LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PS-FRAC

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_P\METHODS\8270-BP101920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	55	62	73	rBV	176134	410465	2.97%	0.741%
2	3.346	73	78	84	rBV	768282	1134755	8.21%	2.047%
3	6.010	520	531	542	rBV	1376774	2089728	15.12%	3.770%
4	7.657	804	811	824	rBV	801739	1363613	9.87%	2.460%
5	8.510	942	956	962	rBV	651421	1040147	7.53%	1.876%
6	9.681	1146	1155	1164	rVB	2245553	3799705	27.49%	6.855%
7	11.351	1430	1439	1454	rBV	826303	1418828	10.27%	2.560%
8	13.739	1838	1845	1854	rBV	6281268	9100810	65.85%	16.418%
9	14.528	1972	1979	1985	rBV	440609	592318	4.29%	1.069%
10	15.110	2071	2078	2085	rVB	1345033	1973044	14.28%	3.559%
11	16.586	2322	2329	2343	rBV	5090816	7307682	52.88%	13.184%
12	17.833	2534	2541	2546	rBV	1660958	2360279	17.08%	4.258%
13	18.645	2674	2679	2687	rBV	773262	1083028	7.84%	1.954%
14	19.839	2878	2882	2892	rBV	209719	328773	2.38%	0.593%
15	20.304	2955	2961	2966	rBV	11343209	13820061	100.00%	24.932%
16	21.474	3156	3160	3171	rBV	1370508	1644119	11.90%	2.966%
17	21.845	3218	3223	3231	rVB	1912427	2642653	19.12%	4.768%
18	24.421	3654	3661	3670	rVB	1142612	2378963	17.21%	4.292%
19	25.033	3760	3765	3779	rVB3	129784	314291	2.27%	0.567%
20	25.592	3853	3860	3873	rBV2	261399	627126	4.54%	1.131%

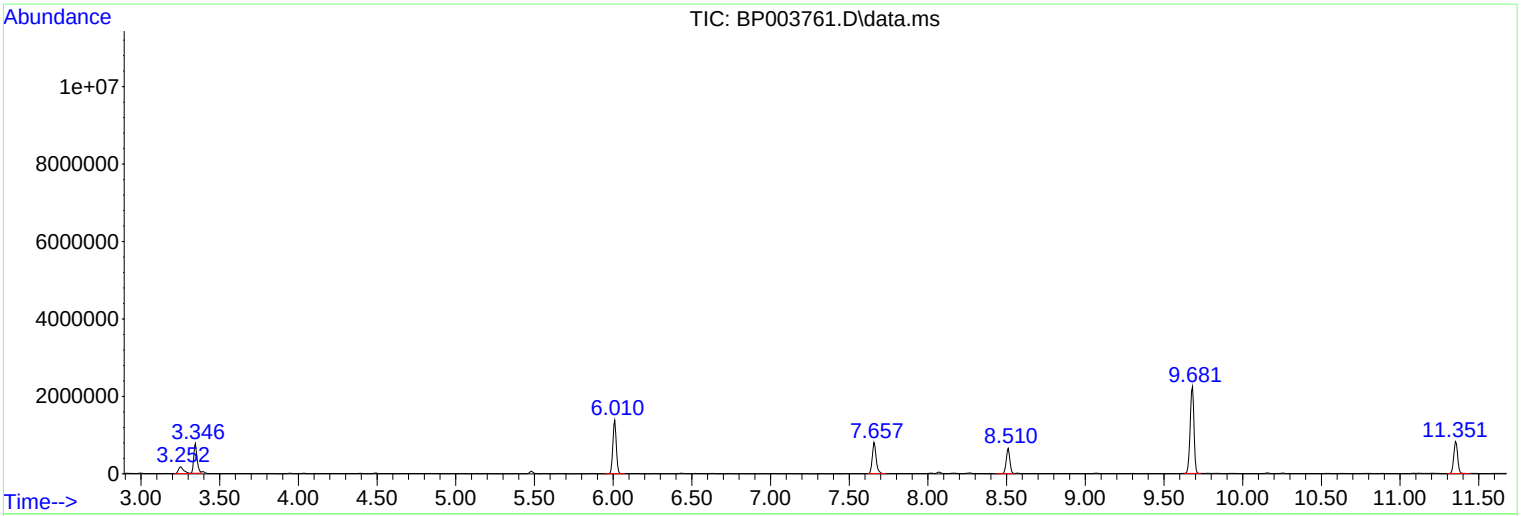
Sum of corrected areas: 55430388

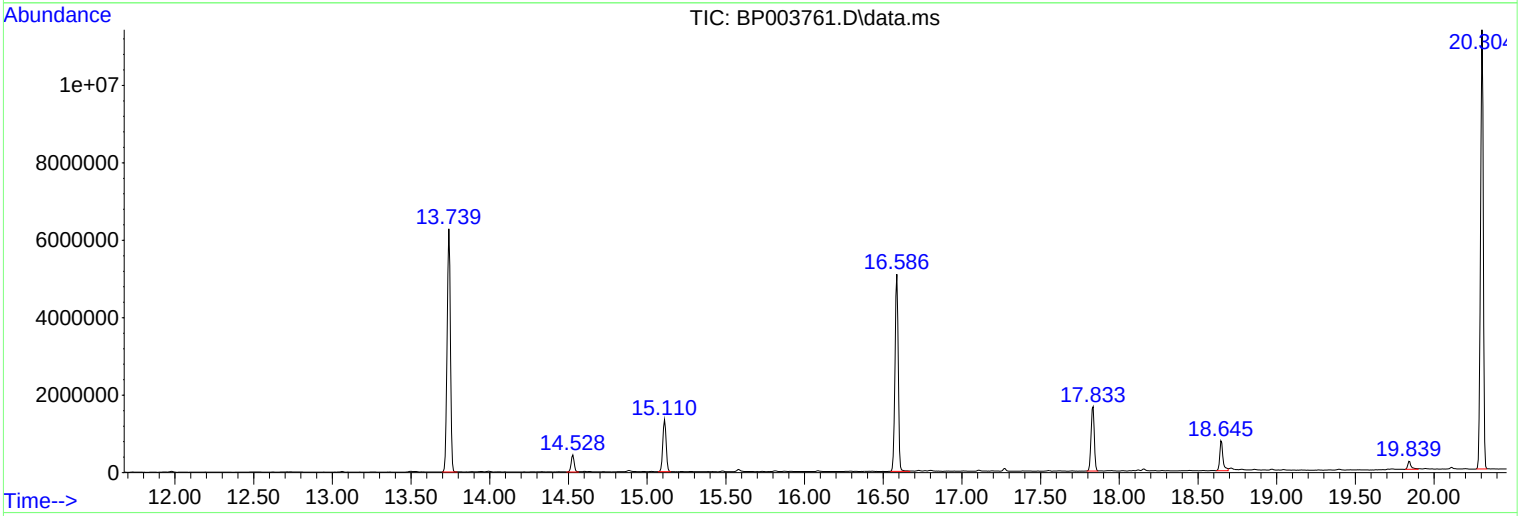
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

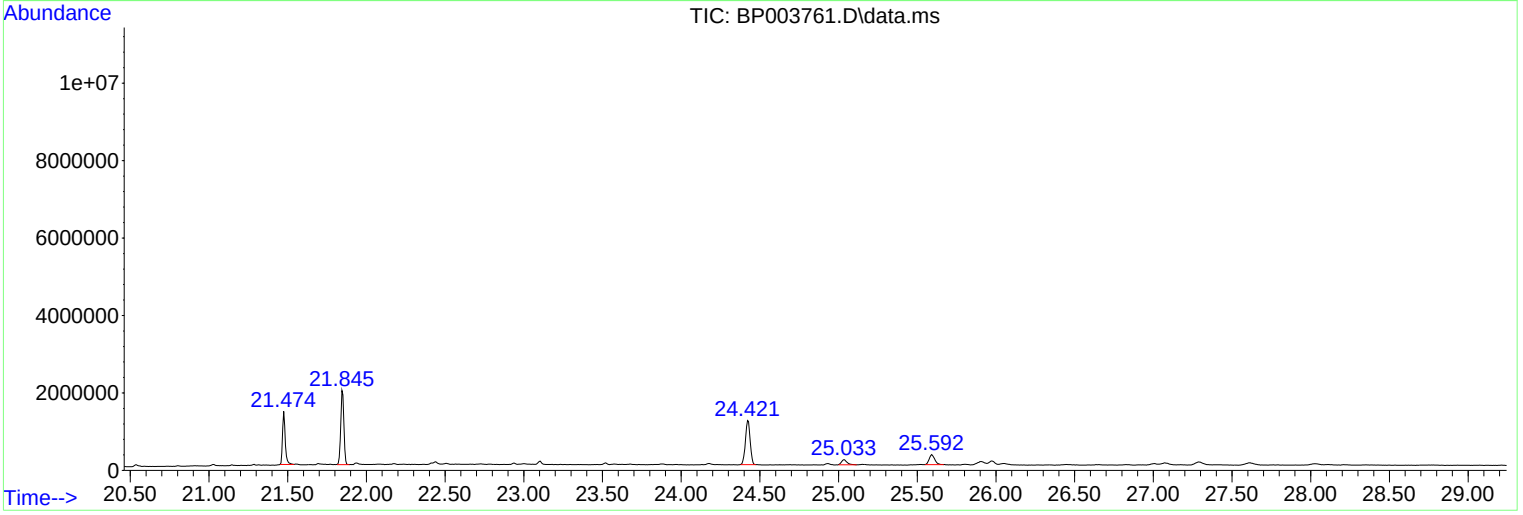
Instrument :
BNA_P
ClientSampleId :
PS-FRAC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PS-FRAC

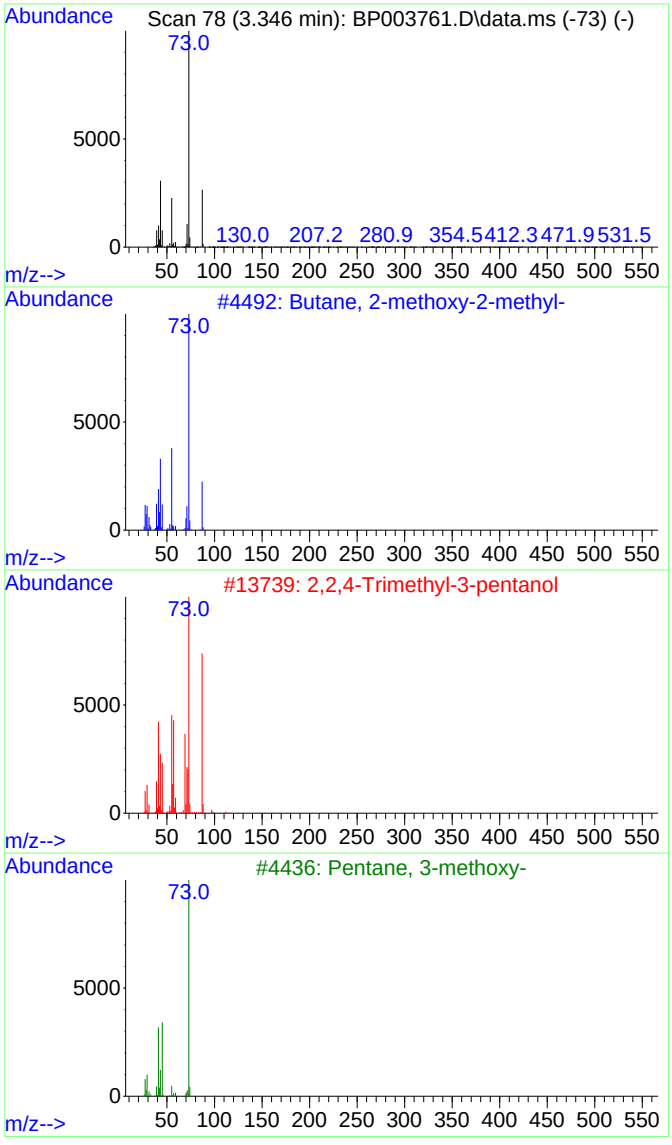
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

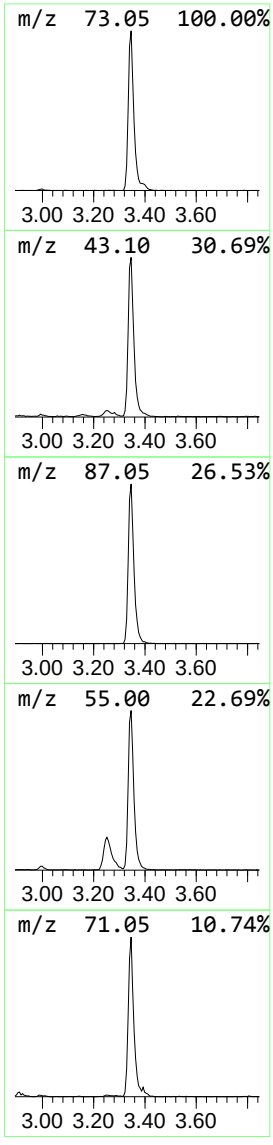
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	21.82 ng	1134760	1,4-Dichlorobenzene-d4	8.510

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PS-FRAC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

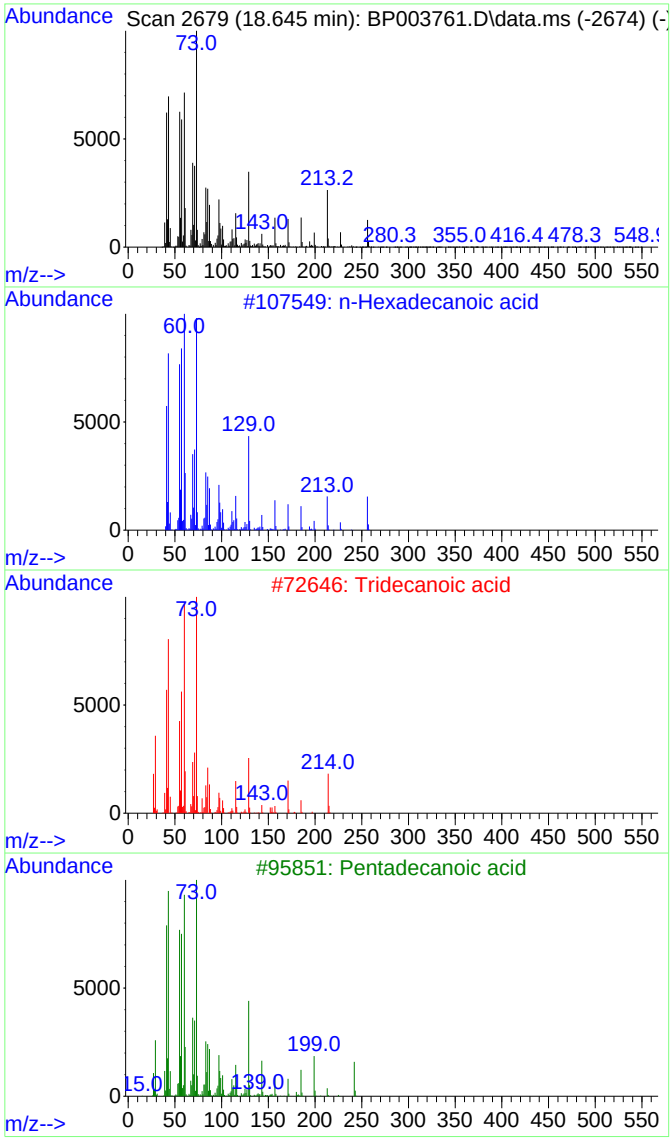
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

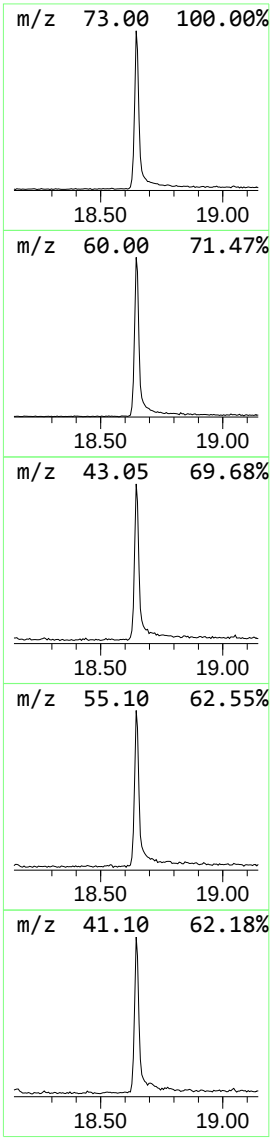
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.645	9.18 ng	1083030	Phenanthrene-d10	17.833

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PS-FRAC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

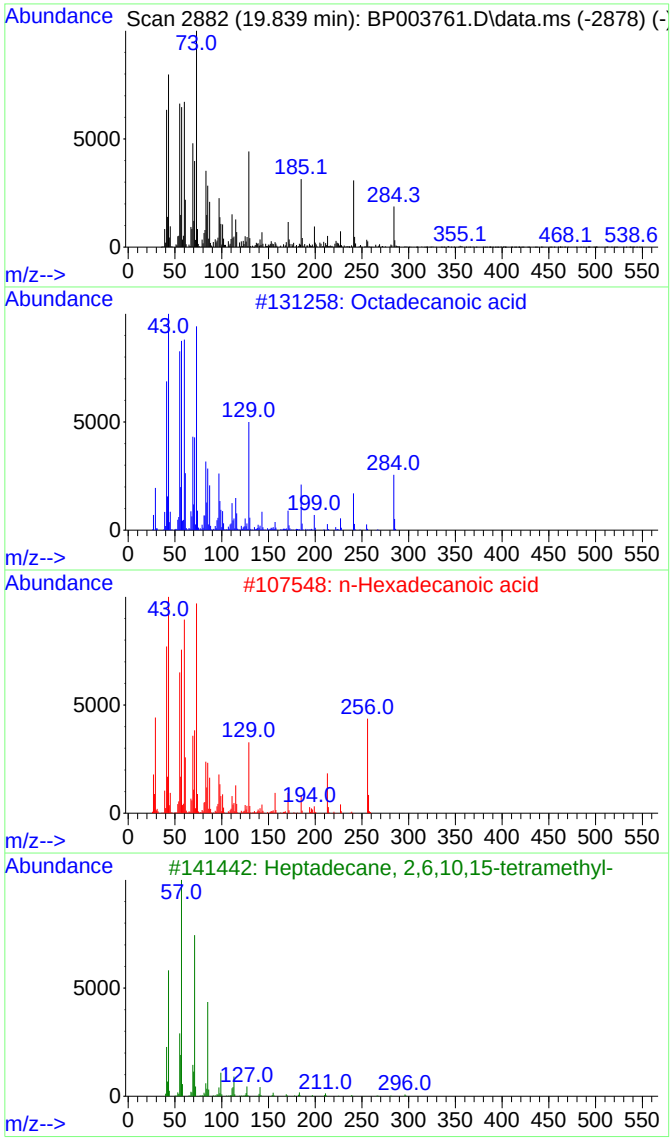
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

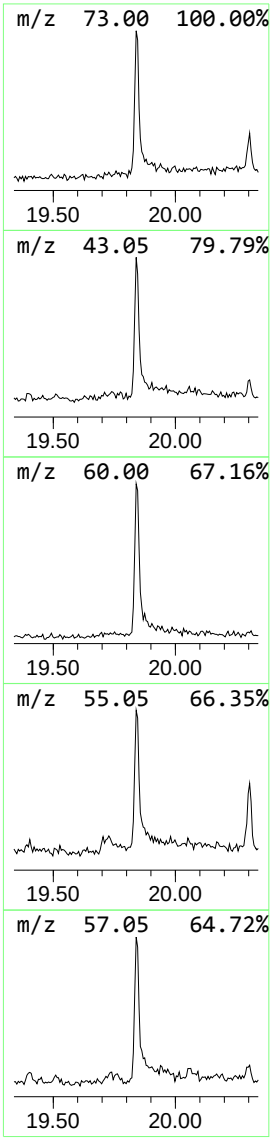
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.839	2.49 ng	328773	Chrysene-d12	21.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PS-FRAC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

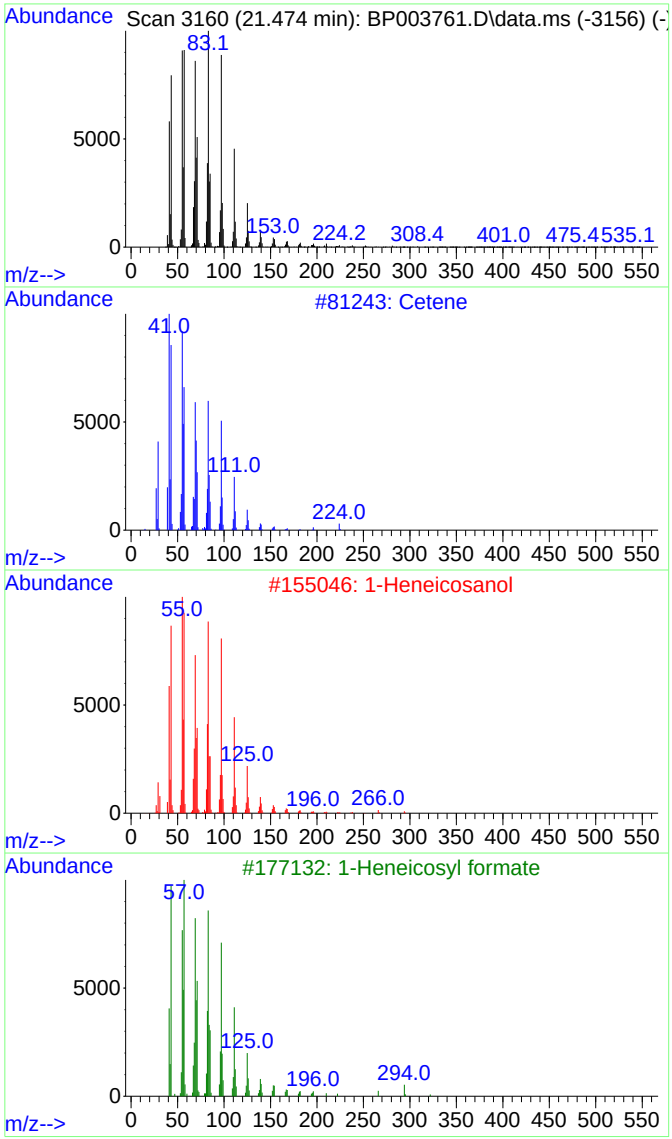
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

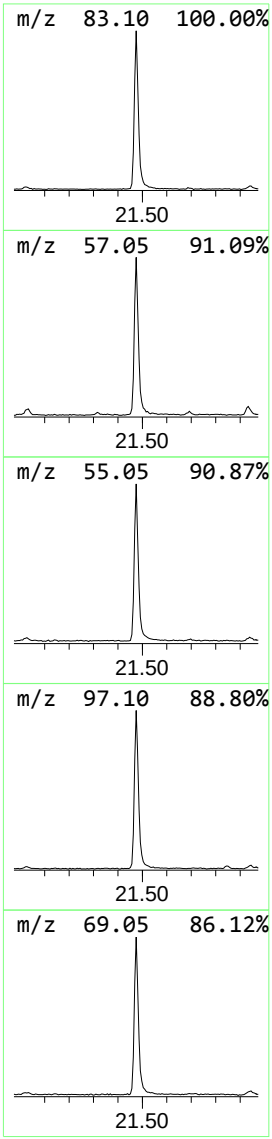
****

Peak Number 5 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	12.44 ng	1644120	Chrysene-d12	21.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PS-FRAC

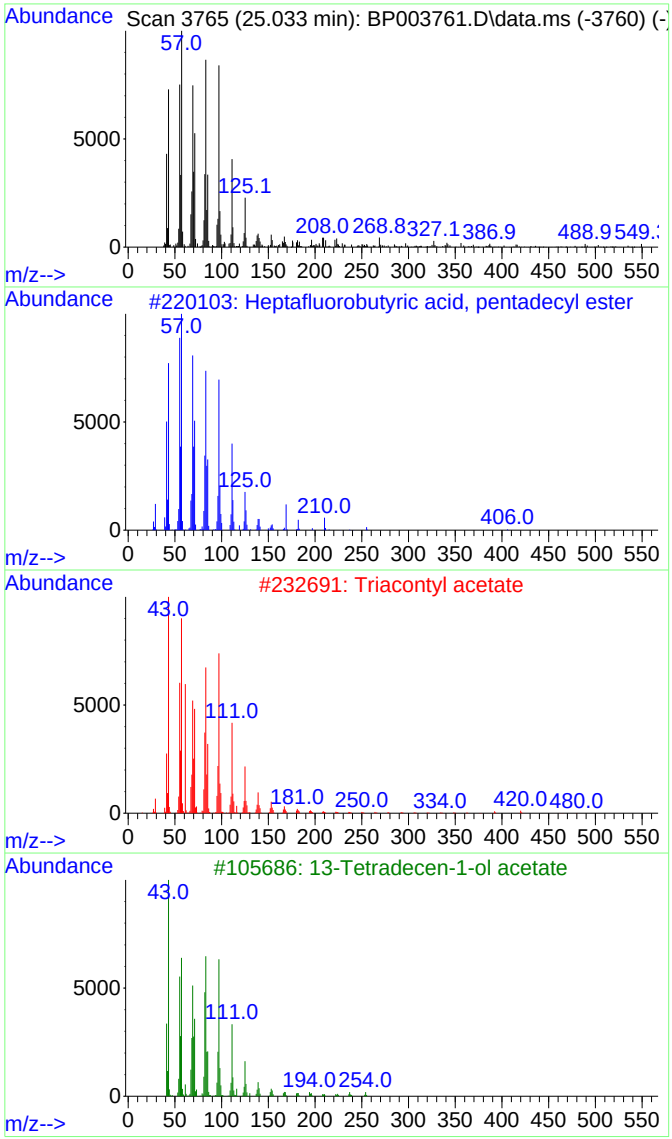
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

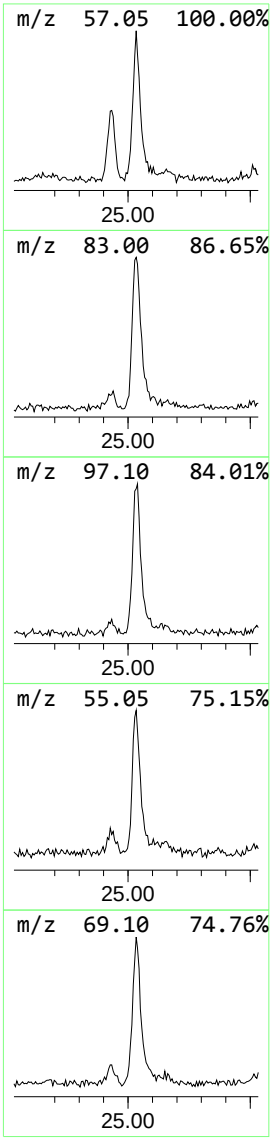
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.033	2.64 ng	314291	Perylene-d12	24.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
2	Triacontyl acetate	480	C32H64O2	041755-58-2	76
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	64
4	1-Octadecene	252	C18H36	000112-88-9	64
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PS-FRAC

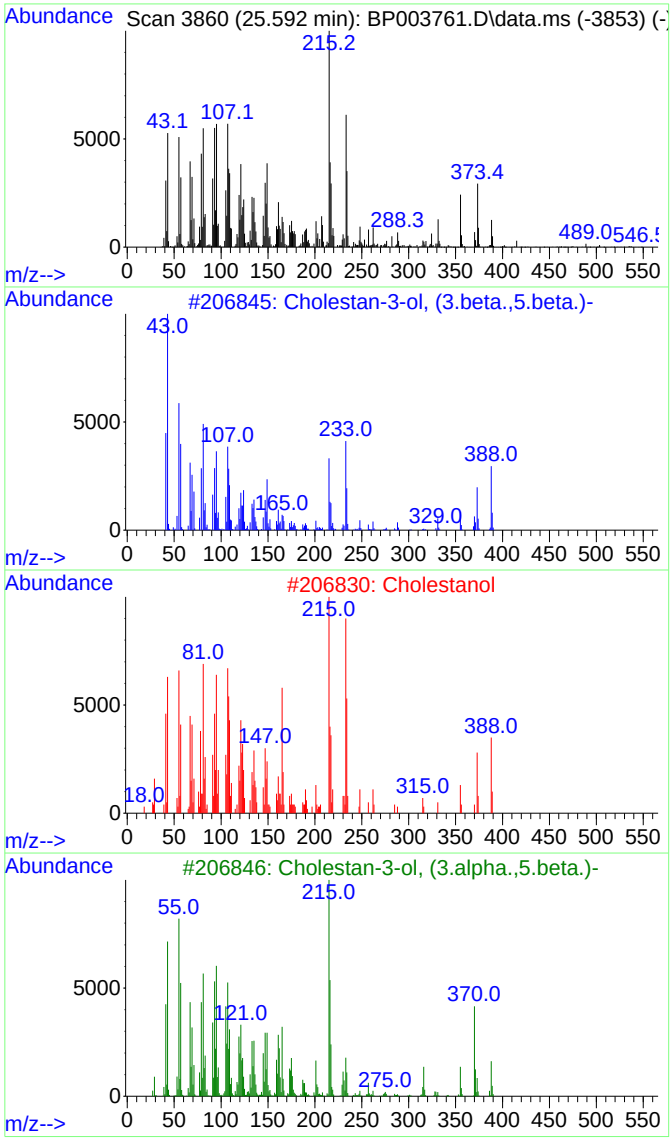
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

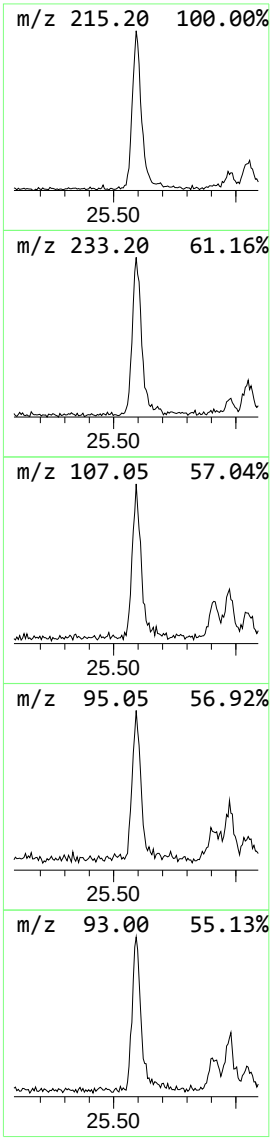
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.592	5.27 ng	627126	Perylene-d12	24.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	78
2	Cholestanol	388	C27H48O	000080-97-7	64
3	Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	62
4	Epicholestanol	388	C27H48O	000516-95-0	55
5	2-((1S,3S)-3-hydroxycyclohexyl)-...	332	C22H36O2	1000372-26-3	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003761.D
Acq On : 27 Oct 2020 18:47
Operator : CG/JU
Sample : L4520-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PS-FRAC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.346	21.8	ng	1134760	1	8.510	1040150	20.0
n-Hexadecanoic ...	18.645	9.2	ng	1083030	4	17.833	2360280	20.0
Octadecanoic acid	19.839	2.5	ng	328773	5	21.845	2642650	20.0
Cetene	21.474	12.4	ng	1644120	5	21.845	2642650	20.0
Heptafluorobuty...	25.033	2.6	ng	314291	6	24.421	2378960	20.0
Cholestan-3-ol,...	25.592	5.3	ng	627126	6	24.421	2378960	20.0