LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	19	rVB	802227	1253906	79.21%	10.349%
2	5.098	507	511	517	rVB	13975	20373	1.29%	0.168%
3	5.498	573	579	584	rBV	1065834	1360653	85.95%	11.230%
4	6.504	744	750	764	rVB	1006162	1315657	83.11%	10.859%
5	6.887	809	815	820	rVB	313283	399913	25.26%	3.301%
6	7.439	904	909	914	rBV	674535	840341	53.08%	6.936%
7	7.692	948	952	958	rBV	20363	24443	1.54%	0.202%
8	8.163	1027	1032	1044	rVB	360485	438910	27.73%	3.623%
9	9.239	1210	1215	1220	rBV	1095977	1332094	84.15%	10.995%
10	9.922	1326	1331	1336	rBV	328912	402778	25.44%	3.324%
11	10.639	1448	1453	1460	rBV	190145	230574	14.57%	1.903%
12	10.716	1460	1466	1477	rBV	576600	749598	47.35%	6.187%
13	10.951	1502	1506	1512	rVB	18146	22795	1.44%	0.188%
14	11.416	1580	1585	1591	rBV	352850	436385	27.57%	3.602%
15	11.492	1592	1598	1602	rVB	11277	16484	1.04%	0.136%
16	11.945	1670	1675	1689	rBV	175502	290915	18.38%	2.401%
17	12.633	1789	1792	1797	rBV	11409	16735	1.06%	0.138%
18	12.733	1805	1809	1818	rBV2	58981	102379	6.47%	0.845%
19	12.863	1827	1831	1848	rBV	36362	68234	4.31%	0.563%
20	13.010	1850	1856	1861	rBV	1234257	1583029	100.00%	13.066%
21	13.921	2007	2011	2022	rVB3	74341	140166	8.85%	1.157%
22	14.074	2032	2037	2048	rVB	368305	555228	35.07%	4.583%
23	15.151	2217	2220	2230	rVB	61735	123514	7.80%	1.019%
24	15.598	2291	2296	2313	rVB	206388	390670	24.68%	3.224%

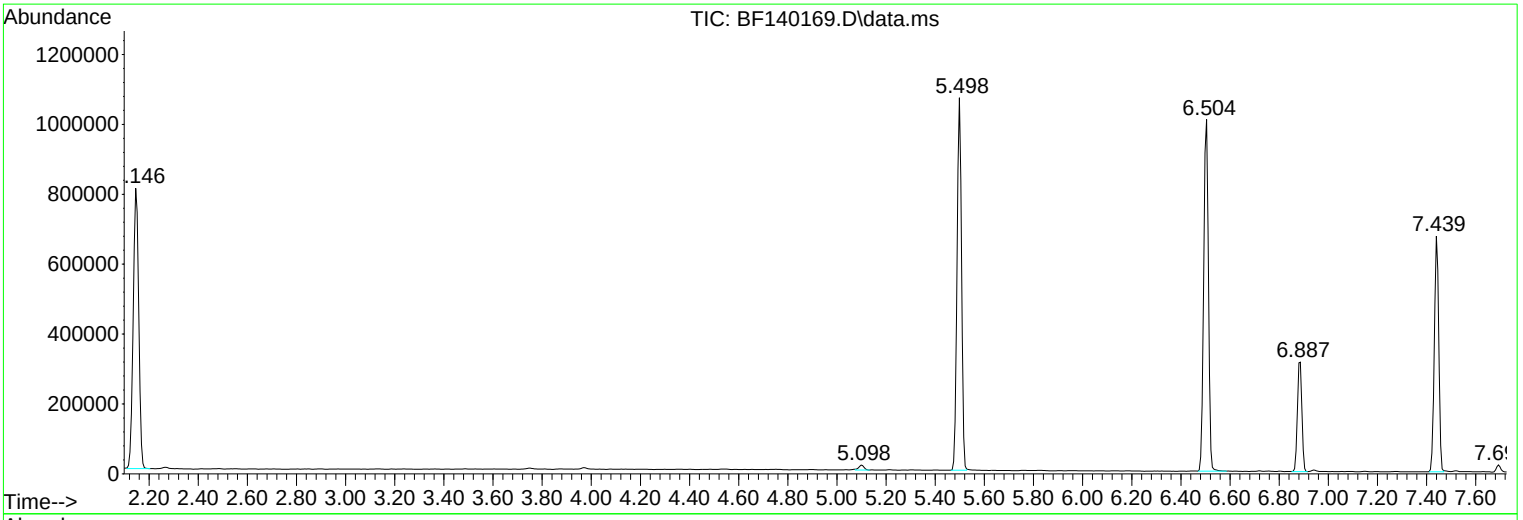
Sum of corrected areas: 12115774

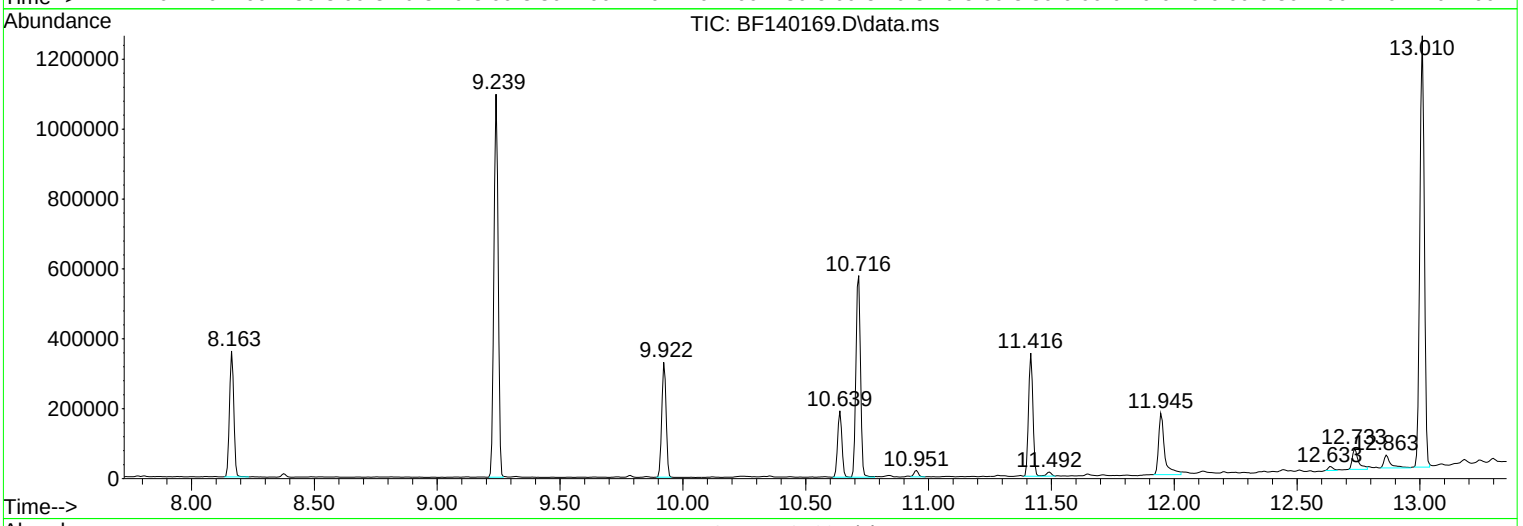
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

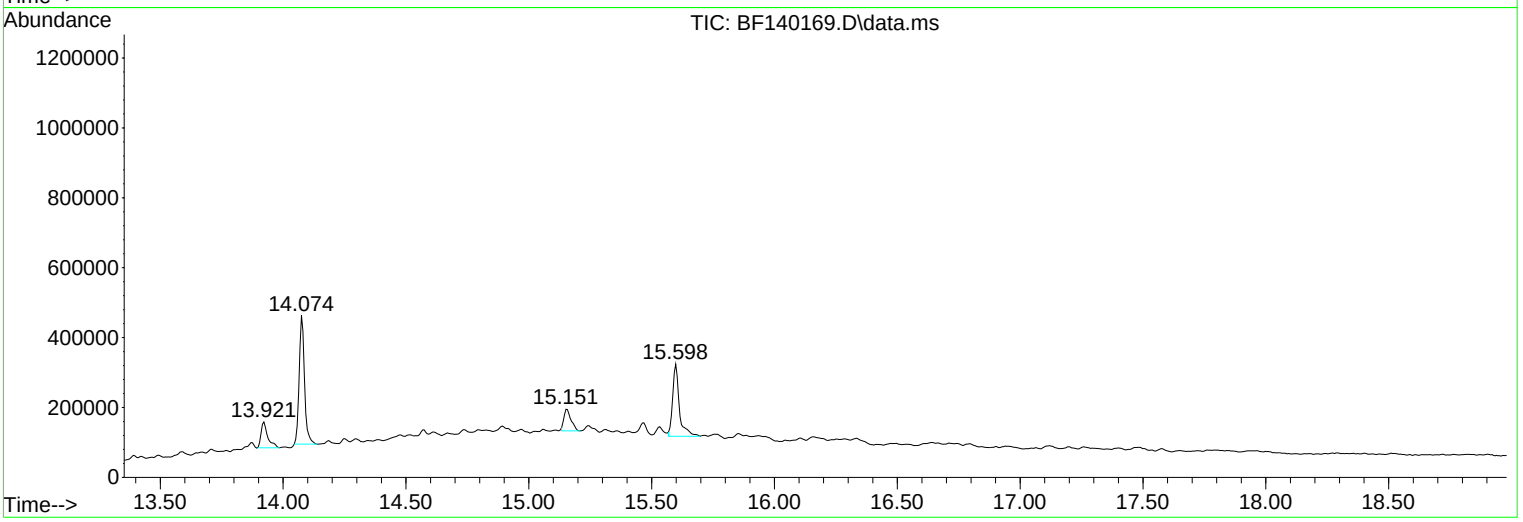
Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

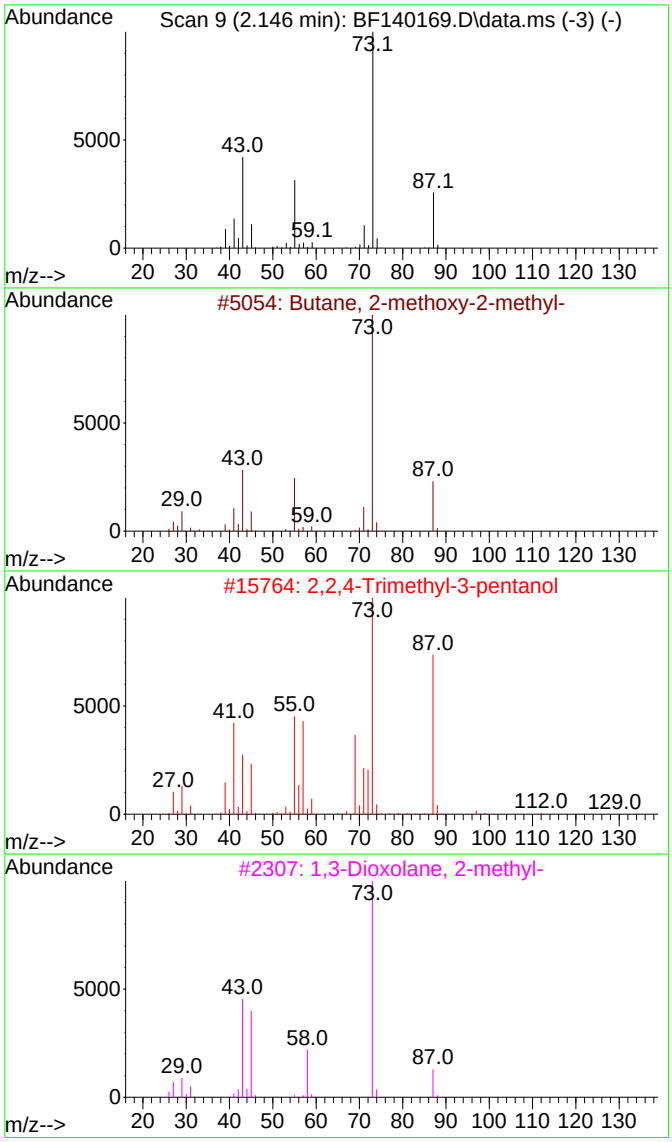
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

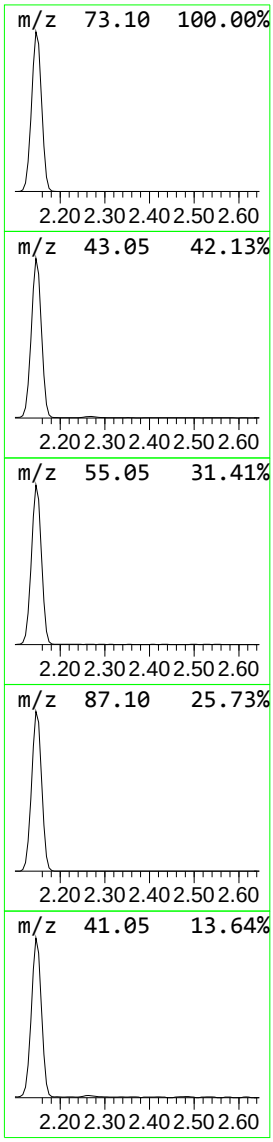
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	62.71 ng	1253910	1,4-Dichlorobenzene-d4	6.887

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

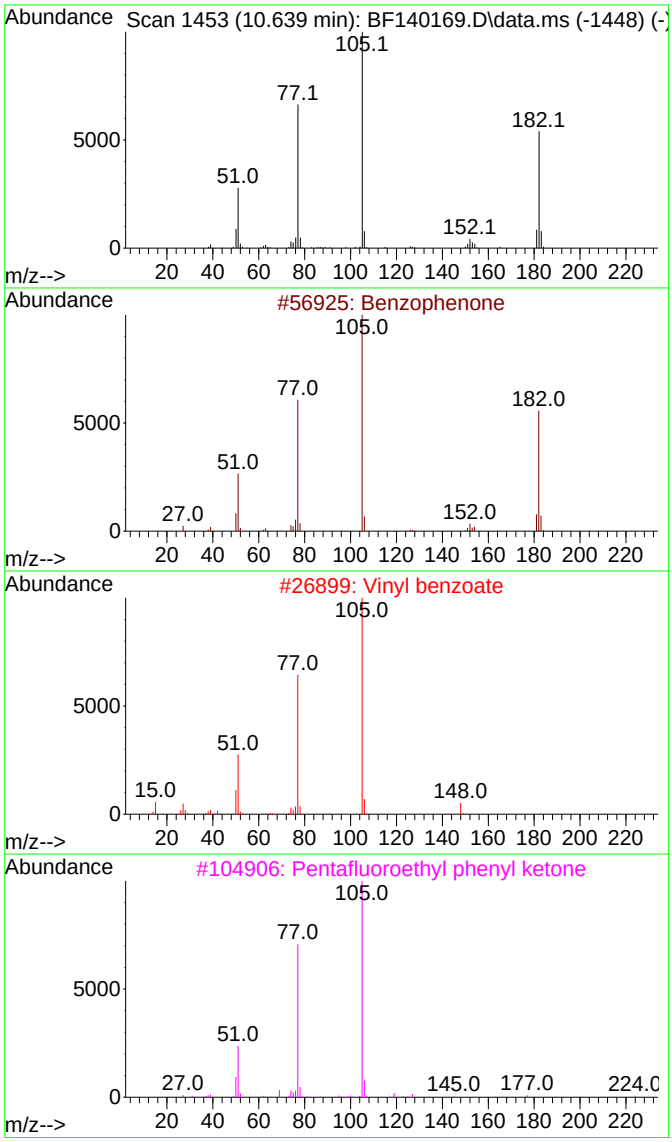
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

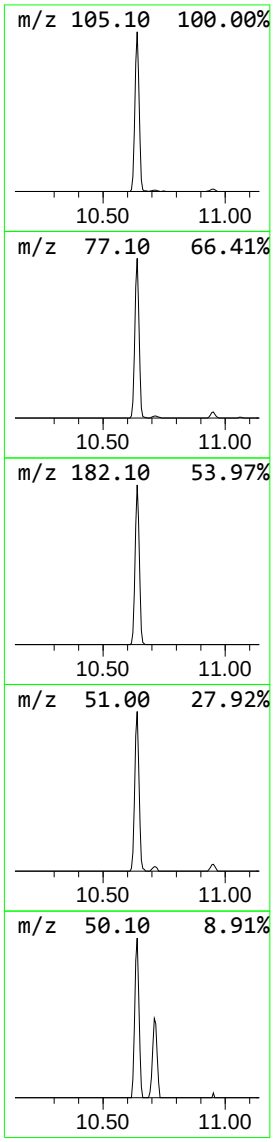
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	11.45 ng	230574	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

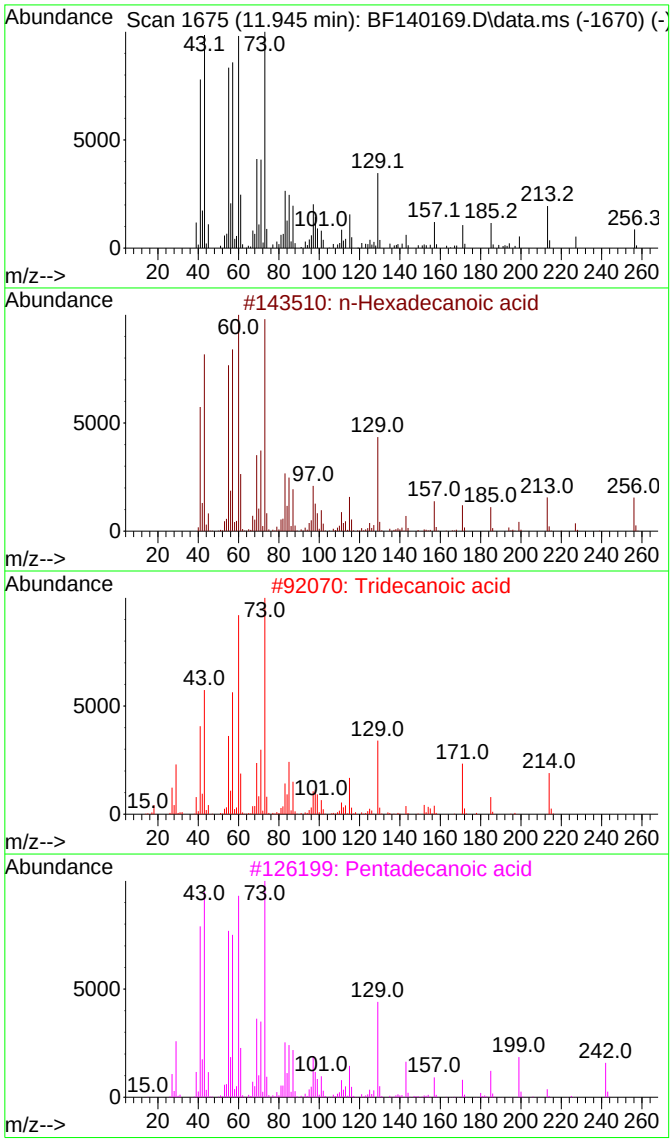
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

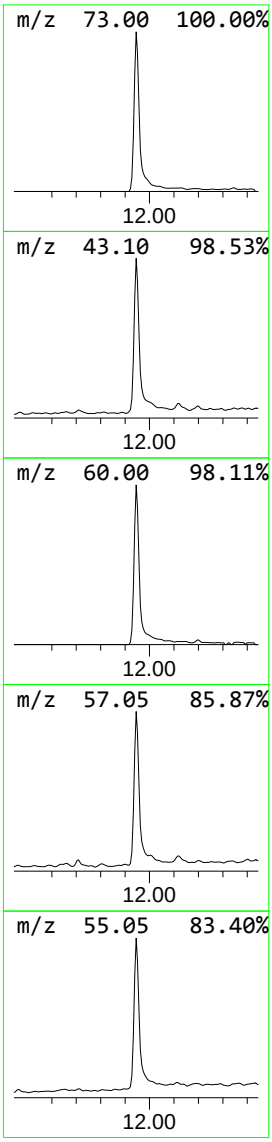
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	13.33 ng	290915	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

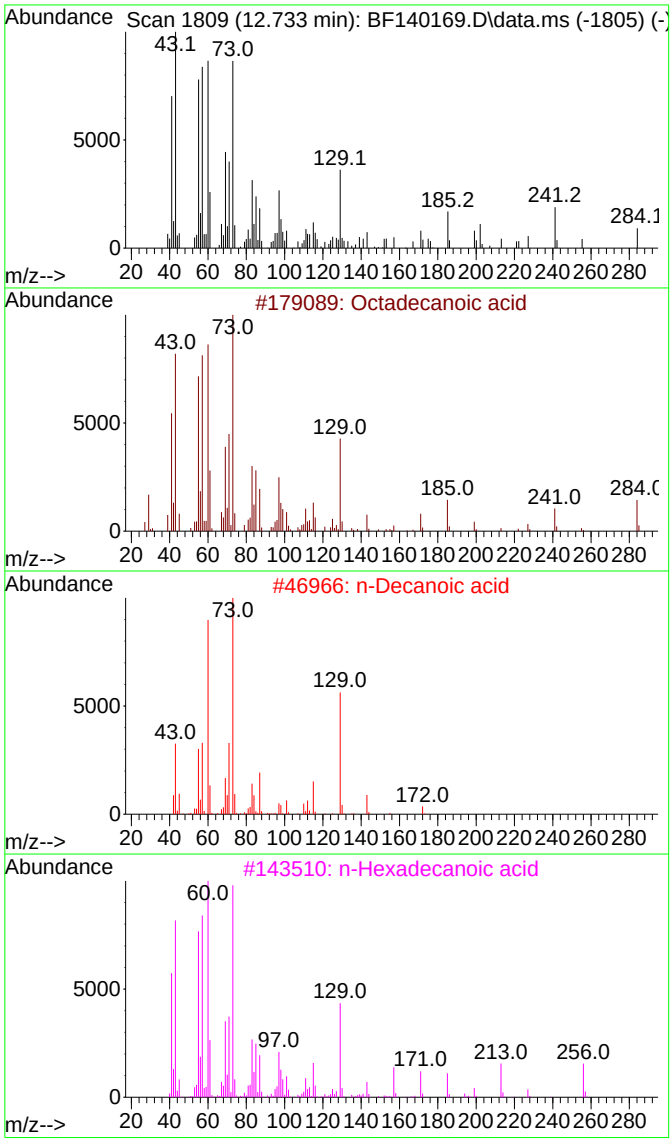
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

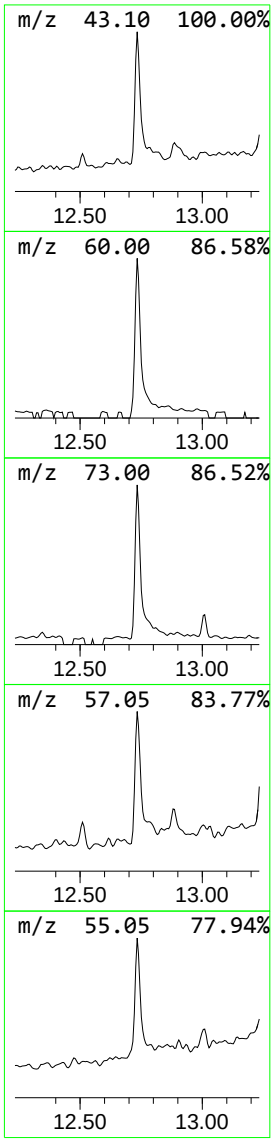
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	4.69 ng	102379	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

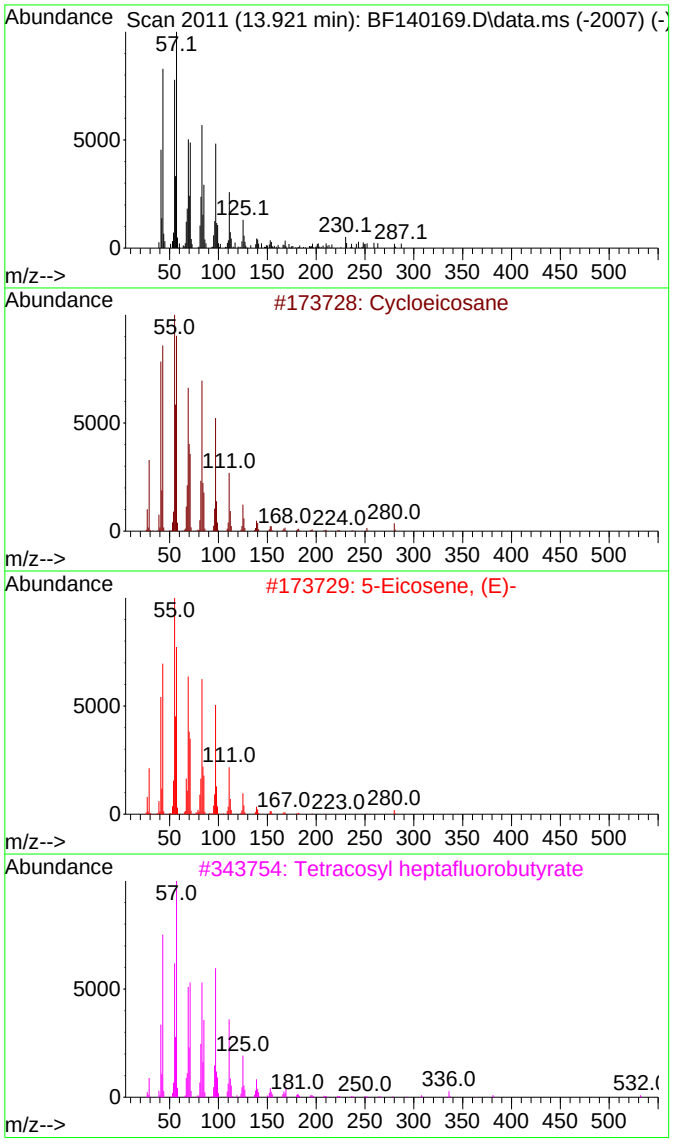
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

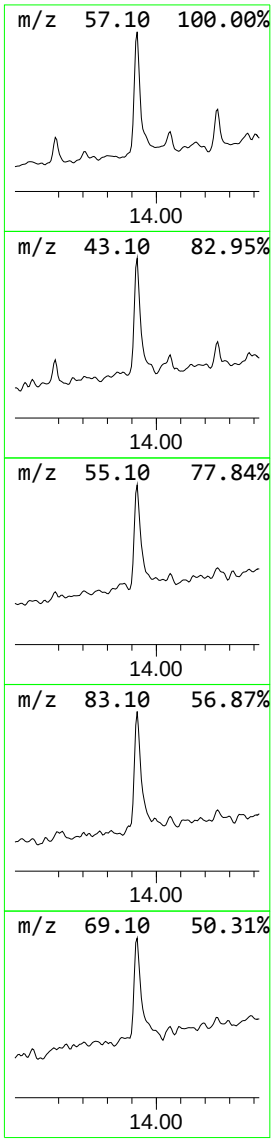
****

Peak Number 6 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.05 ng	140166	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	94
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140169.D
Acq On : 30 Oct 2024 20:25
Operator : RC/JU
Sample : P4611-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.146	62.7	ng	1253910	1	6.887	399913	20.0
Benzophenone	10.639	11.4	ng	230574	3	9.922	402778	20.0
n-Hexadecanoic ...	11.945	13.3	ng	290915	4	11.416	436385	20.0
Octadecanoic acid	12.733	4.7	ng	102379	4	11.416	436385	20.0
Cycloeicosane	13.921	5.0	ng	140166	5	14.074	555228	20.0