LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	15	23	30	rVB	1485576	1872248	42.02%	5.517%
2	5.534	581	586	589	rBV	4347641	4063051	91.20%	11.972%
3	6.533	751	756	759	rBV	3980344	3950403	88.67%	11.640%
4	6.910	817	820	824	rBV	1337404	1195246	26.83%	3.522%
5	7.475	911	916	919	rBV	2896166	2609405	58.57%	7.689%
6	8.092	1018	1021	1035	rBV	139456	279136	6.27%	0.823%
7	8.192	1035	1038	1042	rBV	1722551	1529333	34.33%	4.506%
8	9.269	1216	1221	1224	rBV	5306689	4455256	100.00%	13.128%
9	9.951	1333	1337	1340	rBV	1916220	1730119	38.83%	5.098%
10	10.739	1466	1471	1474	rBV	3003122	2940490	66.00%	8.664%
11	11.433	1586	1589	1593	rBV	1909131	1730778	38.85%	5.100%
12	11.951	1673	1677	1683	rBV	444283	481130	10.80%	1.418%
13	12.739	1807	1811	1819	rBV	151290	176147	3.95%	0.519%
14	13.021	1855	1859	1862	rBV	4768901	4151854	93.19%	12.234%
15	13.945	2012	2016	2019	rBV	123191	151783	3.41%	0.447%
16	14.074	2034	2038	2042	rVB	1374595	1163437	26.11%	3.428%
17	14.833	2164	2167	2175	rBV2	167829	204086	4.58%	0.601%
18	14.927	2180	2183	2188	rVB	68641	75710	1.70%	0.223%
19	15.568	2287	2292	2300	rBV2	896245	1177876	26.44%	3.471%

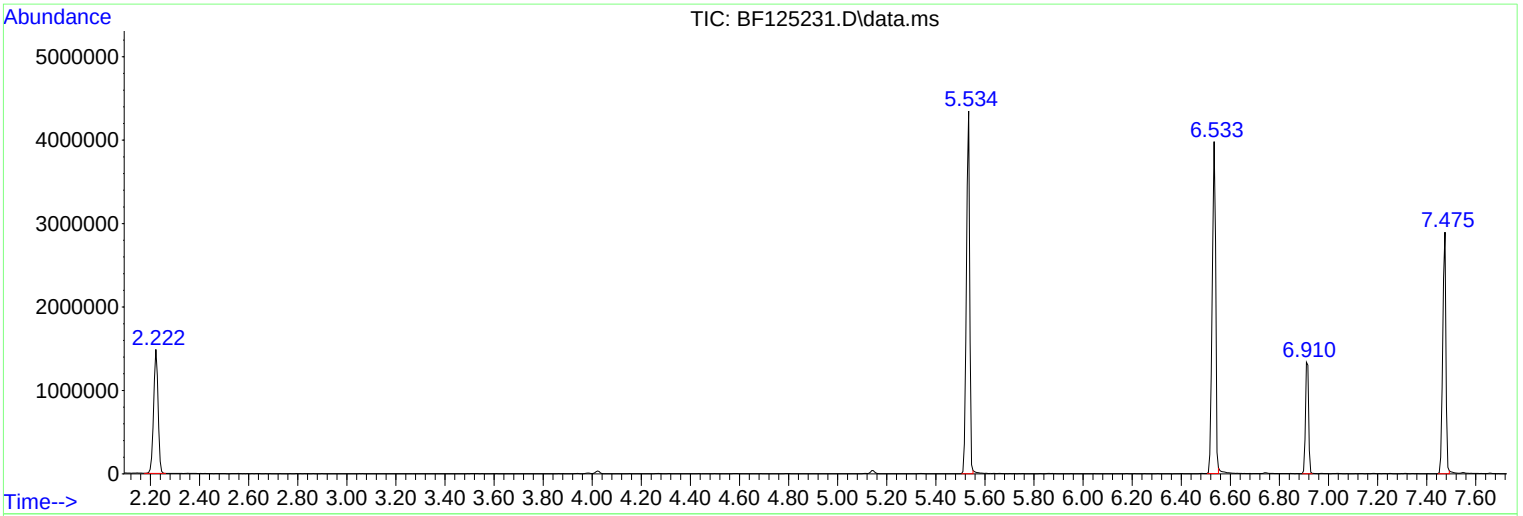
Sum of corrected areas: 33937488

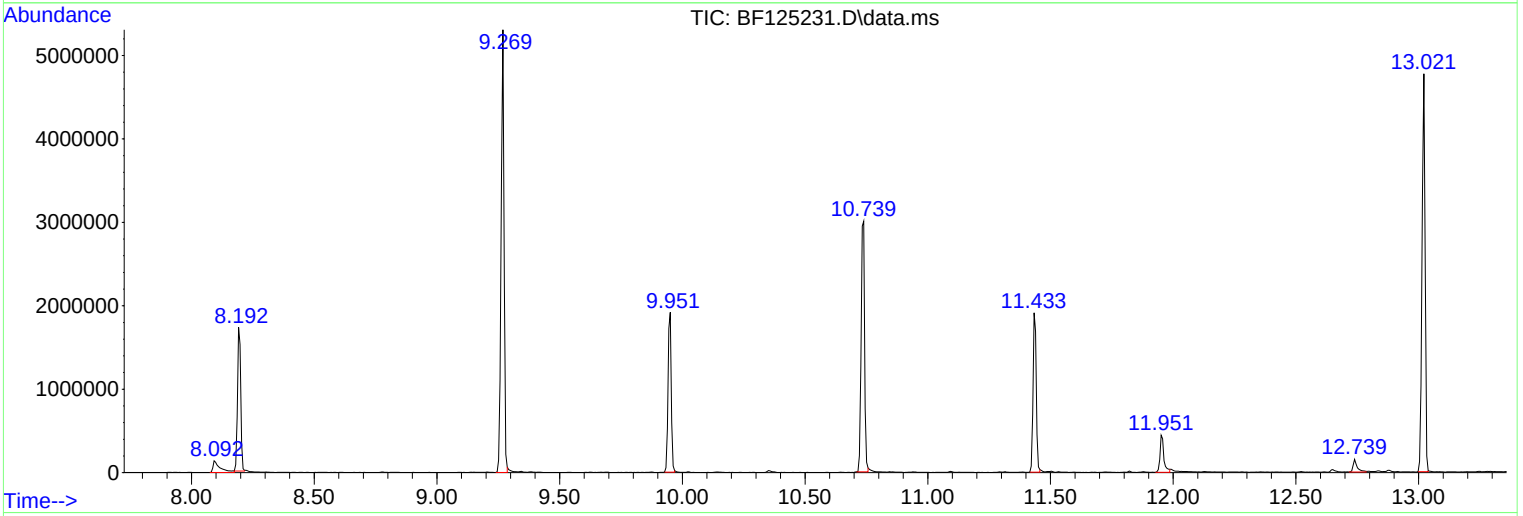
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

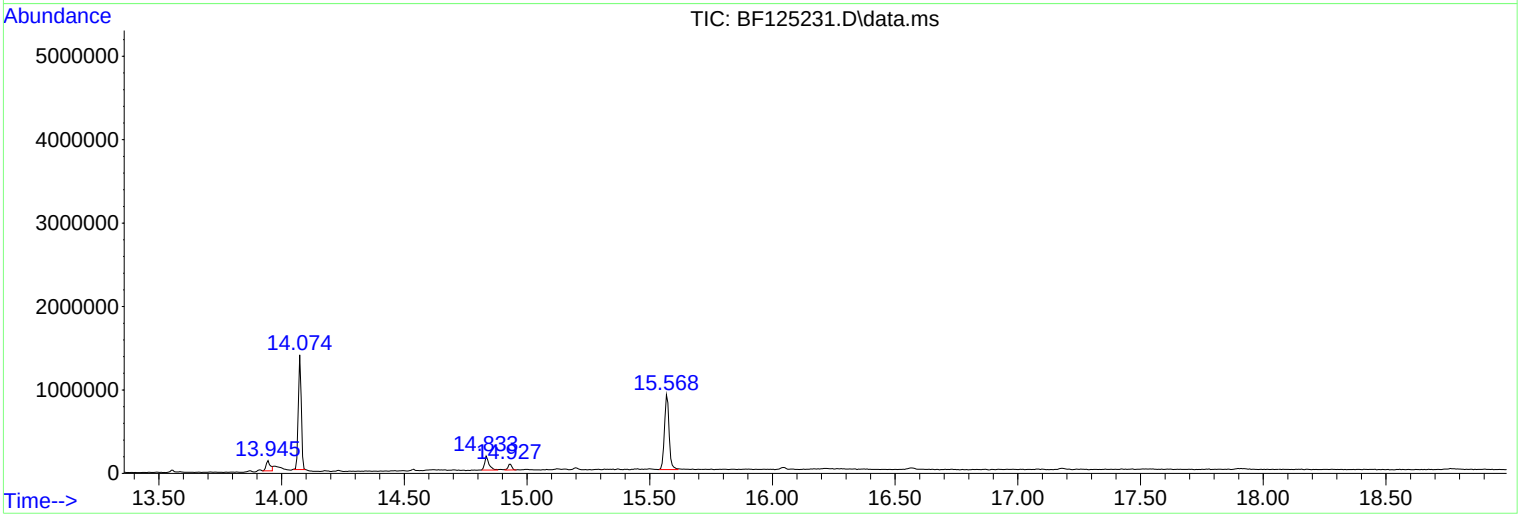
Instrument :
BNA_F
ClientSampleId :
PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

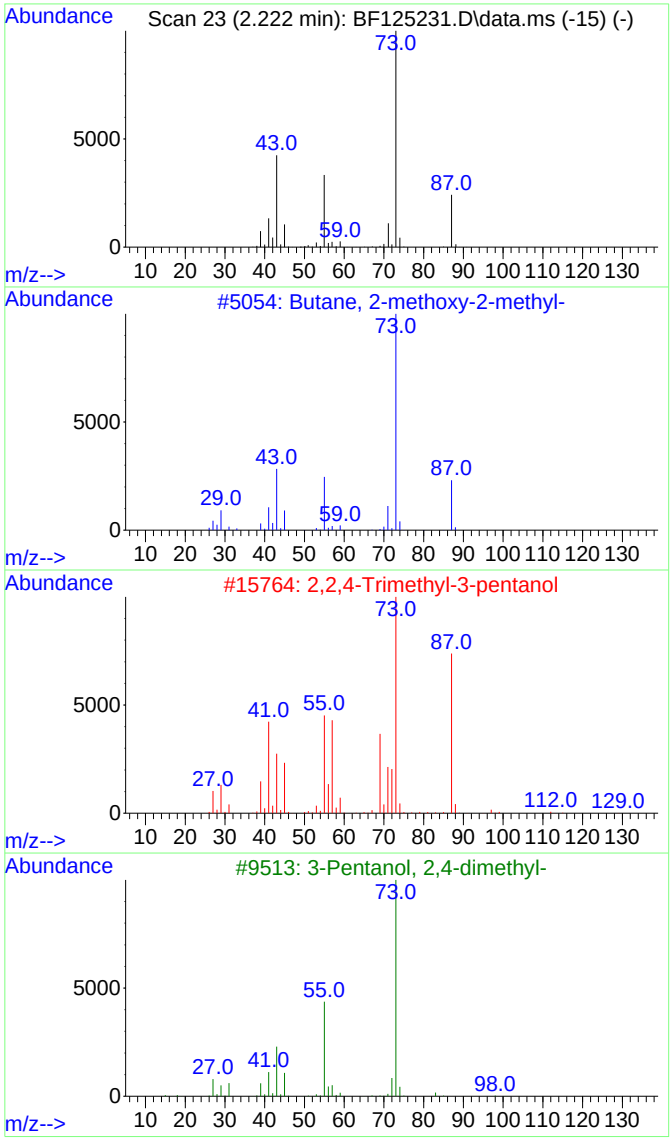
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

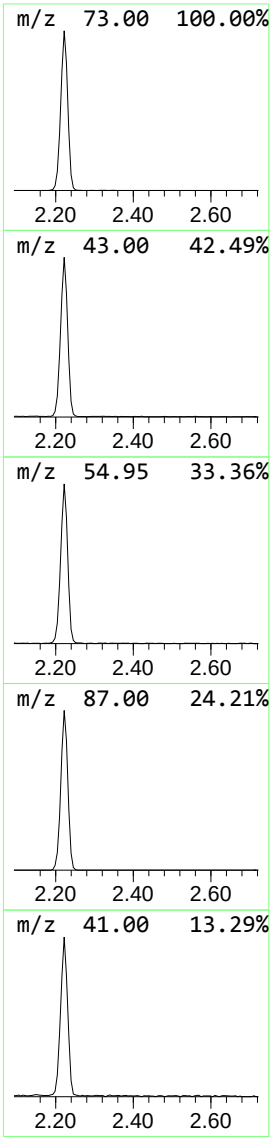
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	31.33 ng	1872250	1,4-Dichlorobenzene-d4	6.916

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

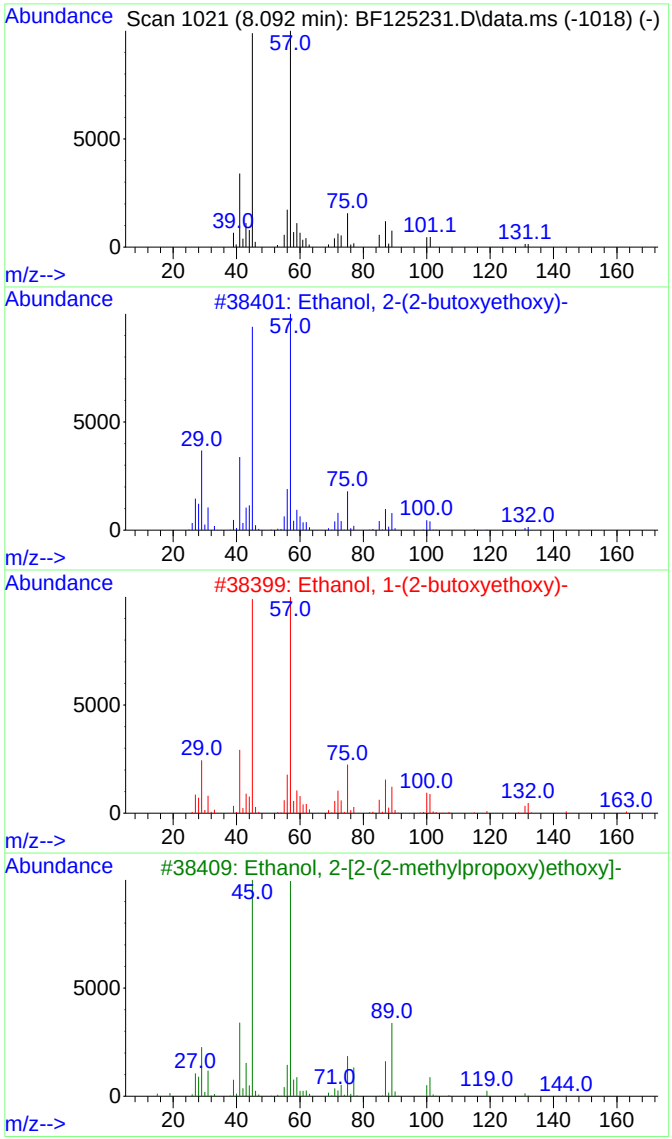
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

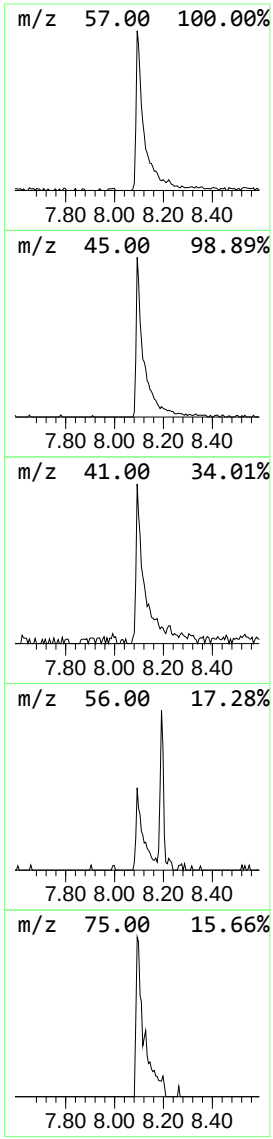
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	3.65 ng	279136	Naphthalene-d8	8.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

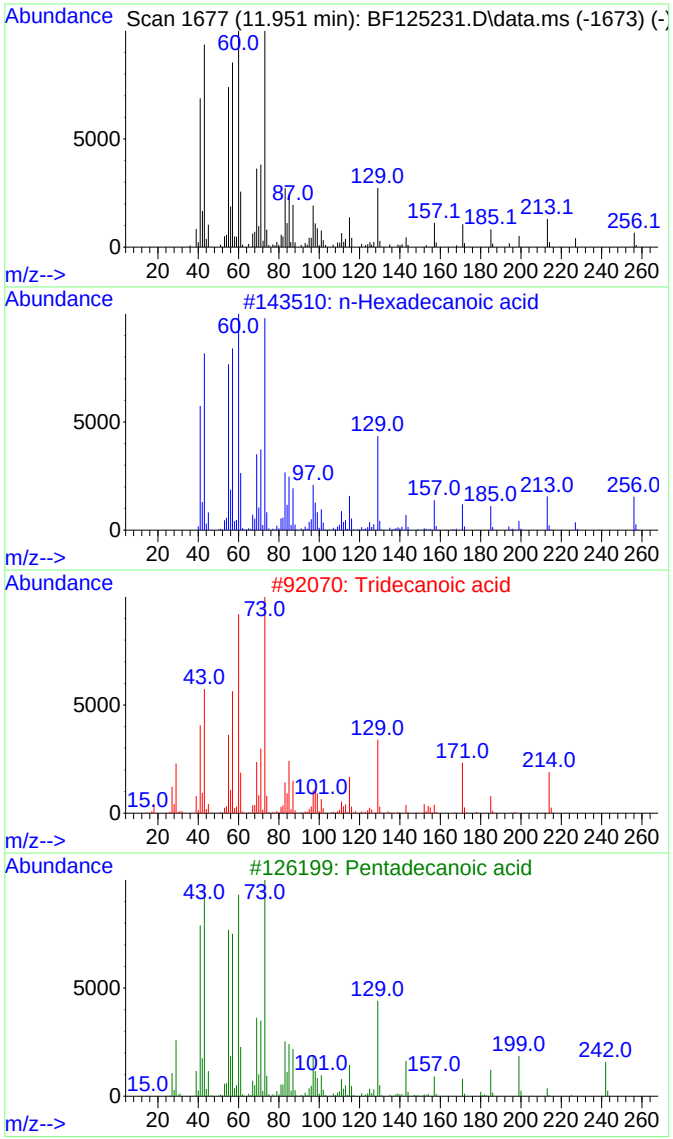
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

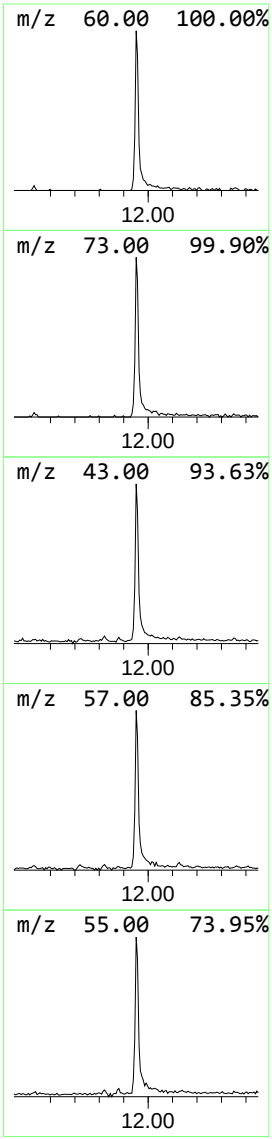
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	5.56 ng	481130	Phenanthrene-d10	11.433

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Nonanoic acid	158	C9H18O2	000112-05-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

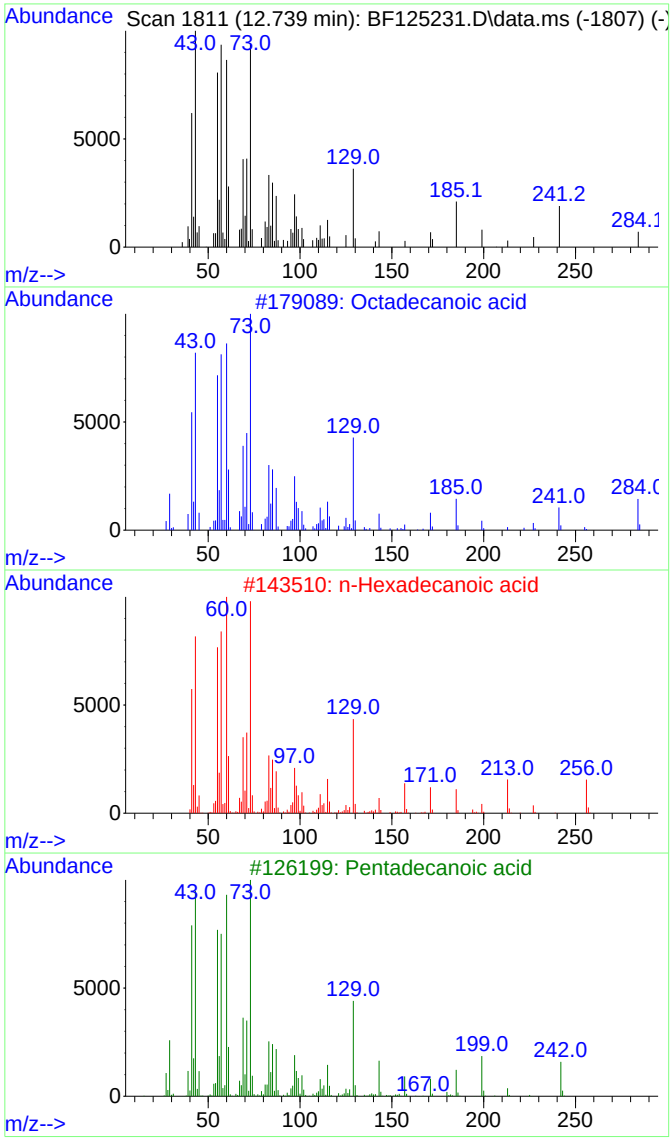
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

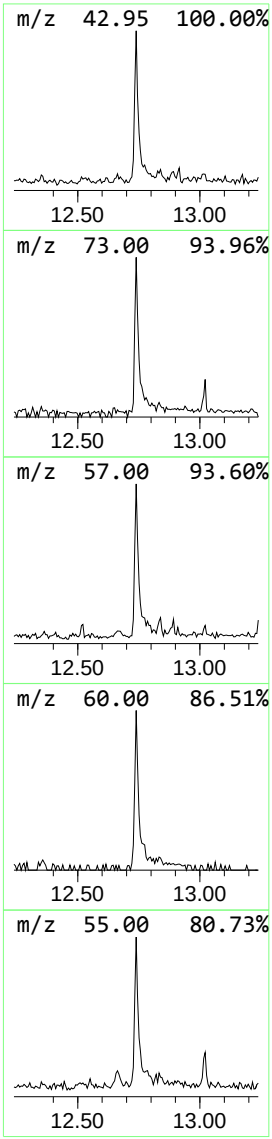
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.04 ng	176147	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

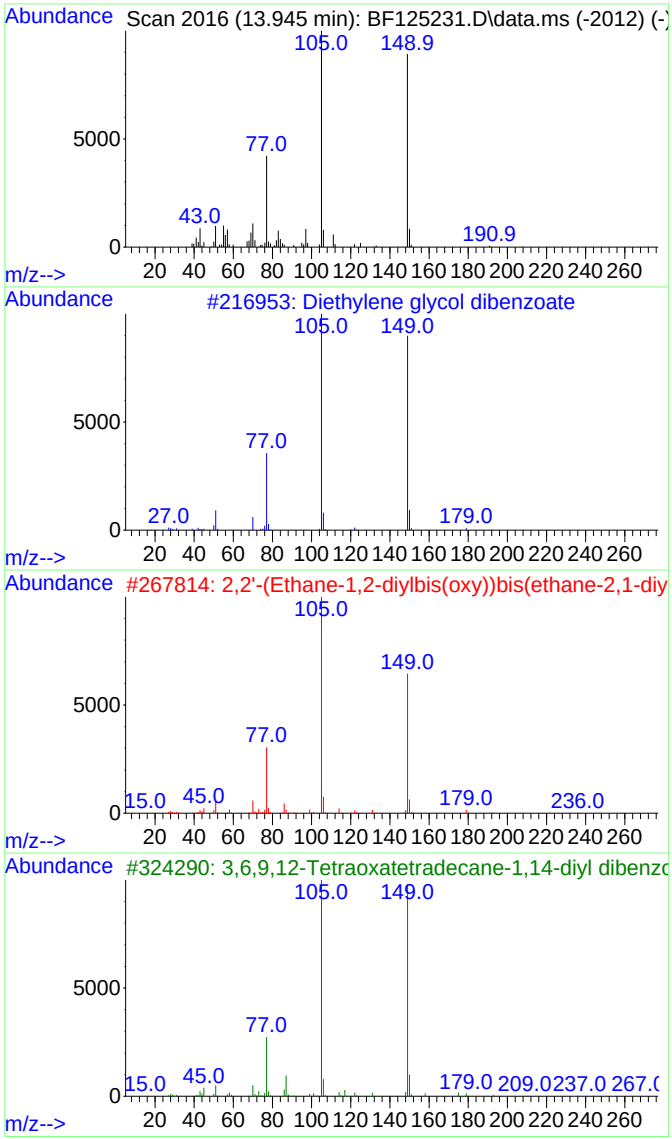
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

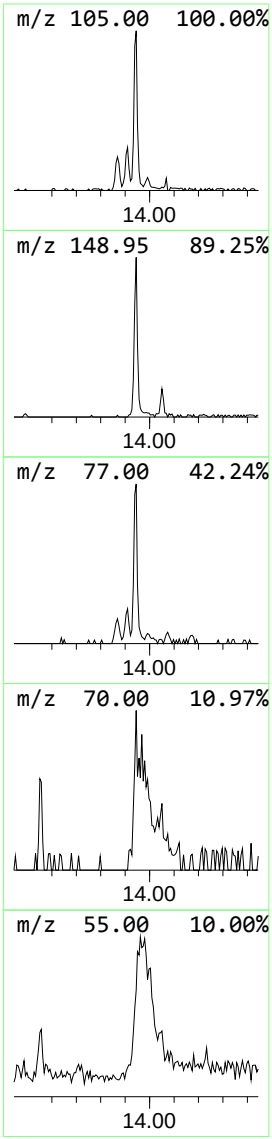
****

Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.61 ng	151783	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	78
3	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
4	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	59
5	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

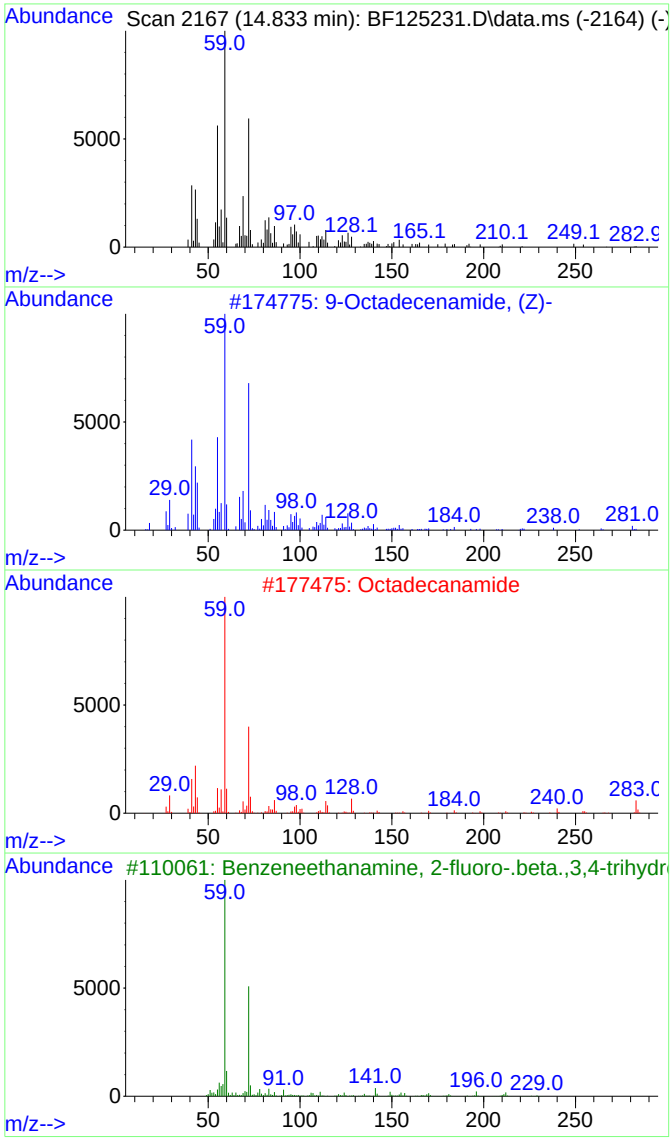
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

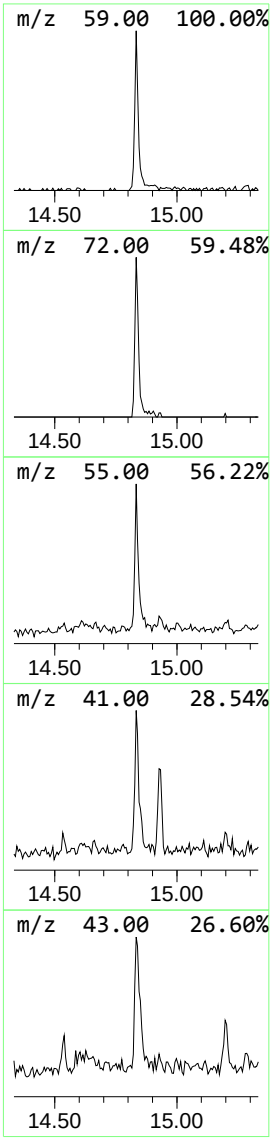
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	3.47 ng	204086	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Octadecanamide	283	C18H37NO	000124-26-5	72
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
4	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	43
5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125231.D
Acq On : 26 Aug 2021 18:26
Operator : JU/CG
Sample : M3547-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PE-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.222	31.3	ng	1872250	1	6.916	1195250	20.0
Ethanol, 2-(2-b...	8.092	3.6	ng	279136	2	8.192	1529330	20.0
n-Hexadecanoic ...	11.951	5.6	ng	481130	4	11.433	1730780	20.0
Octadecanoic acid	12.739	2.0	ng	176147	4	11.433	1730780	20.0
Diethylene glyc...	13.945	2.6	ng	151783	5	14.074	1163440	20.0
9-Octadecenamid...	14.833	3.5	ng	204086	6	15.568	1177880	20.0