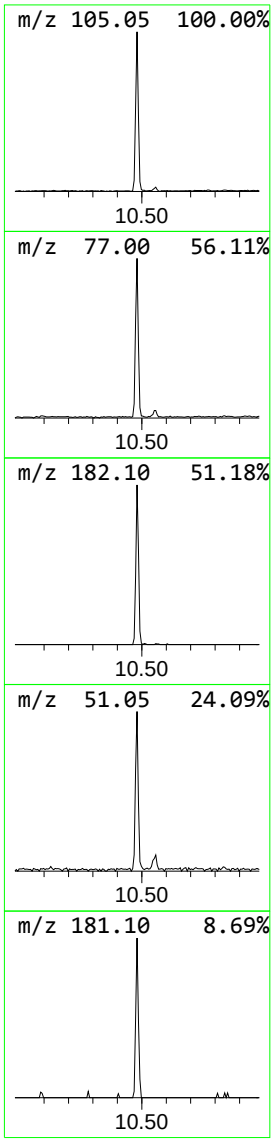
Peak Number 1 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	2.32 ng	171254	Acenaphthene-d10	9.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
3	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	47





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Data File : BF133122.D
Acq On : 28 Apr 2023 14:26
Operator : CG\JU
Sample : 02495-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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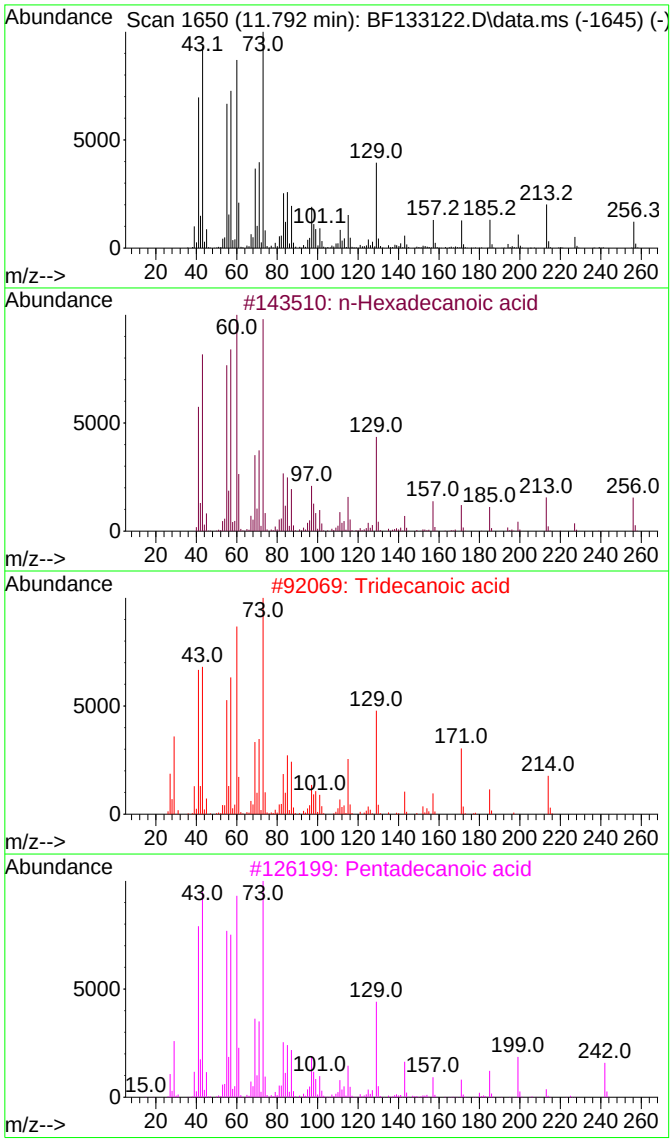
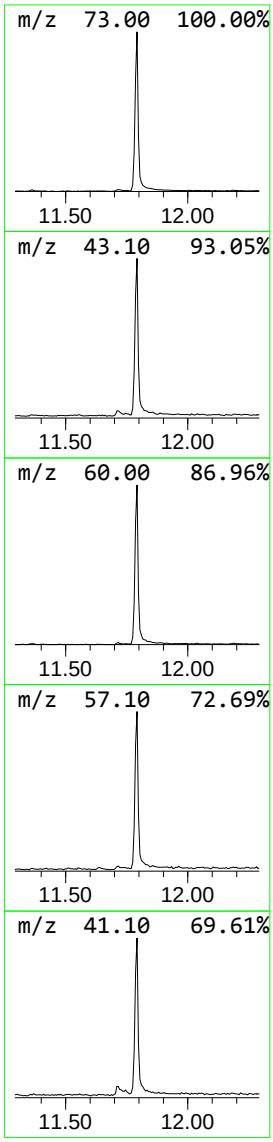
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	16.92 ng	1256660	Phenanthrene-d10	11.251

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	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042823\
Data File : BF133122.D
Acq On : 28 Apr 2023 14:26
Operator : CG\JU
Sample : 02495-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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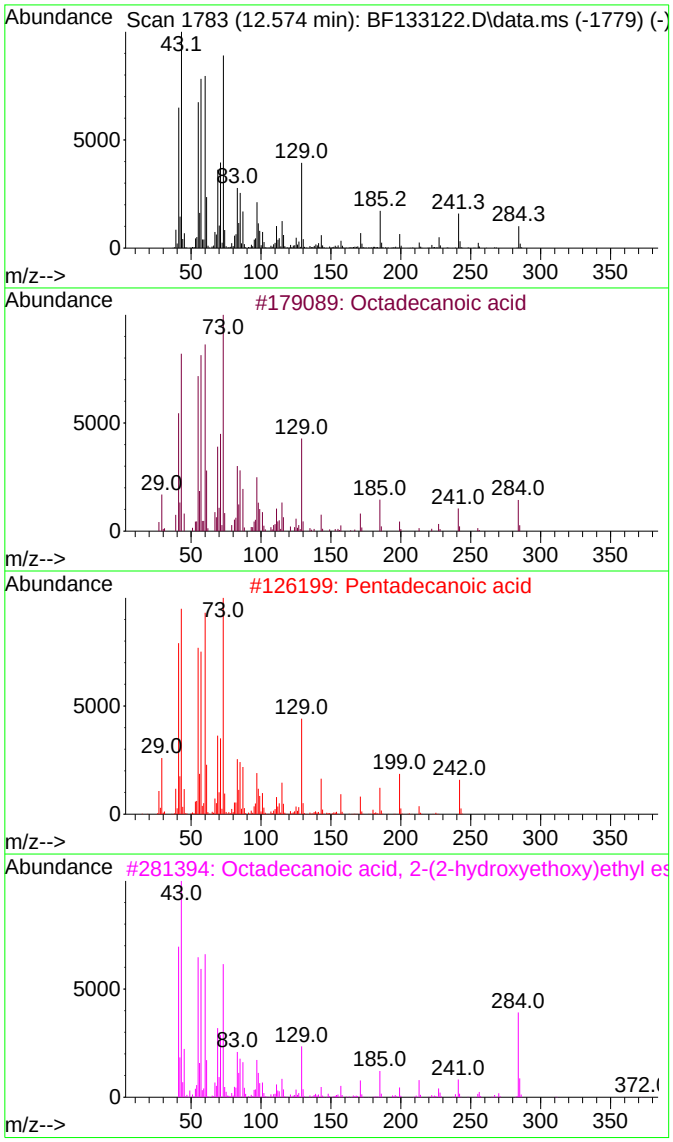
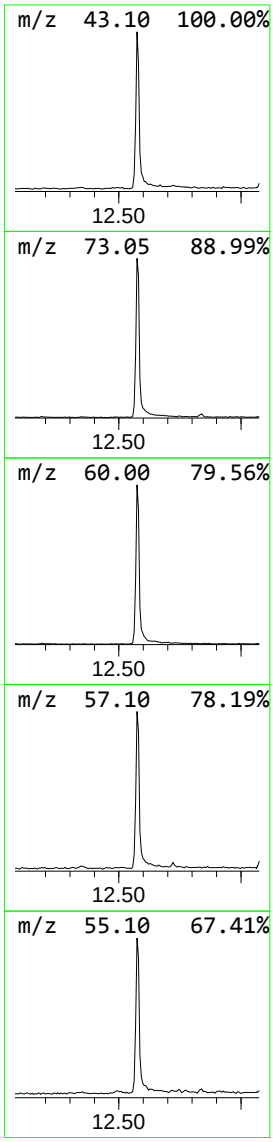
Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	28.53 ng	1496930	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Data File : BF133122.D
Acq On : 28 Apr 2023 14:26
Operator : CG\JU
Sample : 02495-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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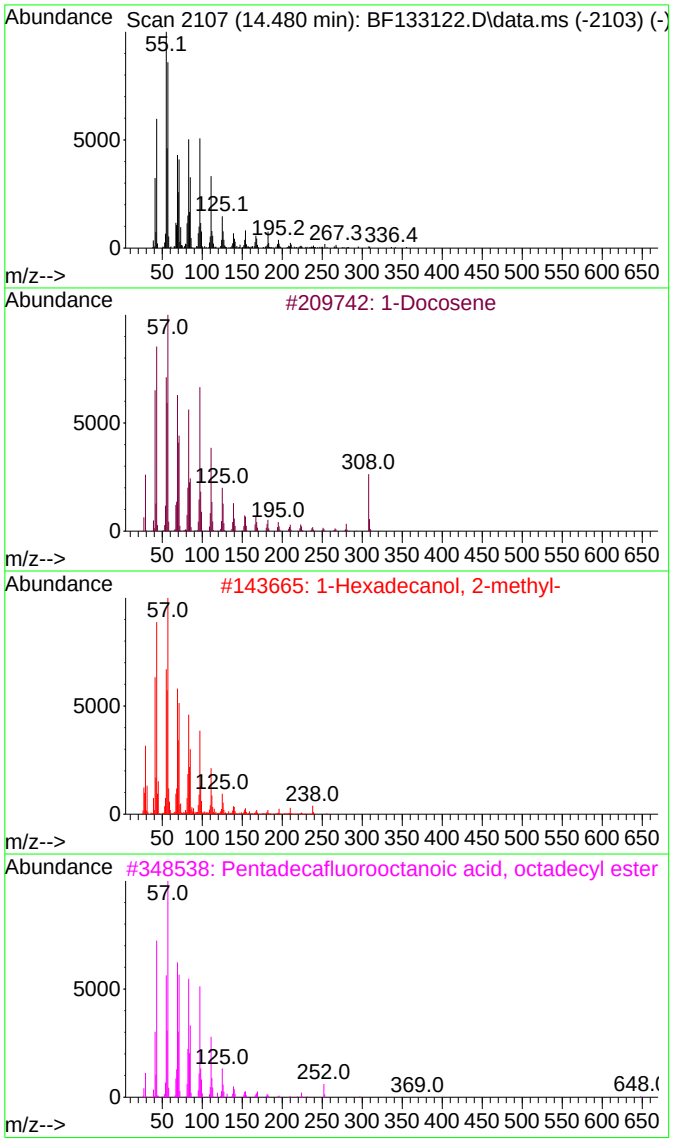
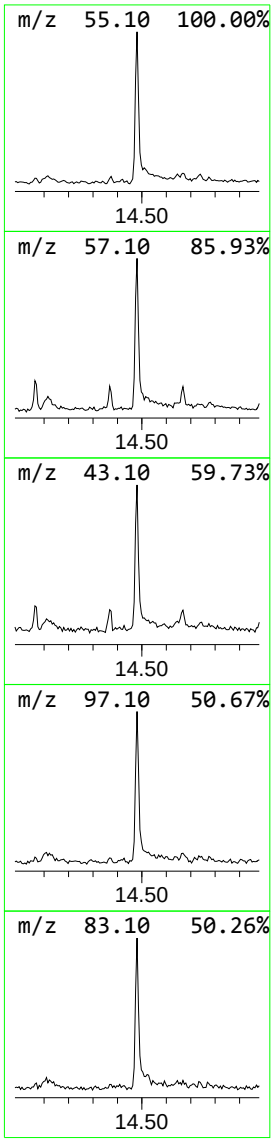
Peak Number 4 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	8.72 ng	457347	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042823\
Data File : BF133122.D
Acq On : 28 Apr 2023 14:26
Operator : CG\JU
Sample : 02495-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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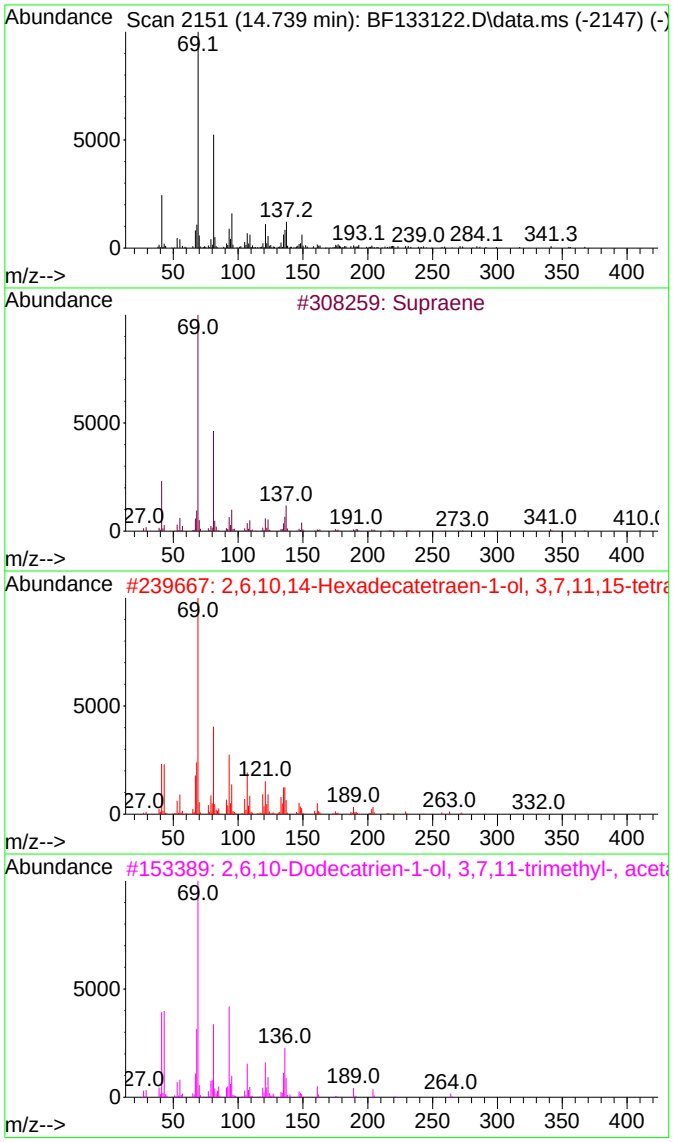
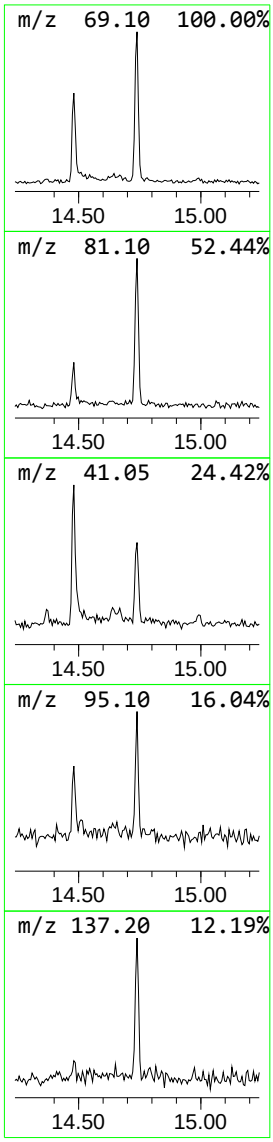
Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	2.69 ng	130169	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4	1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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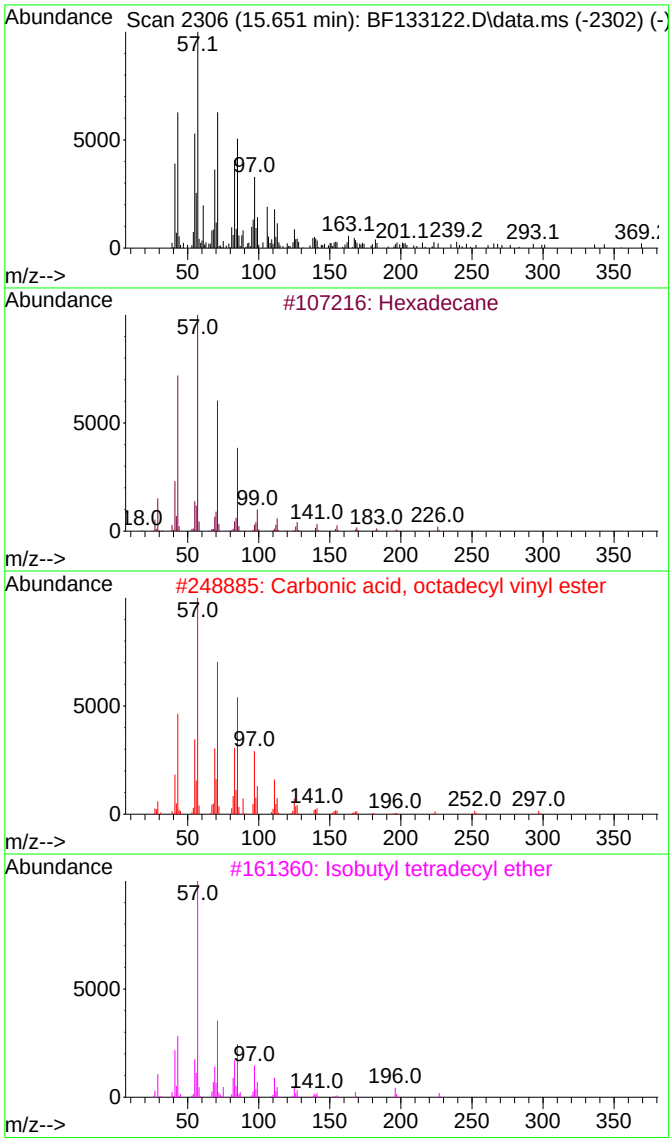
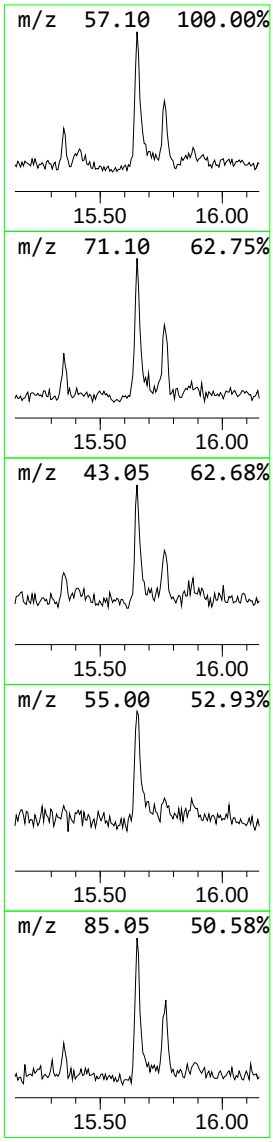
Peak Number 6 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.651	3.51 ng	170176	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	74
3	Isobutyl tetradecyl ether	270	C18H38O	1000406-32-7	74
4	Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	72
5	Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	68





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PZ-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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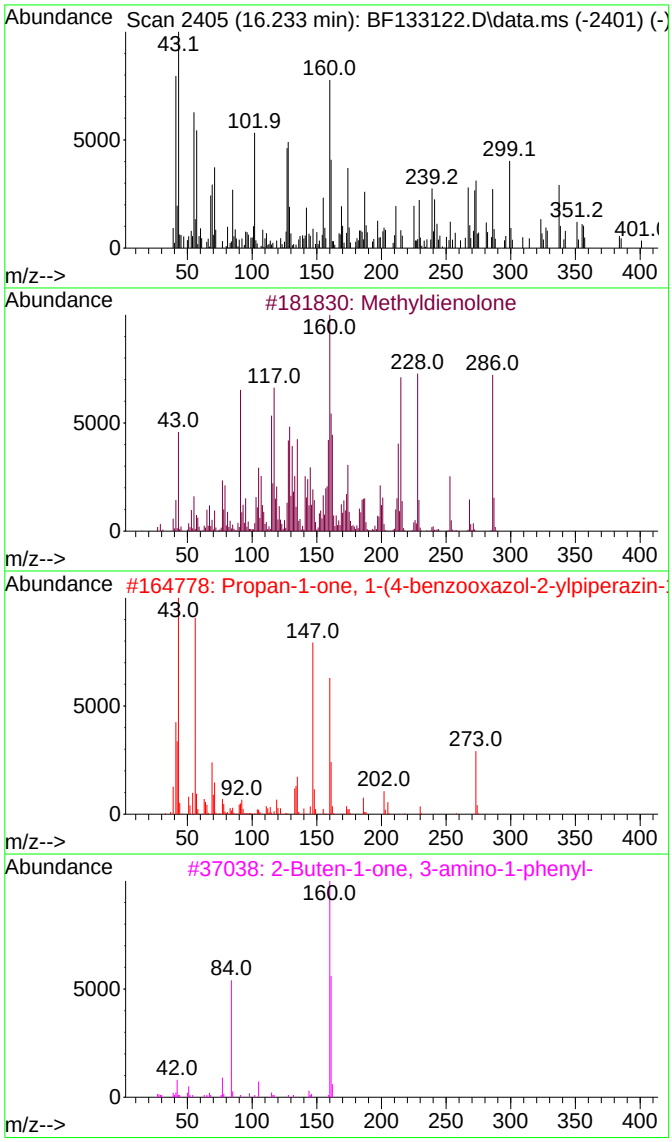
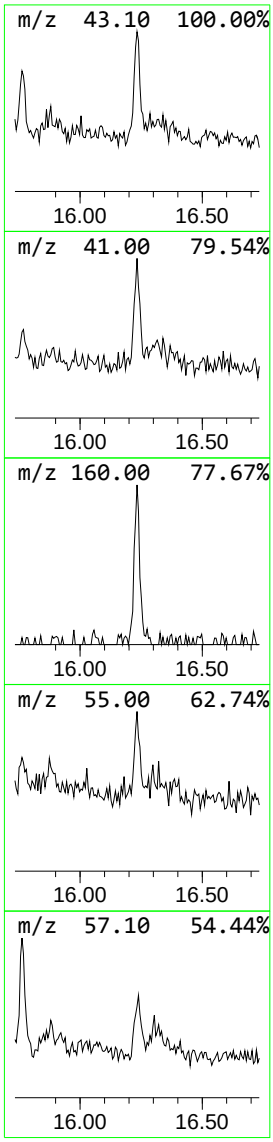
Peak Number 7 unknown16.233 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	2.47 ng	119791	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyldienolone	286	C19H26O2	014531-89-6	25
2	Propan-1-one, 1-(4-benzooxazol-2...	273	C15H19N3O2	1000304-82-1	18
3	2-Buten-1-one, 3-amino-1-phenyl-	161	C10H11NO	001128-85-4	14
4	1H-Indole-6-carboxamide	160	C9H8N2O	001670-88-8	10
5	1,7-Dihydroxynaphthalene, diacetate	244	C14H12O4	051850-49-8	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042823\
Data File : BF133122.D
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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
Benzophenone	10.480	2.3	ng	171254	3	9.769	1477970	20.0
n-Hexadecanoic ...	11.792	16.9	ng	1256660	4	11.251	1485350	20.0
Octadecanoic acid	12.575	28.5	ng	1496930	5	13.880	1049230	20.0
1-Docosene	14.480	8.7	ng	457347	5	13.880	1049230	20.0
Supraene	14.739	2.7	ng	130169	6	15.304	969551	20.0
Hexadecane	15.651	3.5	ng	170176	6	15.304	969551	20.0
unknown16.233	16.233	2.5	ng	119791	6	15.304	969551	20.0