LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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: BF140190.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	12	23	rVB	937510	1503842	62.05%	7.130%
2	5.498	573	579	585	rBV	1623612	2220063	91.60%	10.525%
3	6.504	744	750	755	rBV	1764840	2423524	100.00%	11.490%
4	6.881	809	814	820	rVB	613897	765220	31.57%	3.628%
5	7.439	903	909	914	rBV	1118923	1453576	59.98%	6.891%
6	7.692	948	952	958	rBV	72914	88974	3.67%	0.422%
7	8.163	1026	1032	1040	rBV	850501	1053595	43.47%	4.995%
8	8.375	1064	1068	1075	rVB	27704	36189	1.49%	0.172%
9	9.239	1209	1215	1220	rBV	1900839	2387240	98.50%	11.318%
10	9.922	1326	1331	1344	rVB	950112	1246327	51.43%	5.909%
11	10.639	1447	1453	1460	rBV	190540	237590	9.80%	1.126%
12	10.716	1460	1466	1480	rBV	1399262	1806981	74.56%	8.567%
13	11.416	1580	1585	1593	rBV	935908	1196696	49.38%	5.674%
14	11.486	1593	1597	1600	rVB3	21565	26538	1.10%	0.126%
15	11.945	1670	1675	1690	rBV2	371665	596900	24.63%	2.830%
16	12.674	1795	1799	1804	rVB	39918	51139	2.11%	0.242%
17	12.733	1805	1809	1821	rBV	66775	129437	5.34%	0.614%
18	12.827	1821	1825	1829	rBV	131643	163935	6.76%	0.777%
19	13.010	1850	1856	1861	rBV	1560451	2011287	82.99%	9.536%
20	13.398	1919	1922	1927	rVB	22331	27197	1.12%	0.129%
21	13.539	1942	1946	1951	rBV2	86332	117834	4.86%	0.559%
22	13.586	1951	1954	1957	rBV2	20563	27089	1.12%	0.128%
23	13.927	2007	2012	2021	rBV	84157	161509	6.66%	0.766%
24	14.080	2033	2038	2047	rVB	556384	743563	30.68%	3.525%
25	15.609	2292	2298	2303	rBV	398729	616188	25.43%	2.921%

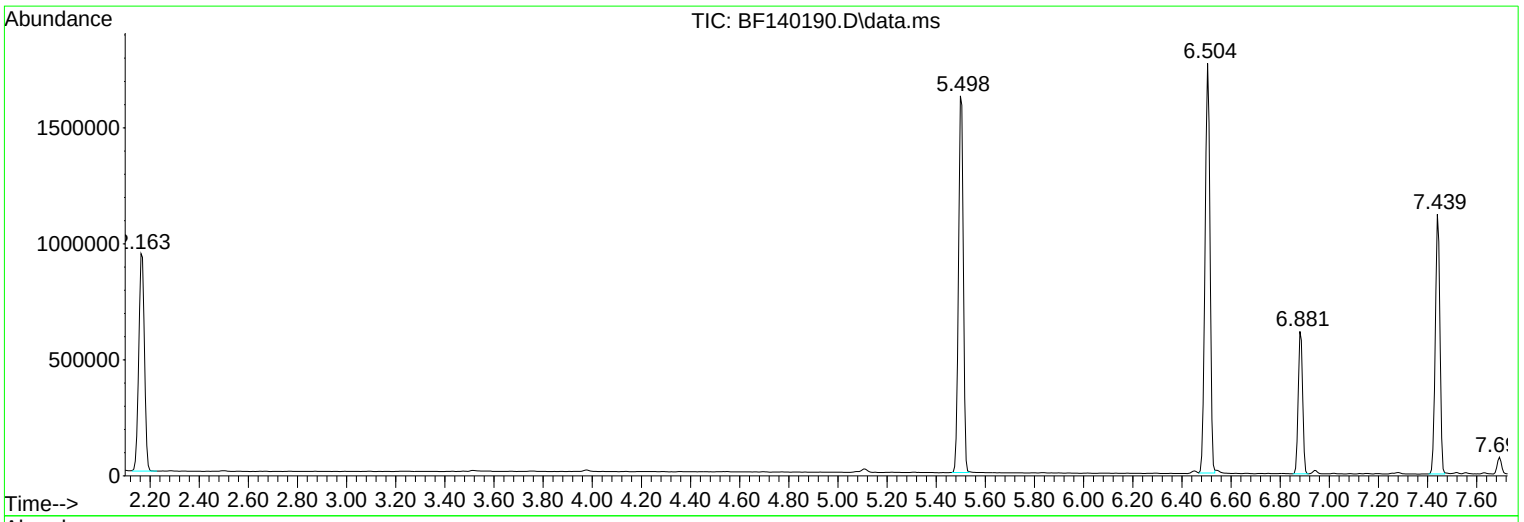
Sum of corrected areas: 21092433

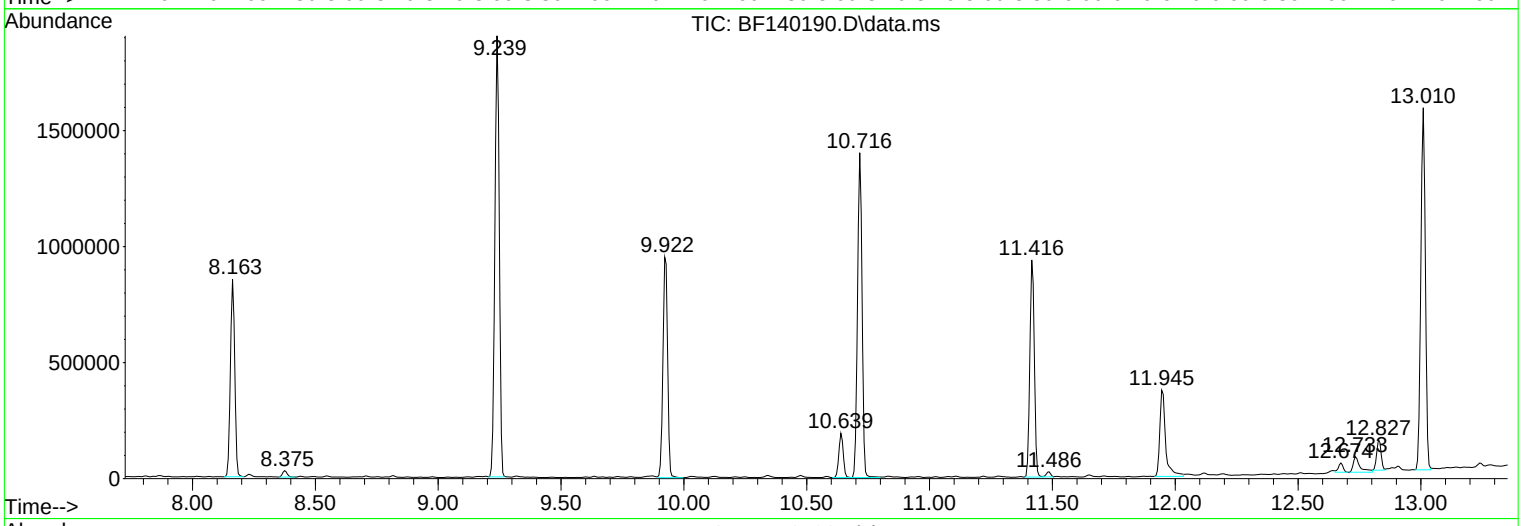
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

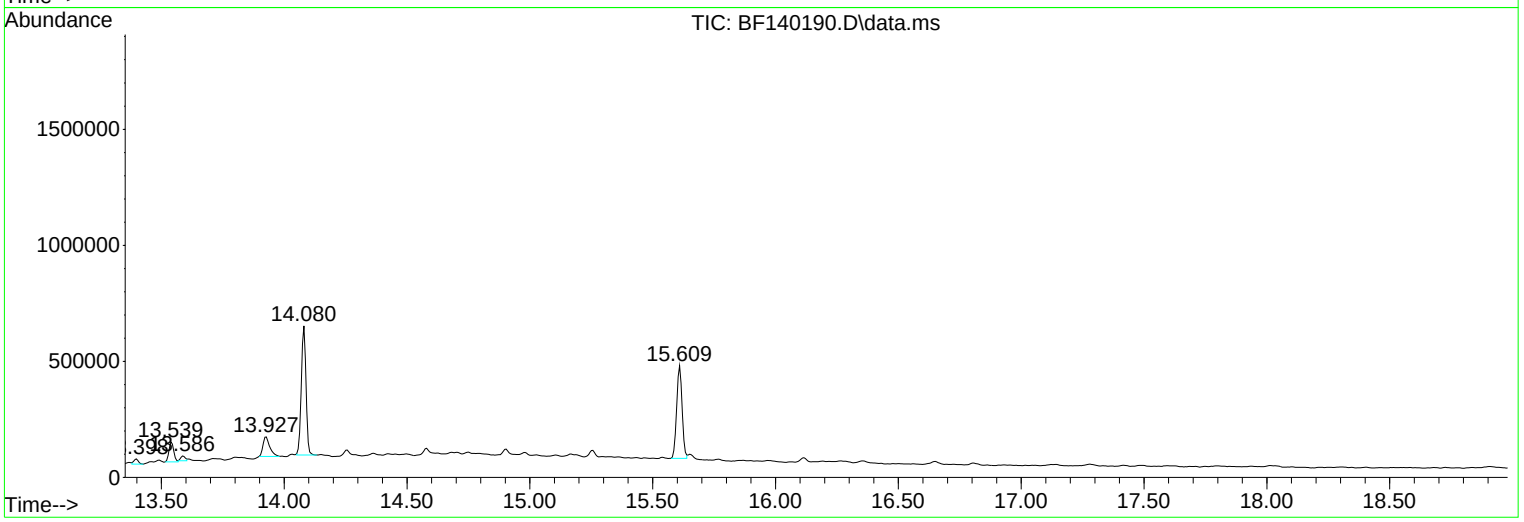
Instrument :
BNA_F
ClientSampleId :
BP-F16

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\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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

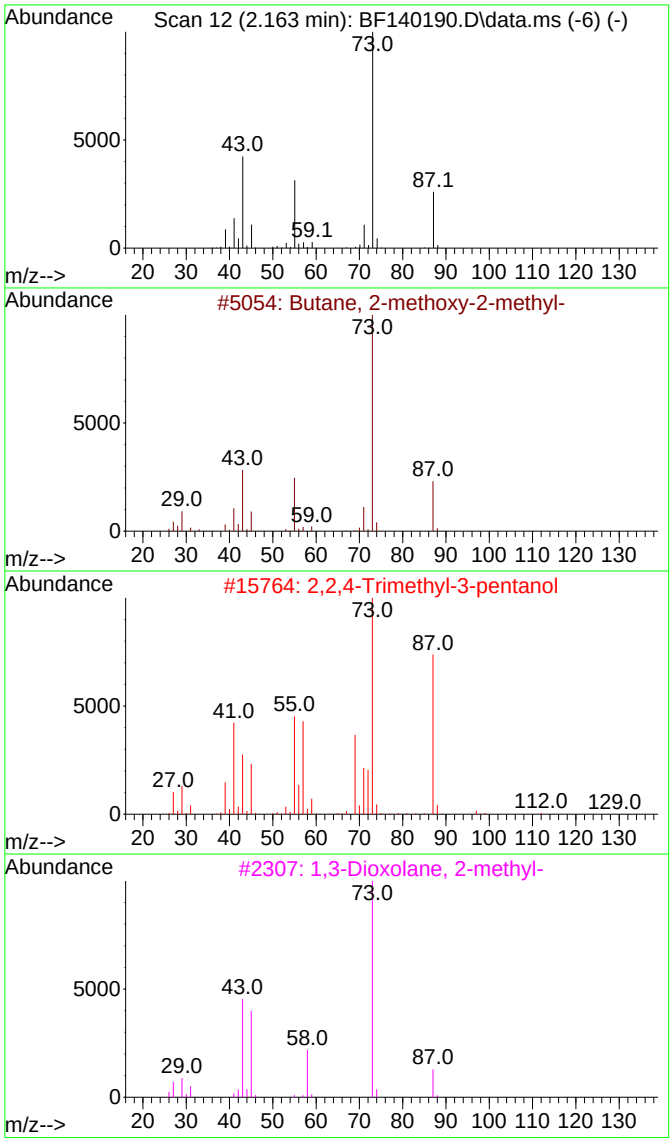
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

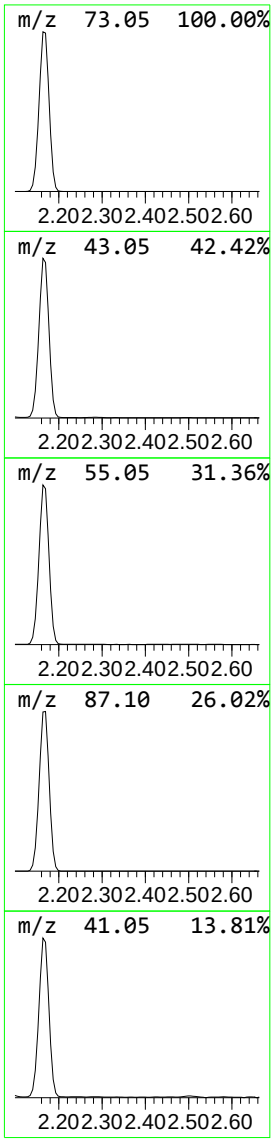
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	39.30 ng	1503840	1,4-Dichlorobenzene-d4	6.881

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
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\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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

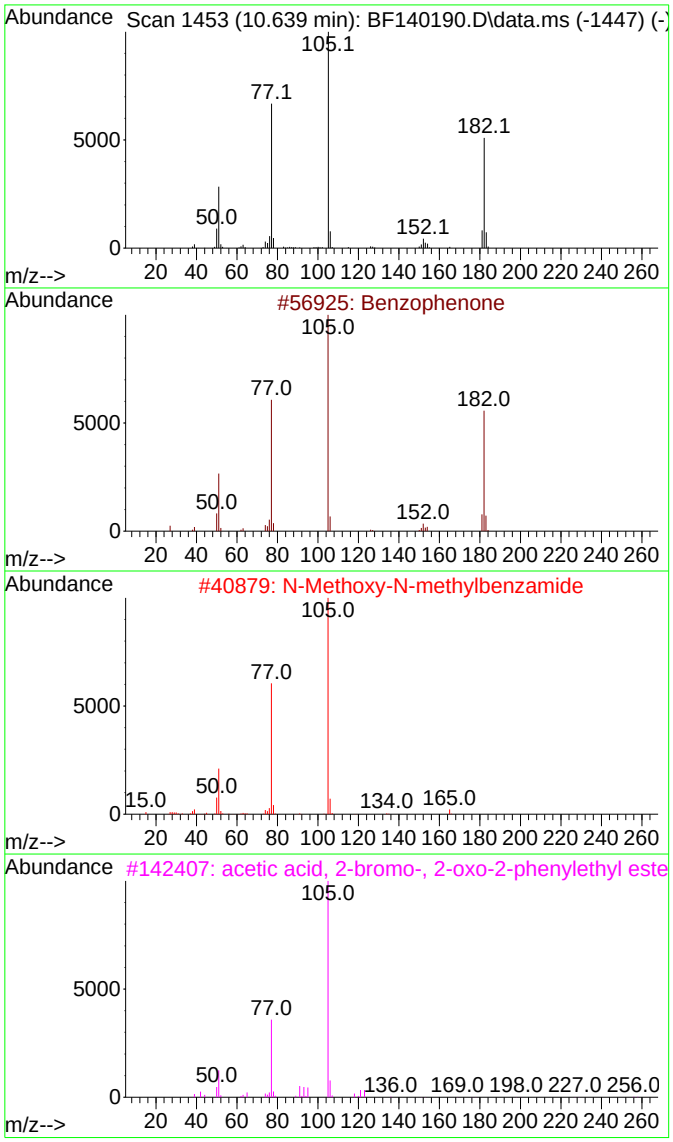
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

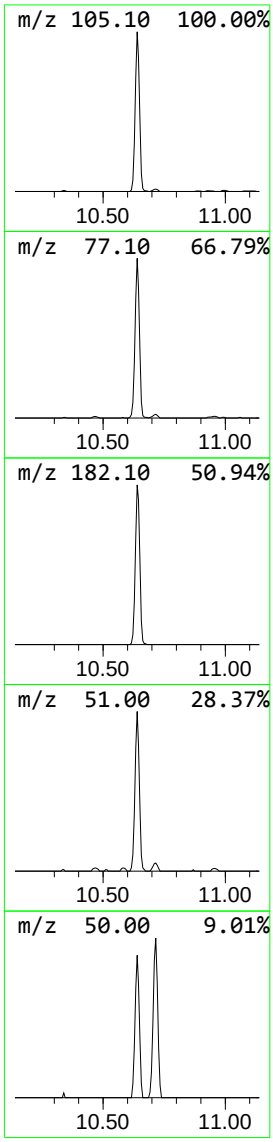
****

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	3.81 ng	237590	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
3	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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

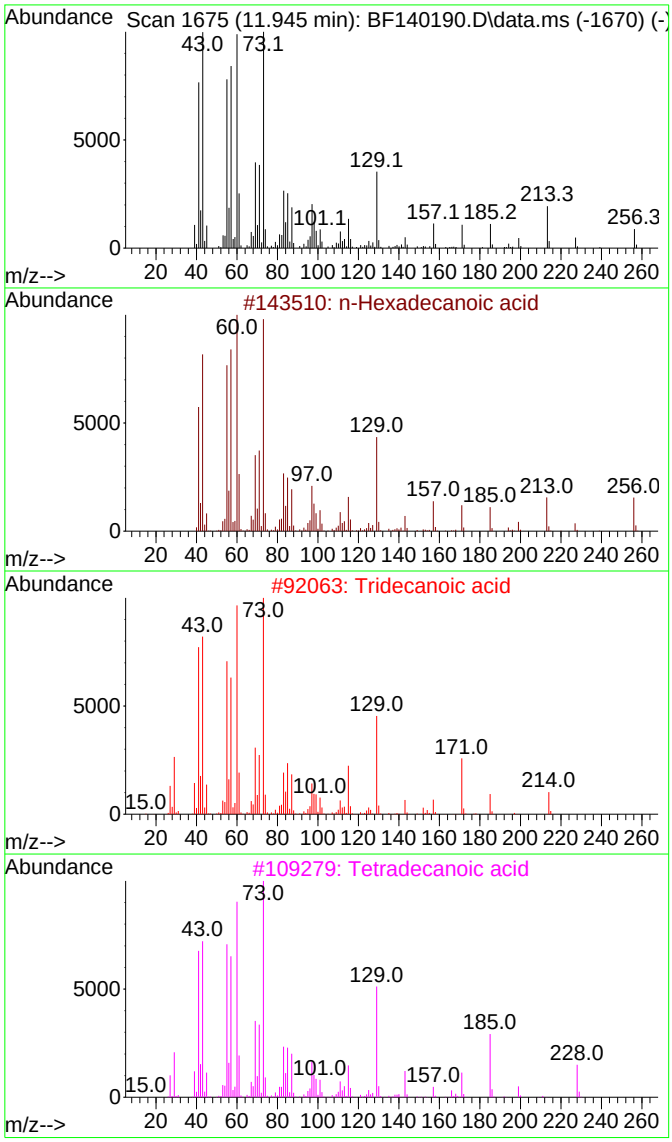
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

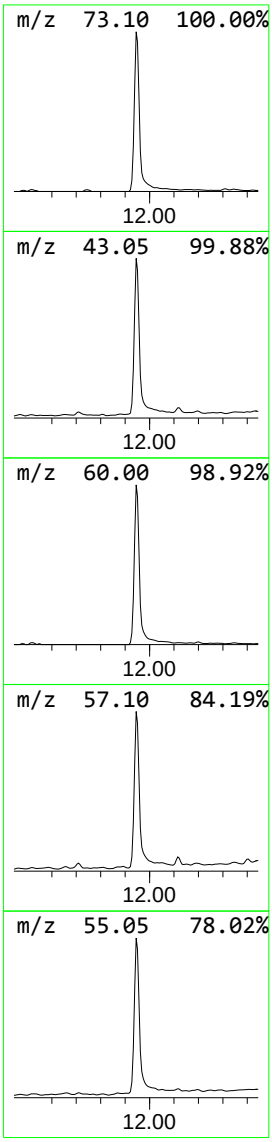
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	9.98 ng	596900	Phenanthrene-d10	11.416

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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

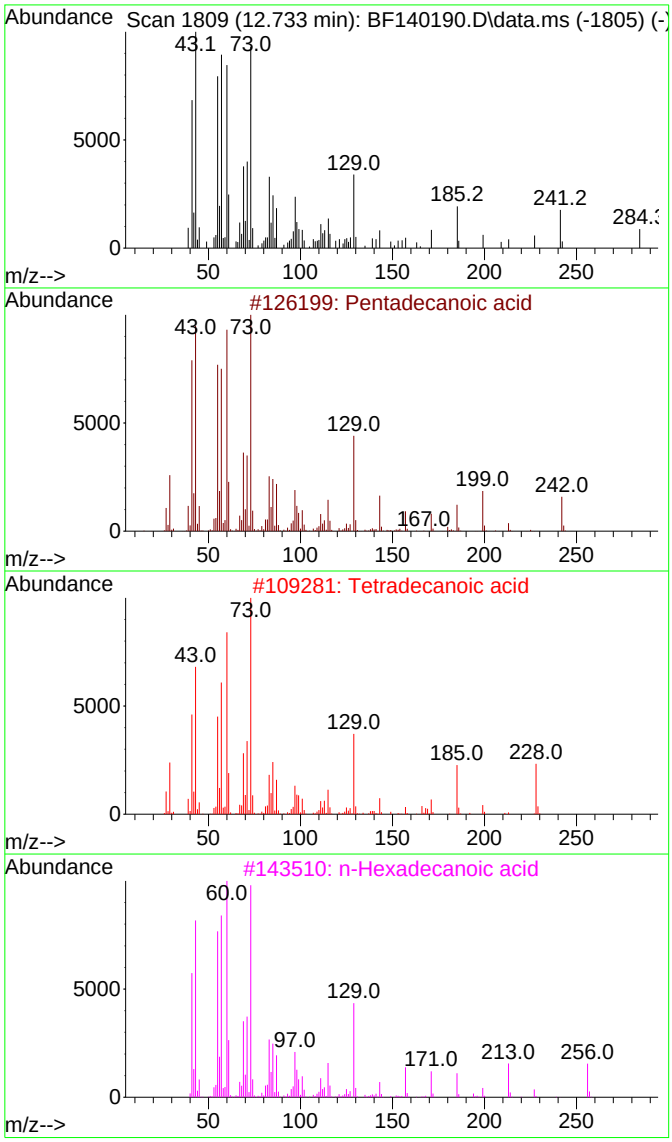
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

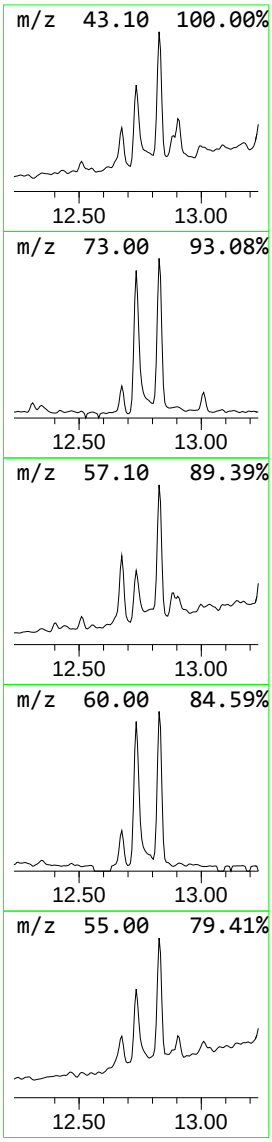
****

Peak Number 4 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.16 ng	129437	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

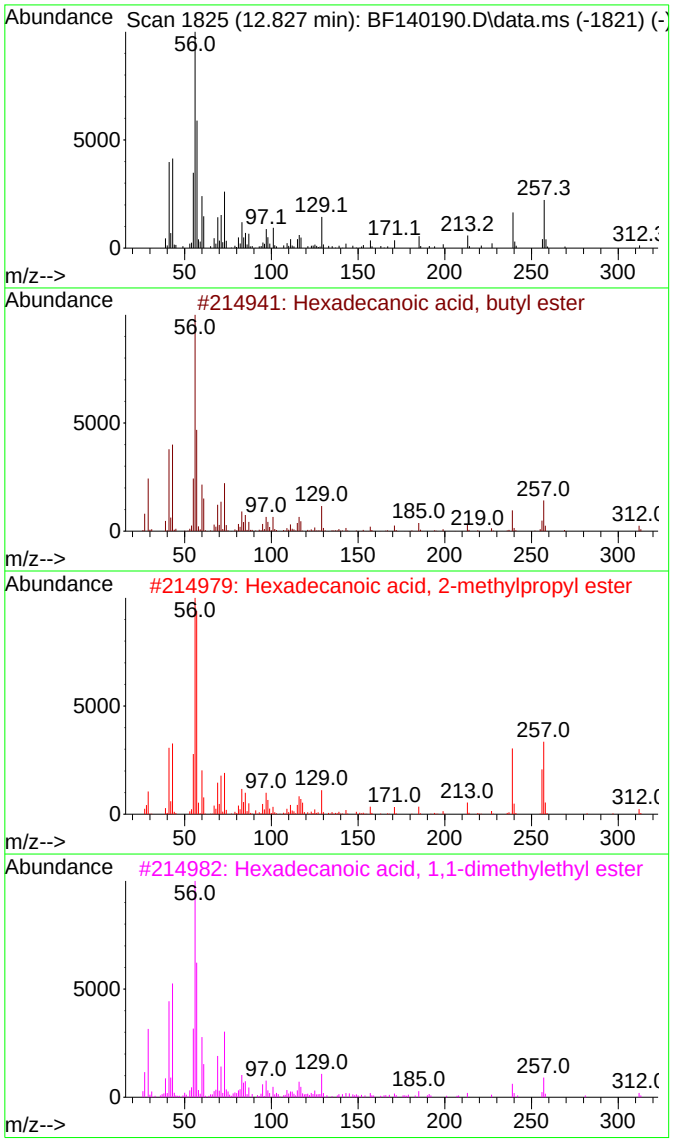
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

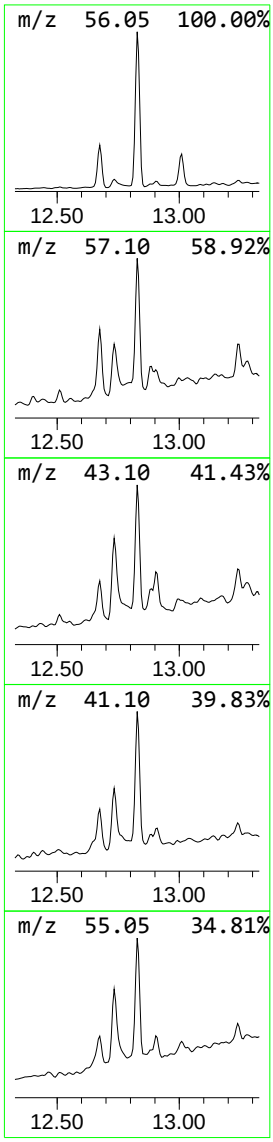
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	4.41 ng	163935	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	89
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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

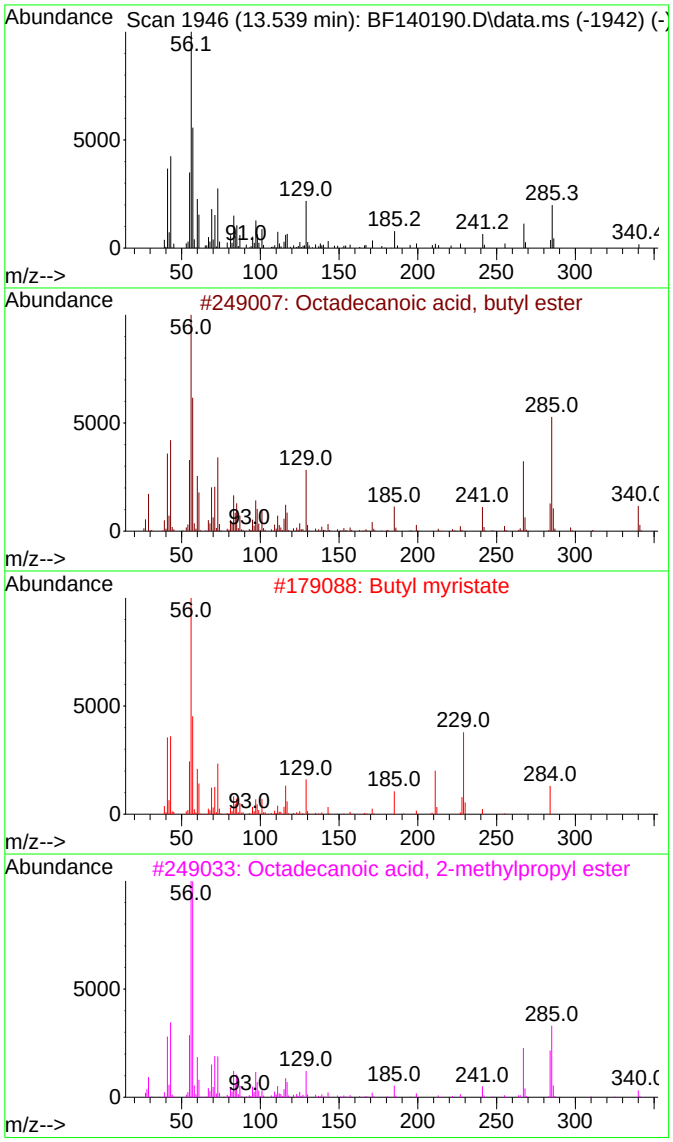
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

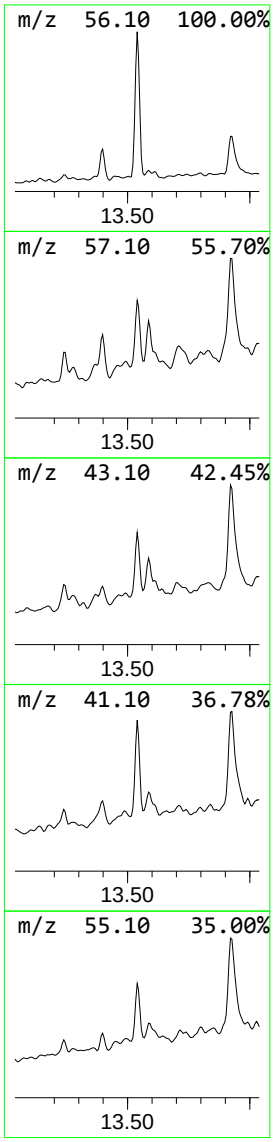
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.539	3.17 ng	117834	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Butyl myristate	284	C18H36O2	000110-36-1	59
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	49
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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

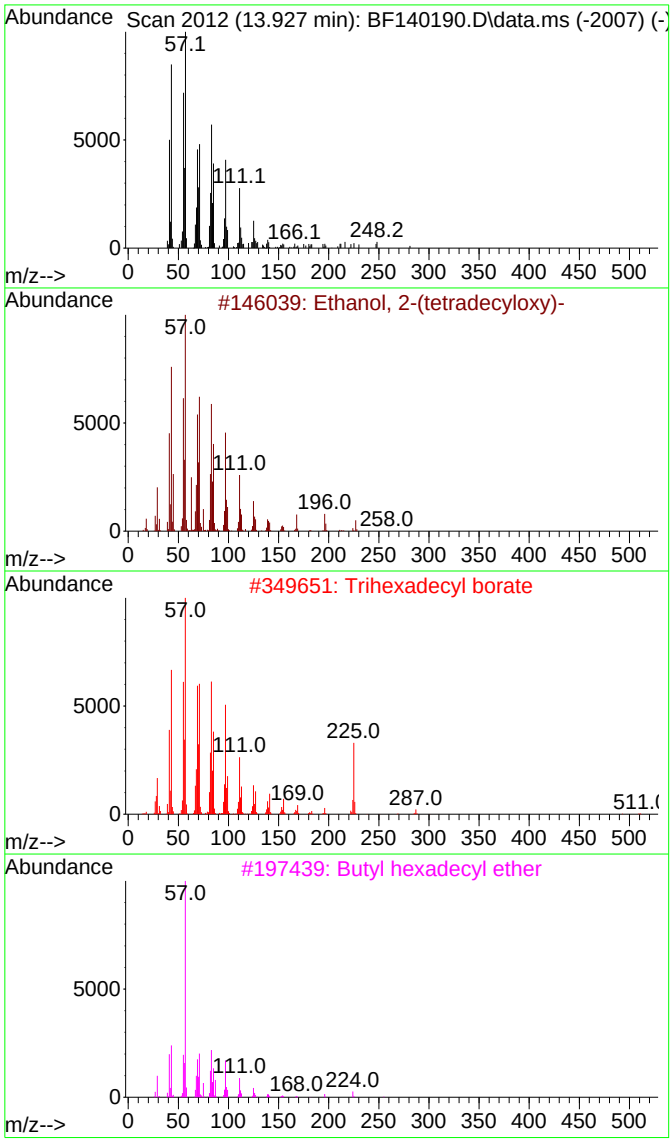
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

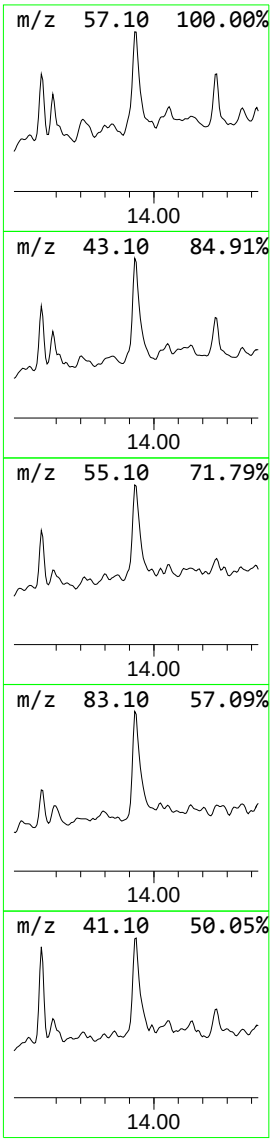
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	4.34 ng	161509	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Trihexadecyl borate	735	C48H99BO3	002665-11-4	91
3	Butyl hexadecyl ether	298	C20H42O	1010406-40-5	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140190.D
Acq On : 31 Oct 2024 15:42
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

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...	2.163	39.3	ng	1503840	1	6.881	765220	20.0
Benzophenone	10.639	3.8	ng	237590	3	9.922	1246330	20.0
n-Hexadecanoic ...	11.945	10.0	ng	596900	4	11.416	1196700	20.0
Pentadecanoic acid	12.733	2.2	ng	129437	4	11.416	1196700	20.0
Hexadecanoic ac...	12.827	4.4	ng	163935	5	14.080	743563	20.0
Octadecanoic ac...	13.539	3.2	ng	117834	5	14.080	743563	20.0
Ethanol, 2-(tet...	13.927	4.3	ng	161509	5	14.080	743563	20.0