LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TPR-10-COMP

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: BF125316.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	25	rVB	1017431	1314847	29.02%	4.179%
2	5.528	580	585	589	rBV	3980911	4093329	90.33%	13.010%
3	6.540	752	757	760	rBV	3974203	4085656	90.16%	12.986%
4	6.910	816	820	823	rBV	1212572	1071550	23.65%	3.406%
5	7.475	911	916	919	rBV	2671911	2677724	59.09%	8.511%
6	8.092	1017	1021	1032	rBV	250507	448273	9.89%	1.425%
7	8.192	1034	1038	1041	rBV	1755800	1412425	31.17%	4.489%
8	9.269	1217	1221	1224	rBV	5430424	4531560	100.00%	14.403%
9	9.375	1236	1239	1249	rVB	119025	137744	3.04%	0.438%
10	9.951	1333	1337	1340	rBV	1686920	1549016	34.18%	4.923%
11	10.739	1467	1471	1474	rBV	2839282	2421110	53.43%	7.695%
12	11.439	1586	1590	1593	rBV	1496374	1314846	29.02%	4.179%
13	11.822	1652	1655	1657	rBV	74452	59311	1.31%	0.189%
14	11.951	1674	1677	1686	rBV3	151435	186187	4.11%	0.592%
15	12.527	1770	1775	1778	rBV2	202853	200720	4.43%	0.638%
16	12.616	1787	1790	1794	rVB2	70056	76679	1.69%	0.244%
17	12.739	1808	1811	1815	rBV4	50227	81007	1.79%	0.257%
18	13.021	1855	1859	1863	rBV	3843382	3596616	79.37%	11.432%
19	13.204	1888	1890	1894	rBV4	52371	53413	1.18%	0.170%
20	14.080	2035	2039	2042	rBV	1136917	1033611	22.81%	3.285%
21	15.586	2291	2295	2305	rVB	559082	771303	17.02%	2.452%
22	16.310	2415	2418	2424	rVB2	237478	345095	7.62%	1.097%

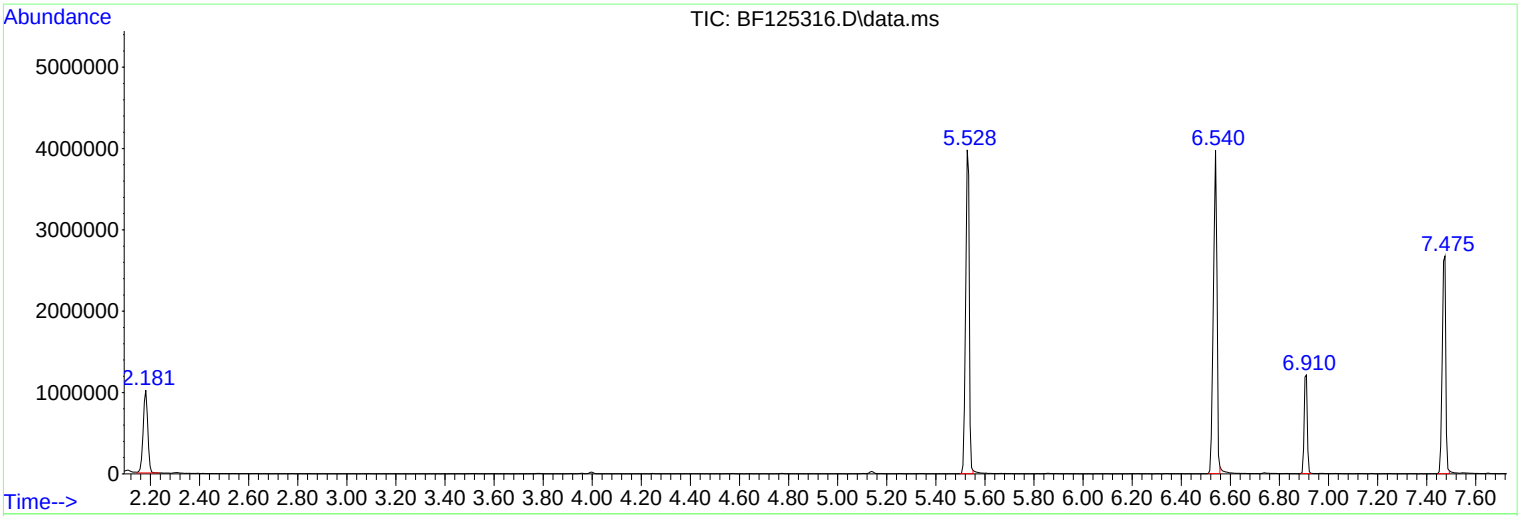
Sum of corrected areas: 31462022

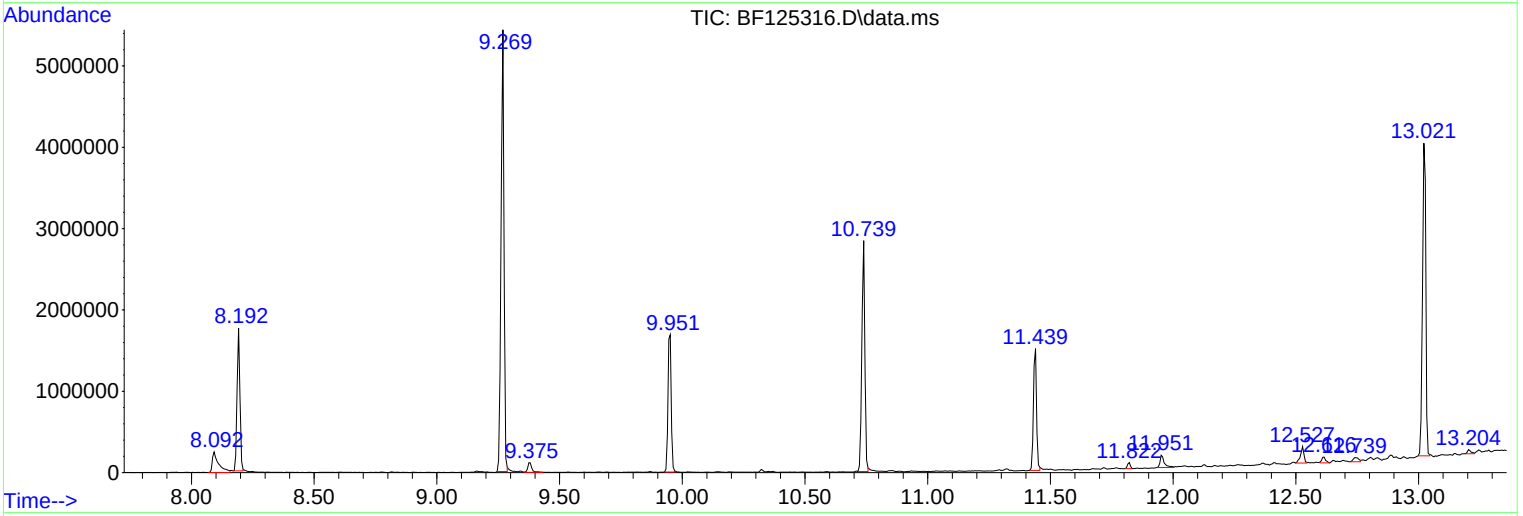
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

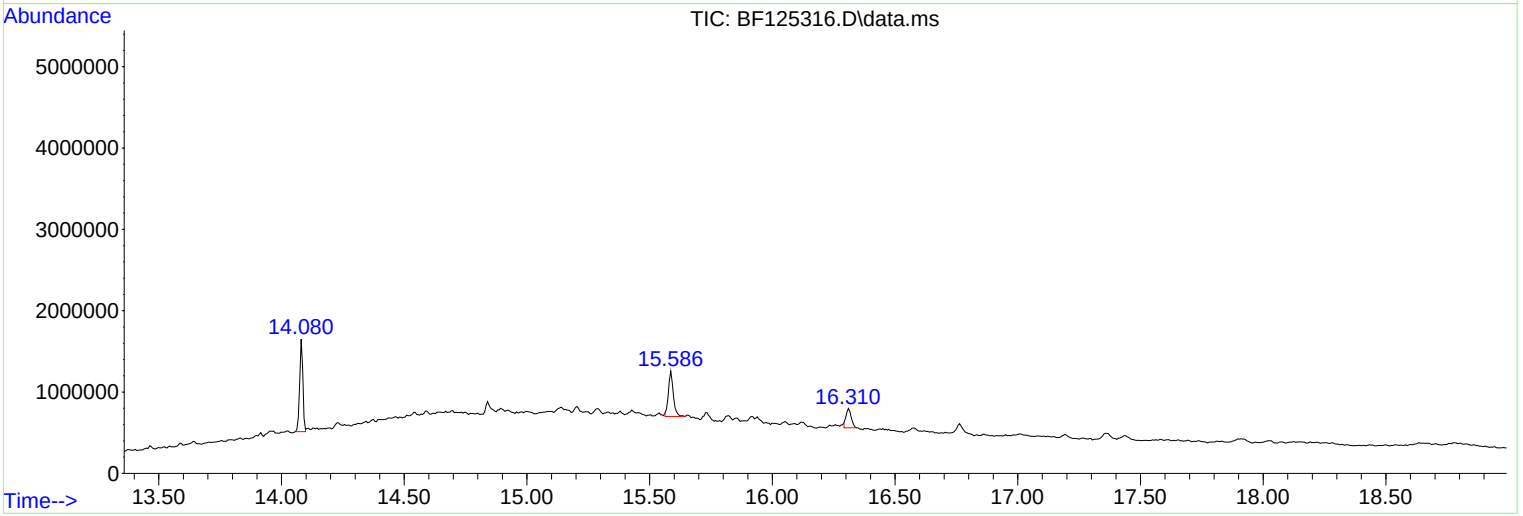
Instrument :
BNA_F
ClientSampleId :
TPR-10-COMP

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\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TPR-10-COMP

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

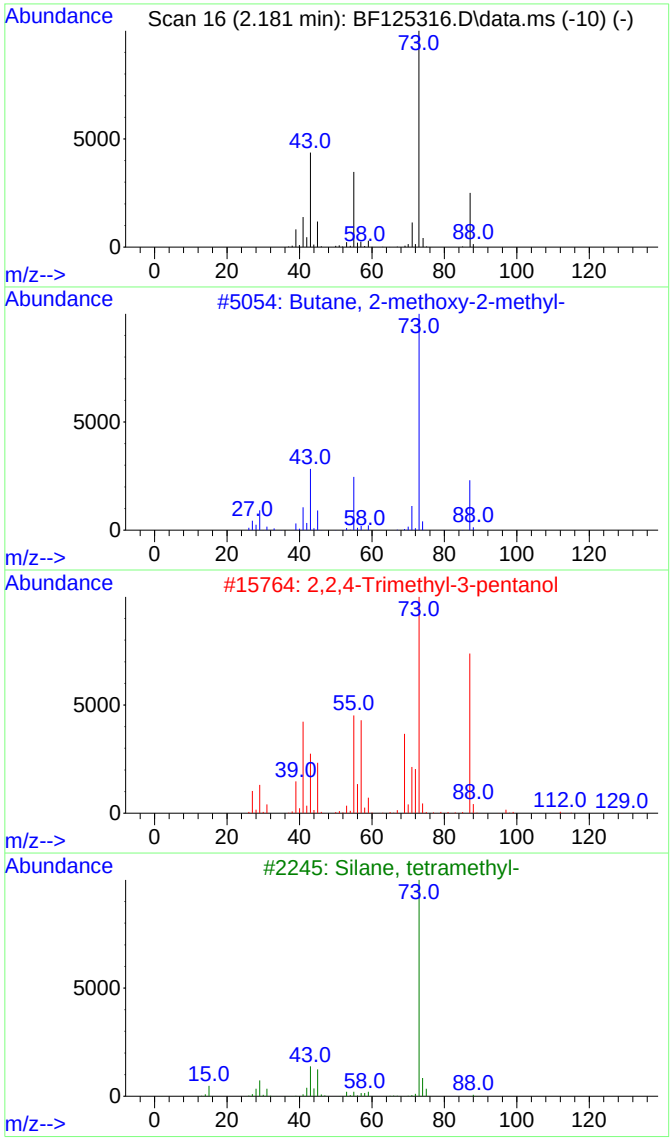
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

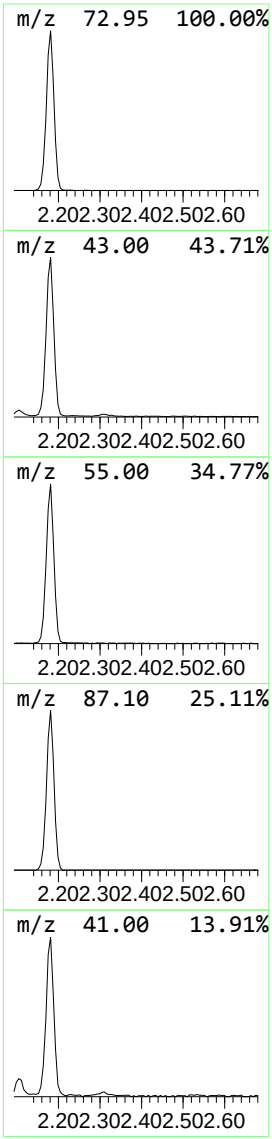
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	24.54 ng	1314850	1,4-Dichlorobenzene-d4	6.910

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TPR-10-COMP

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

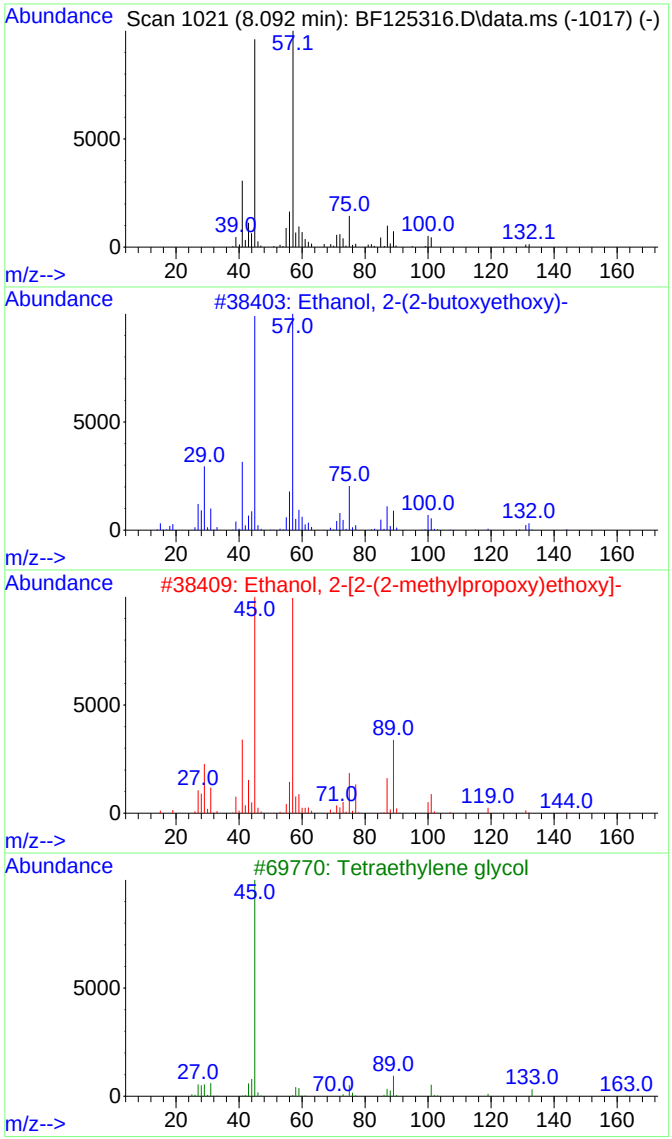
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

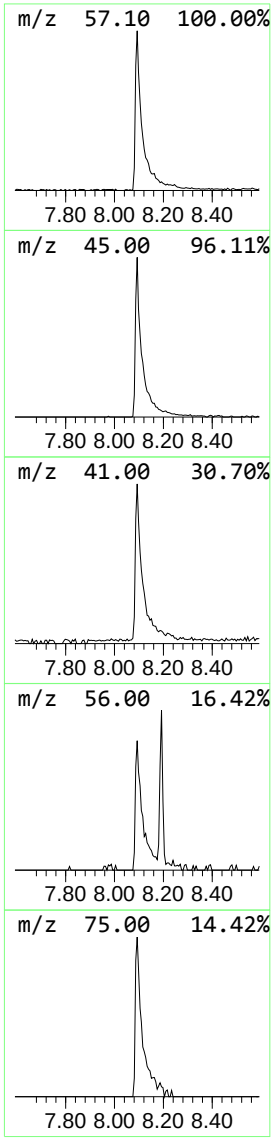
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	6.35 ng	448273	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, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
5	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TPR-10-COMP

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

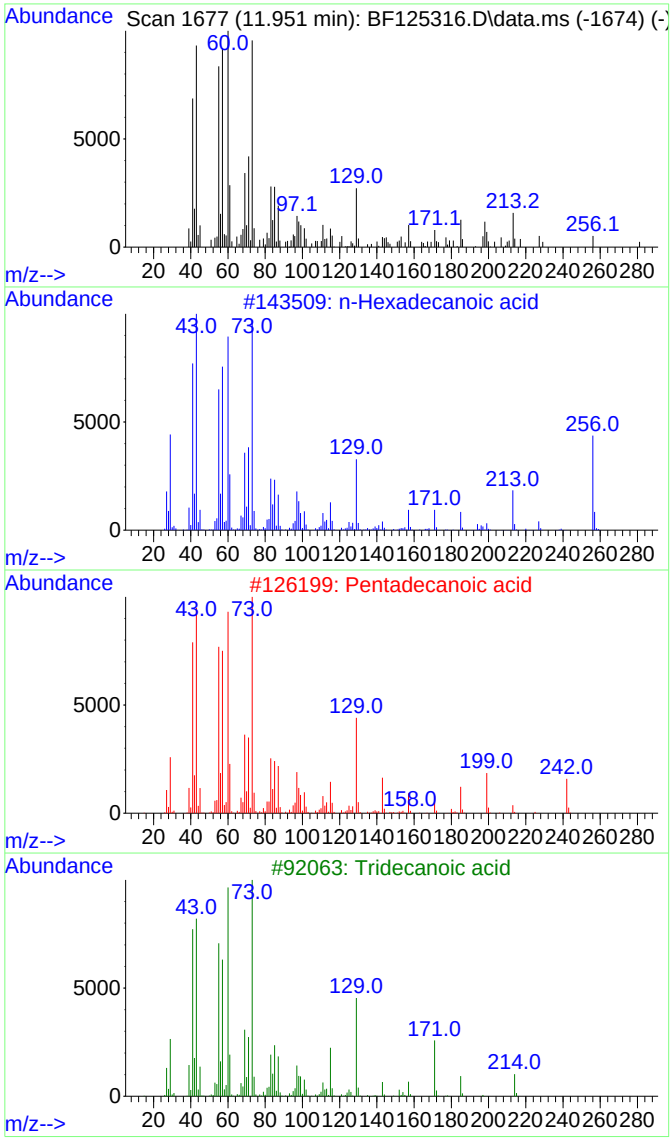
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

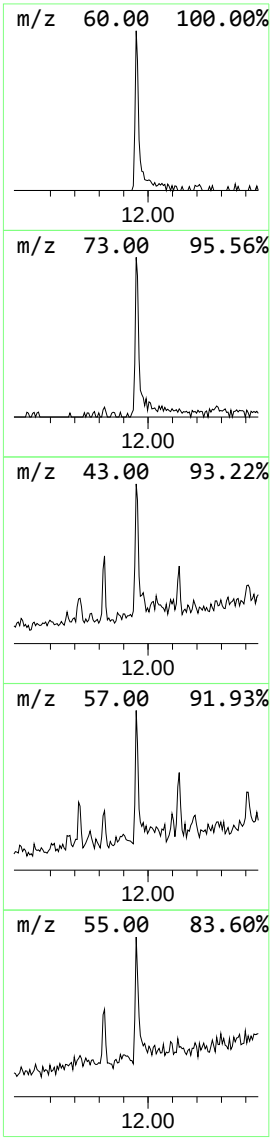
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.83 ng	186187	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TPR-10-COMP

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

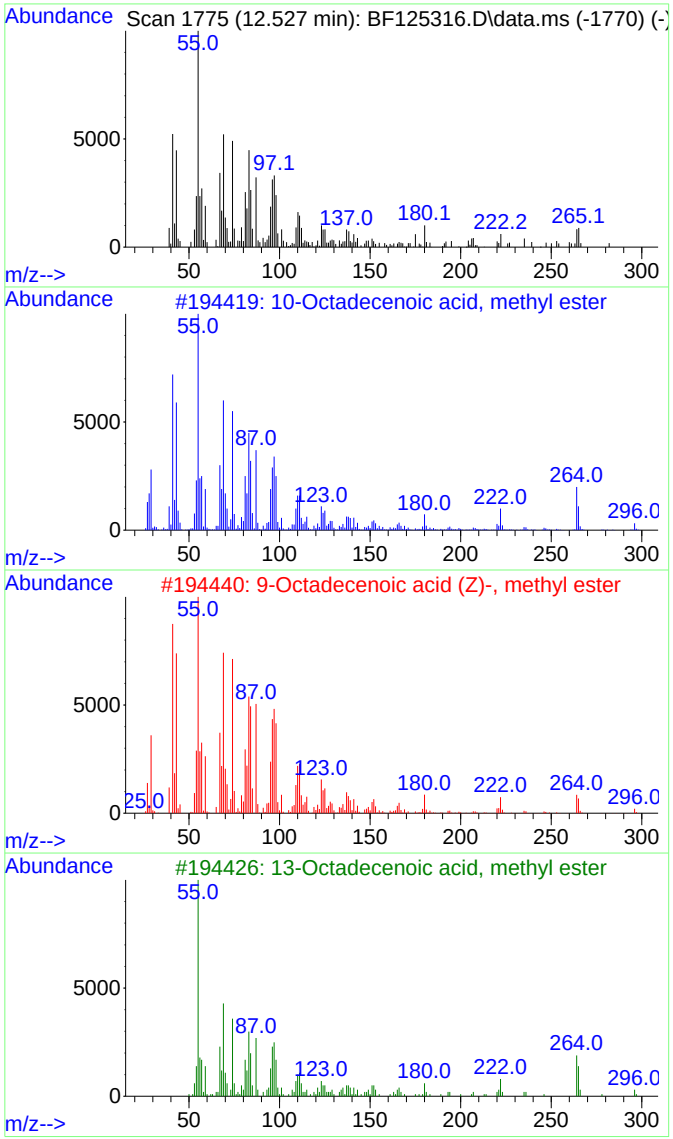
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

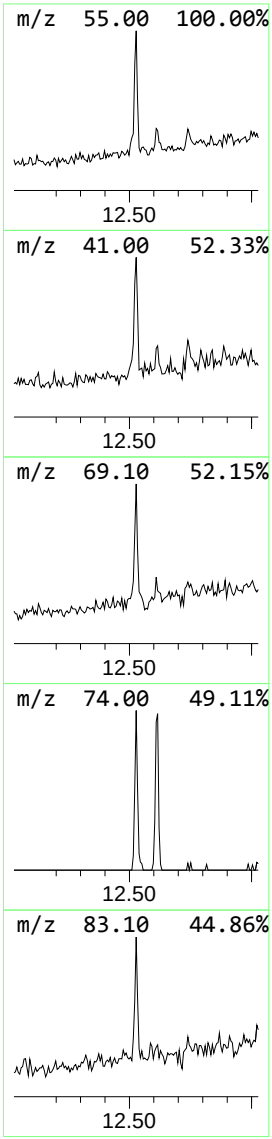
****

Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	3.05 ng	200720	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	91
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TPR-10-COMP

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

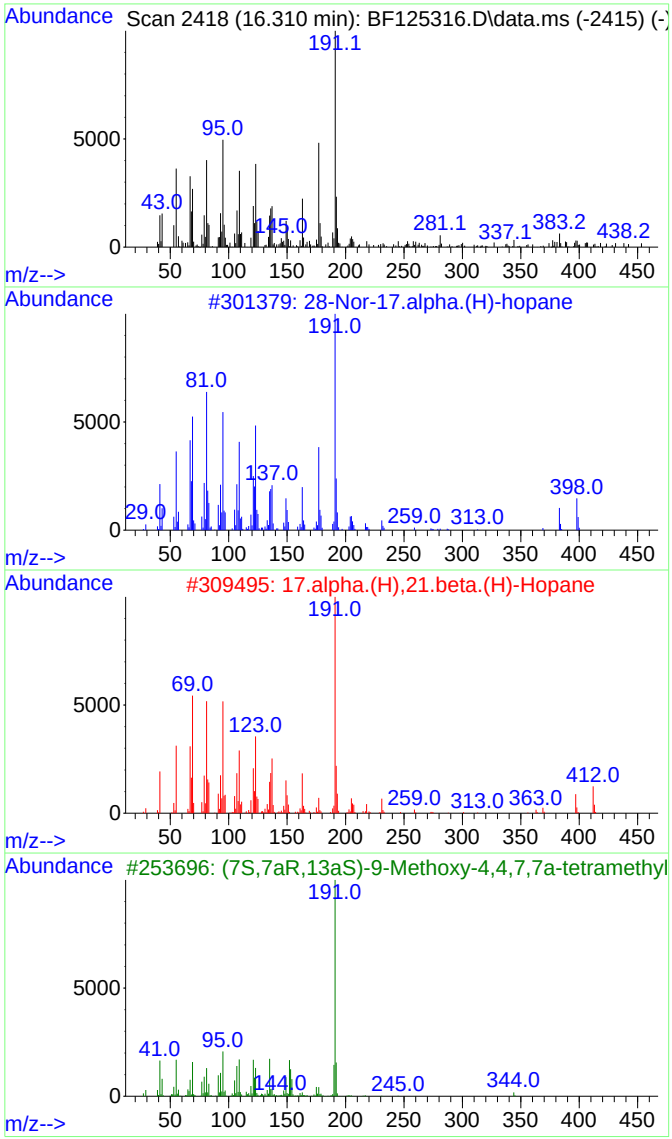
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

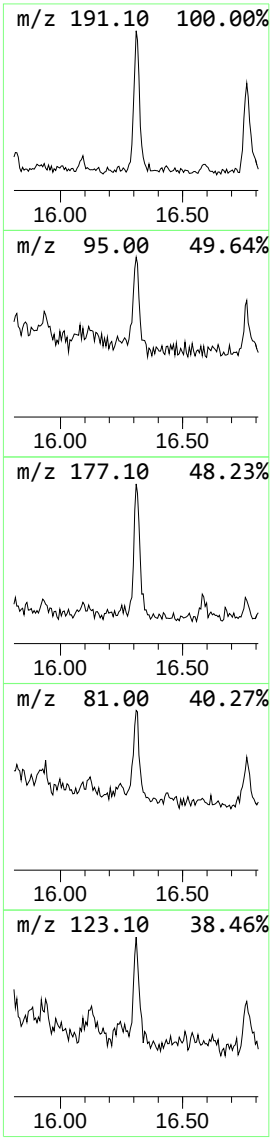
****

Peak Number 5 28-Nor-17.alpha.(H)-hopane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	8.95 ng	345095	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	90
2	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	64
3	(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	46
4	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
5	Benzamide, 3-trifluoromethyl-2-f...	453	C20H15F8NO2	1000407-71-9	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125316.D
Acq On : 1 Sep 2021 20:17
Operator : JU/CG
Sample : M3615-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TPR-10-COMP

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...	2.181	24.5	ng	1314850	1	6.910	1071550	20.0
Ethanol, 2-(2-b...	8.092	6.3	ng	448273	2	8.192	1412430	20.0
n-Hexadecanoic ...	11.951	2.8	ng	186187	4	11.439	1314850	20.0
10-Octadecenoic...	12.527	3.0	ng	200720	4	11.439	1314850	20.0
28-Nor-17.alpha...	16.310	8.9	ng	345095	6	15.586	771303	20.0