LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : FB020724

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\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019743.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	323	329	336	rVB	87817	128796	1.96%	0.497%
2	5.475	397	406	413	rBV	191724	282090	4.30%	1.087%
3	7.075	669	678	684	rBV	128449	215018	3.28%	0.829%
4	7.904	812	819	826	rVB	230159	379458	5.78%	1.463%
5	9.075	1010	1018	1029	rBV	761622	1322943	20.16%	5.100%
6	10.704	1287	1295	1304	rBV	286013	510147	7.77%	1.967%
7	13.169	1705	1714	1723	rBV	2160966	3338751	50.88%	12.871%
8	14.539	1940	1947	1958	rBV	463315	719433	10.96%	2.773%
9	14.963	2007	2019	2023	rBV6	62257	179730	2.74%	0.693%
10	15.563	2095	2121	2141	rBV3	1232528	6157574	93.84%	23.738%
11	16.033	2191	2201	2214	rBV	985613	1562947	23.82%	6.025%
12	16.339	2248	2253	2262	rVB3	36639	68246	1.04%	0.263%
13	16.698	2309	2314	2327	rVB6	53345	125710	1.92%	0.485%
14	17.298	2410	2416	2422	rBV	672093	951637	14.50%	3.669%
15	18.192	2563	2568	2576	rBV	365232	523200	7.97%	2.017%
16	18.463	2610	2614	2617	rBV	122356	183272	2.79%	0.707%
17	18.504	2618	2621	2633	rVB3	130287	226599	3.45%	0.874%
18	19.427	2774	2778	2788	rVB	174289	255765	3.90%	0.986%
19	19.863	2847	2852	2858	rBV	5171216	6561716	100.00%	25.296%
20	21.392	3107	3112	3122	rVB	849862	1164636	17.75%	4.490%
21	23.815	3518	3524	3533	rVB	516384	1082569	16.50%	4.173%

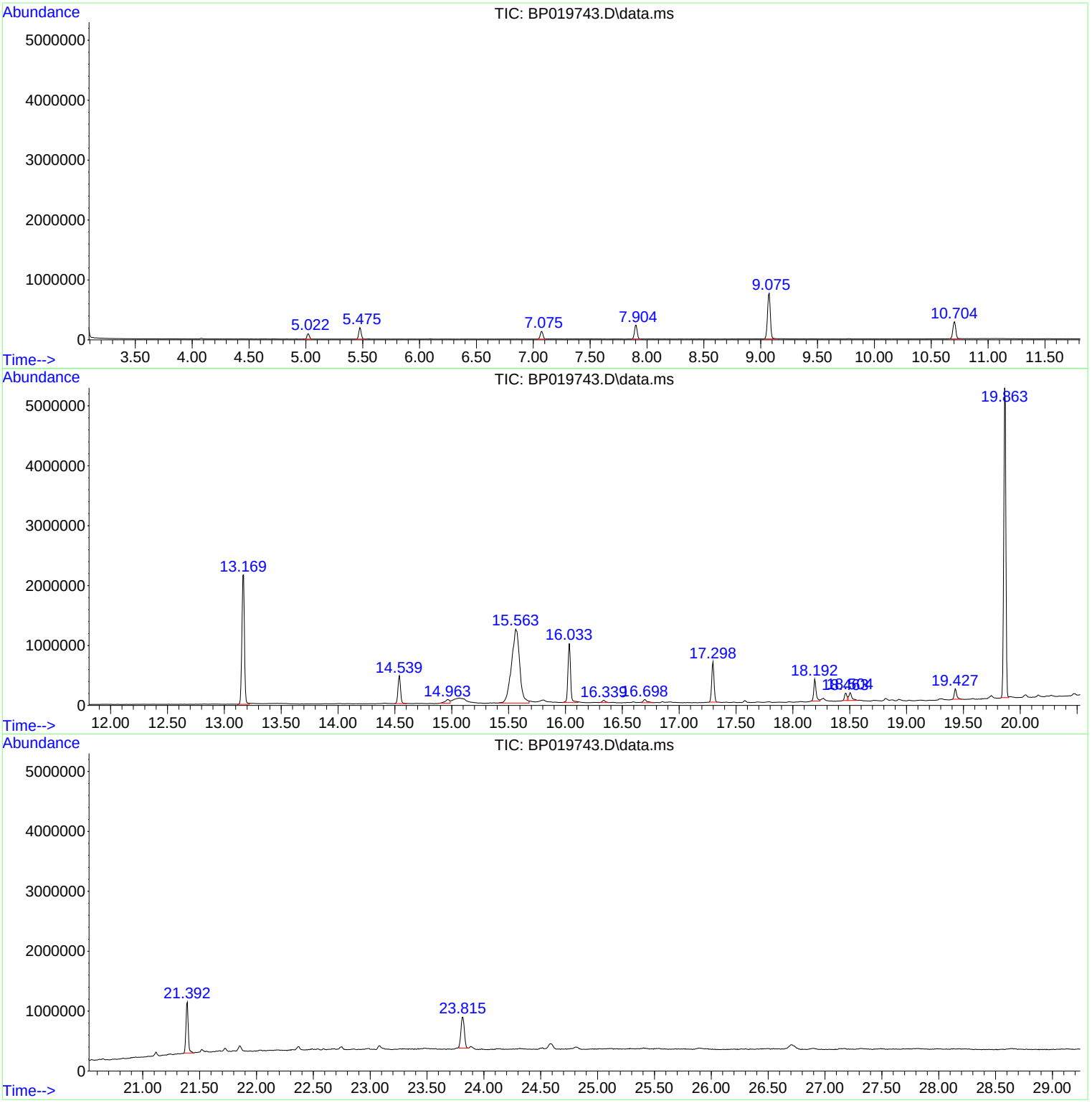
Sum of corrected areas: 25940237

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

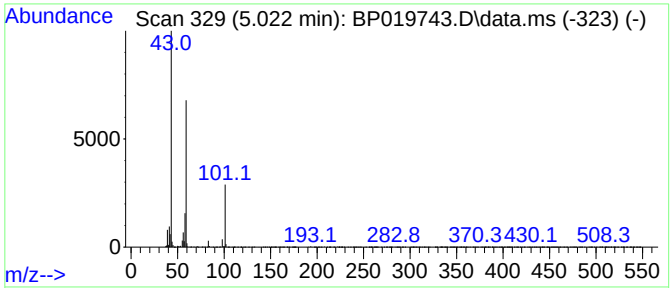
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

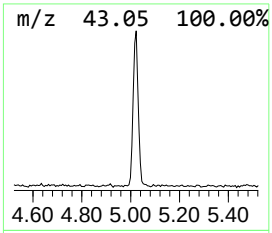
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

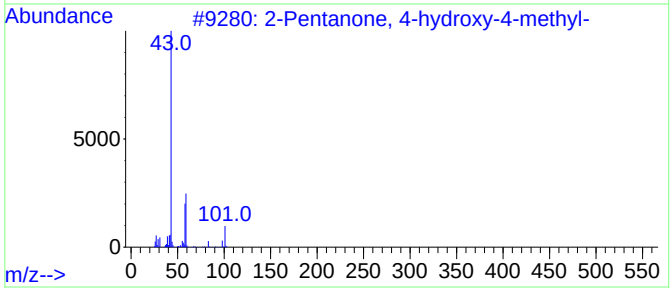
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

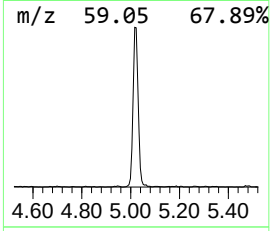
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	6.79 ng	128796	1,4-Dichlorobenzene-d4	7.899

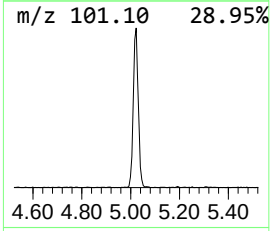
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Acetone	58	C3H6O	000067-64-1	9

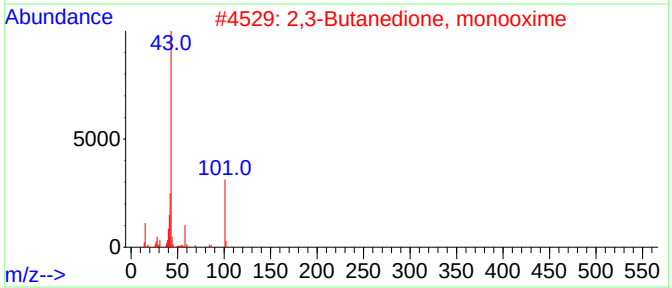


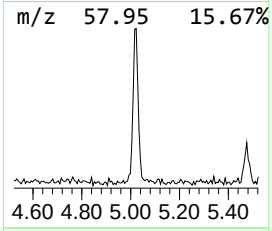


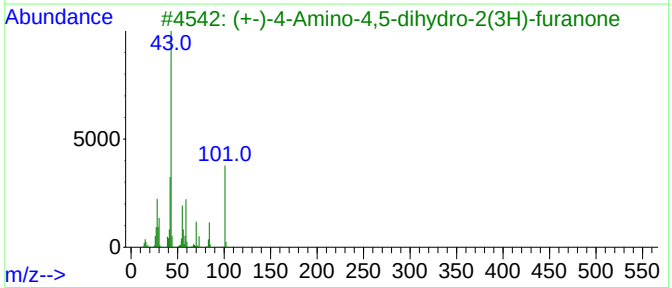


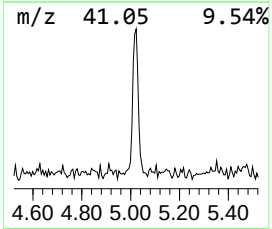












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

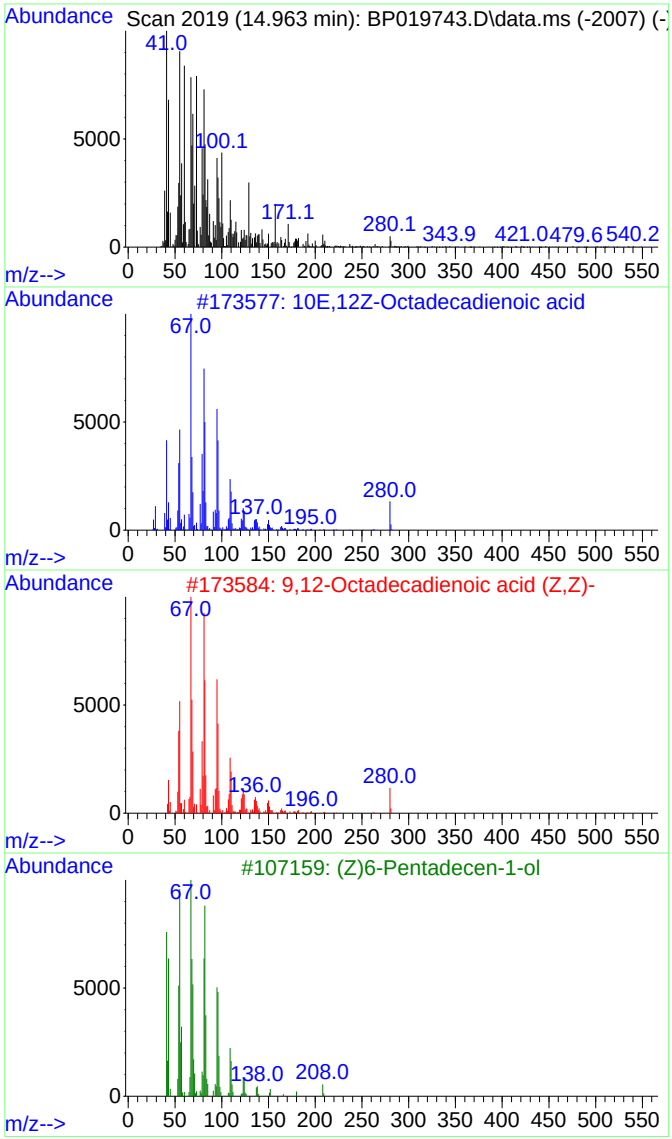
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

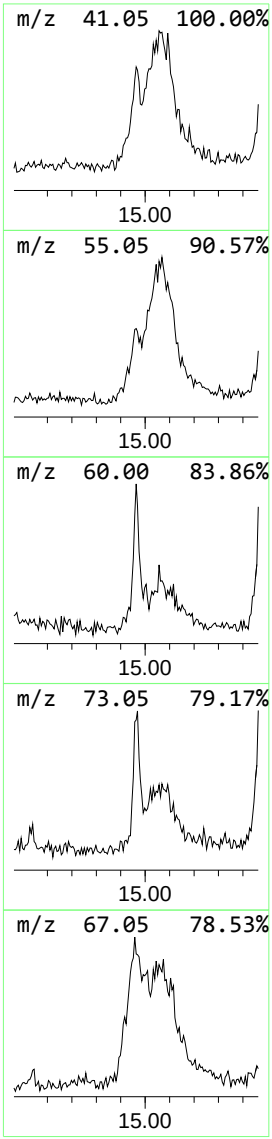
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 10E,12Z-Octadecadienoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	5.00 ng	179730	Acenaphthene-d10	14.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	66
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	60
3	(Z)6-Pentadecen-1-ol	226	C15H30O	068797-95-5	53
4	1,11-Dodecadiene	166	C12H22	005876-87-9	47
5	Linoelaidic acid	280	C18H32O2	000506-21-8	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

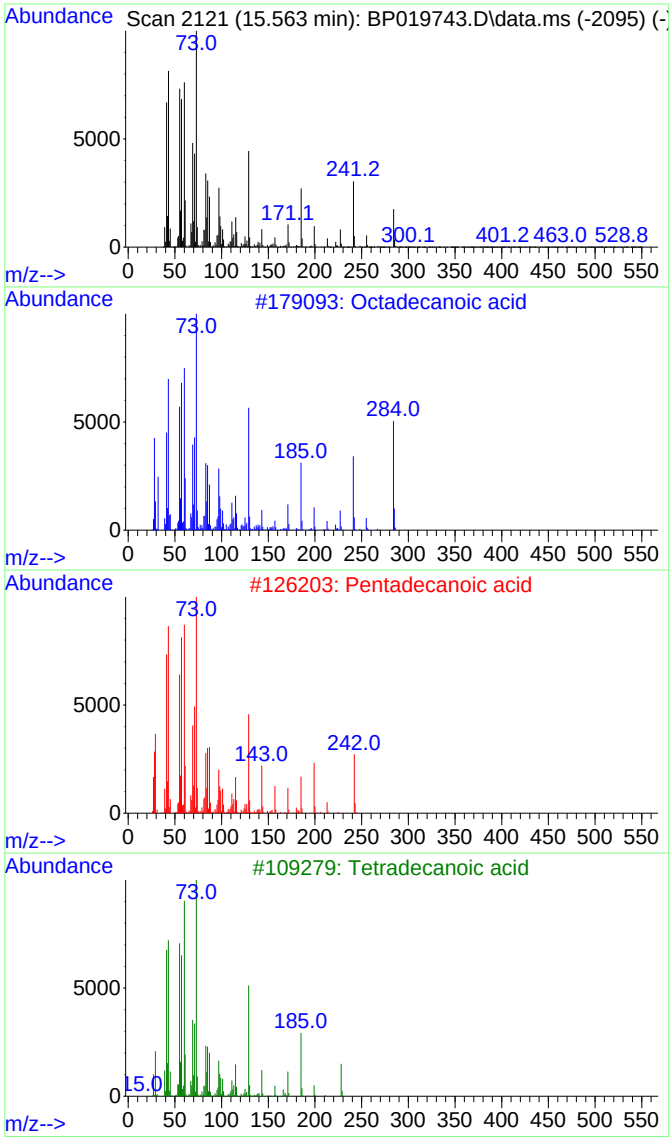
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

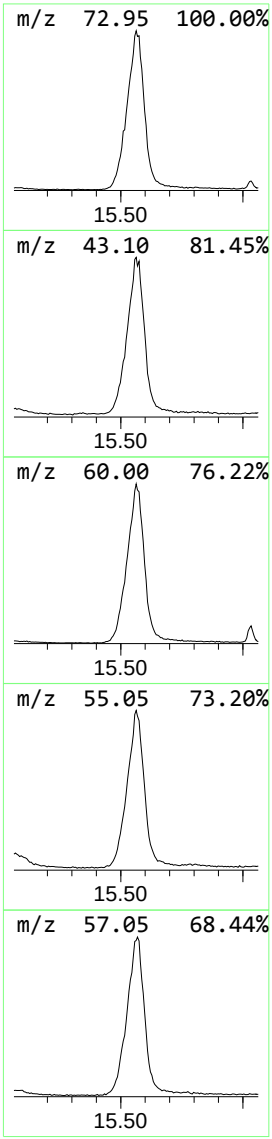
****

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.563	171.18 ng	6157570	Acenaphthene-d10	14.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

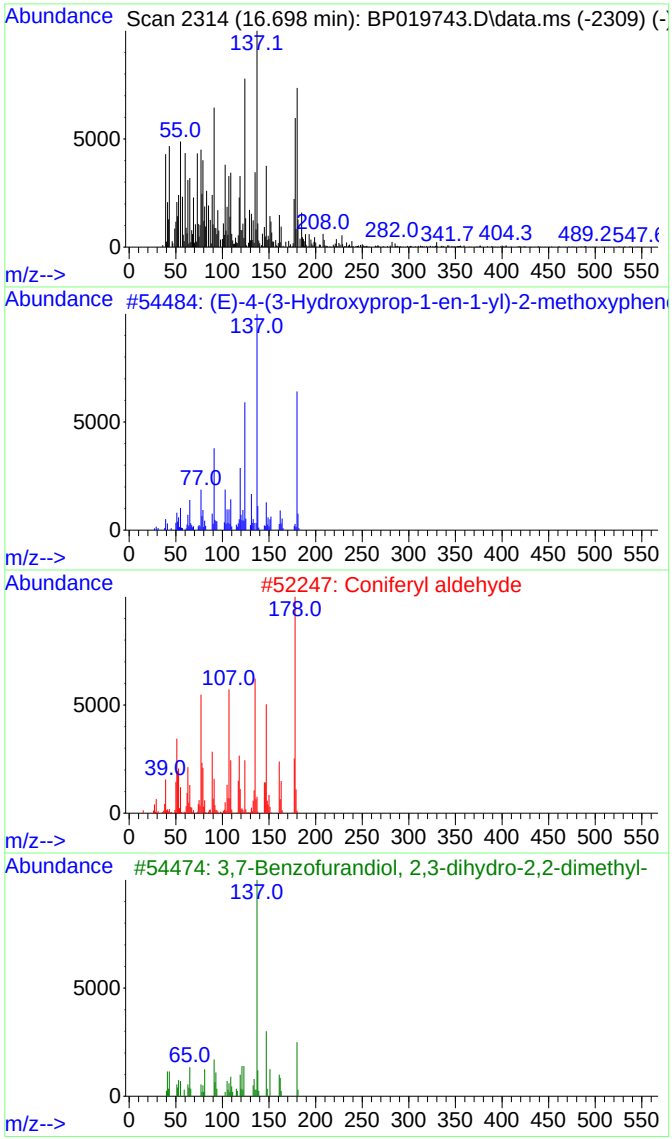
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

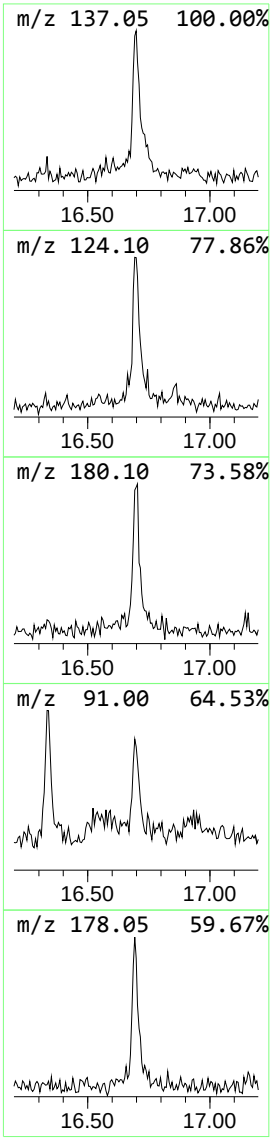
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.698	2.64 ng	125710	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	70
2	Coniferyl aldehyde	178	C10H10O3	000458-36-6	46
3	3,7-Benzofurandiol, 2,3-dihydro-...	180	C10H12O3	017781-15-6	42
4	2-Butanone, 3-(phenylthio)-	180	C10H12OS	013023-53-5	38
5	Benzene, 1-methyl-3-[(2-methylpr...	180	C11H16S	054576-36-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

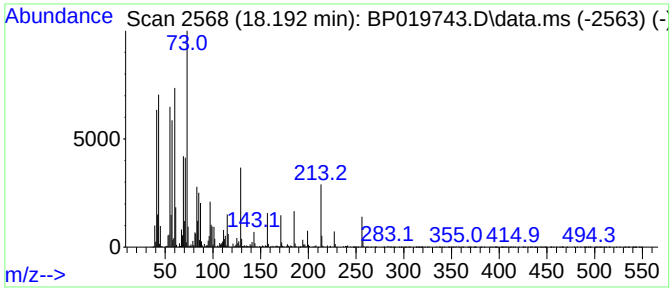
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

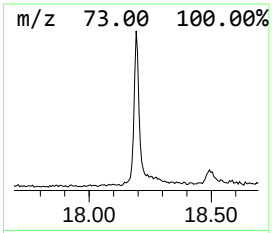
****

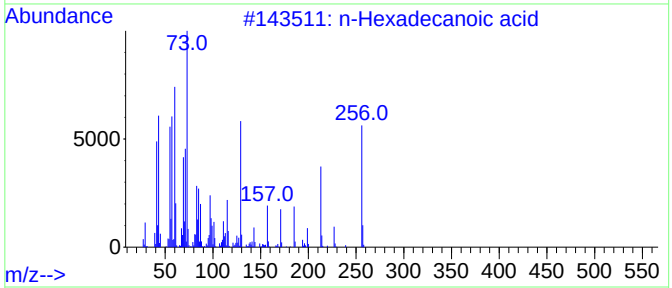
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

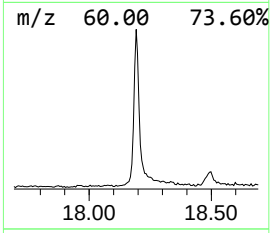
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	11.00 ng	523200	Phenanthrene-d10	17.298

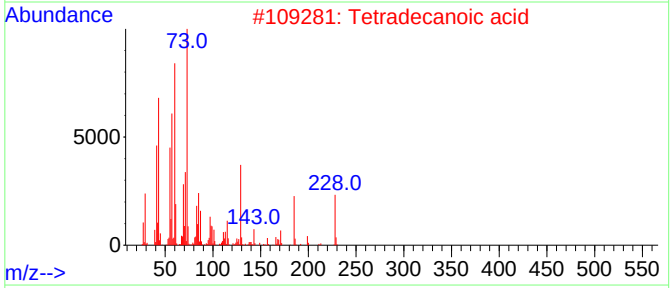
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70

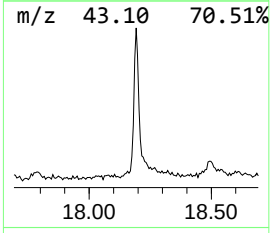


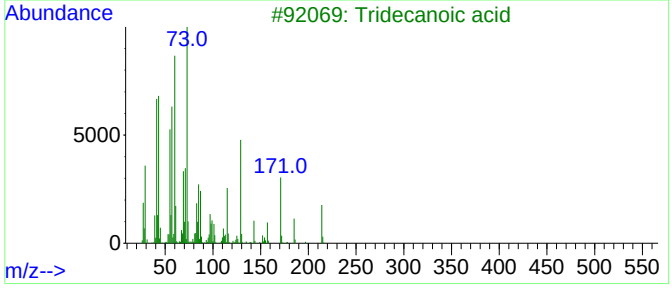


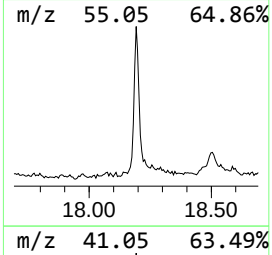


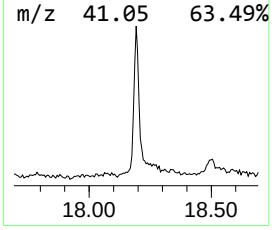












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

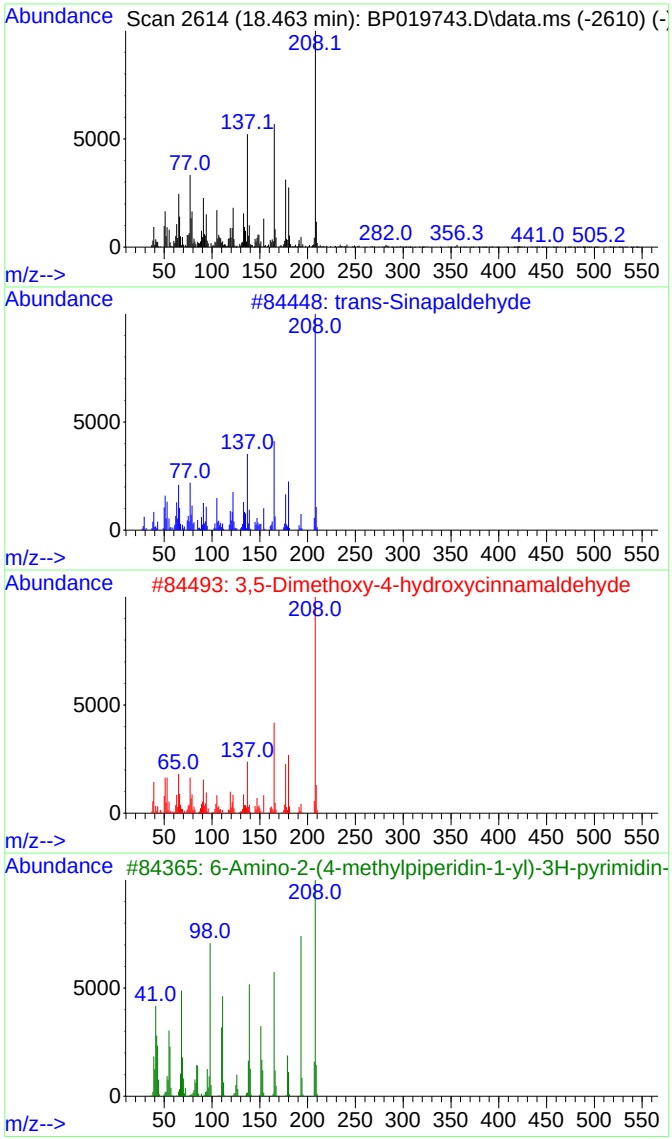
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

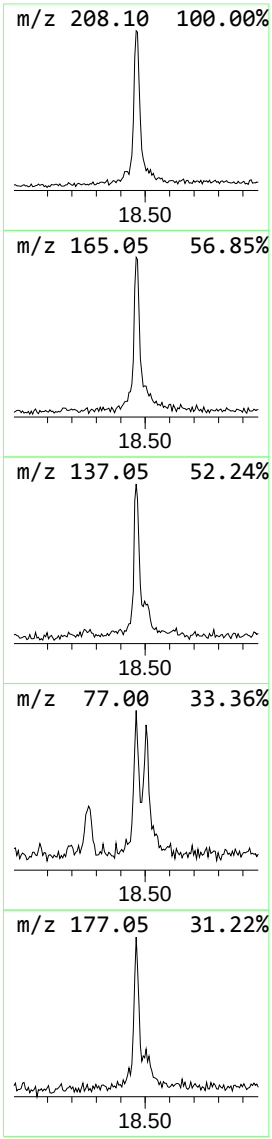
****

Peak Number 6 trans-Sinapaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.463	3.85 ng	183272	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	94
2	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	90
3	6-Amino-2-(4-methylpiperidin-1-y...	208	C10H16N4O	1000388-65-9	83
4	Butan-1-one, 1-(3,4-dimethoxyphe...	208	C12H16O3	054419-21-5	53
5	2,5-Dimethoxycinnamic acid	208	C11H12O4	010538-51-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

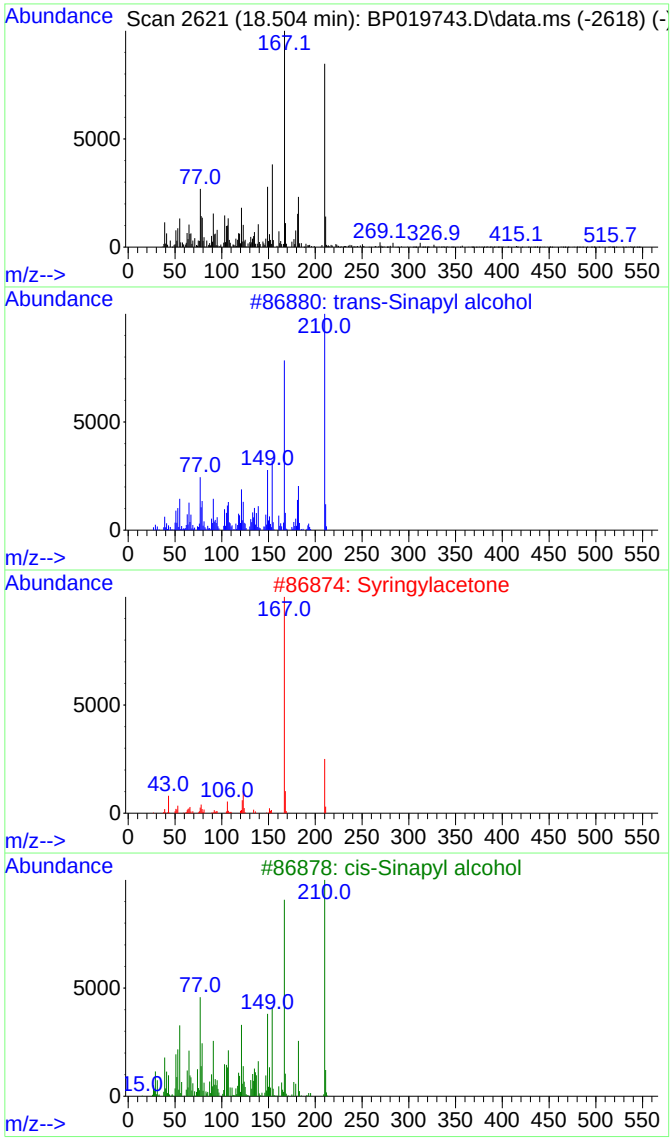
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

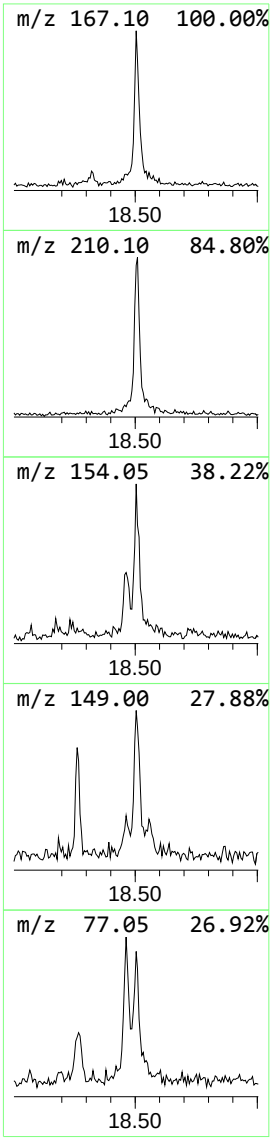
****

Peak Number 7 trans-Sinapyl alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.504	4.76 ng	226599	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	90
2	Syringylacetone	210	C11H14O4	019037-58-2	64
3	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	58
4	9H-fluoren-9-one, 2,7-diamino-	210	C13H10N2O	1000400-61-7	43
5	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

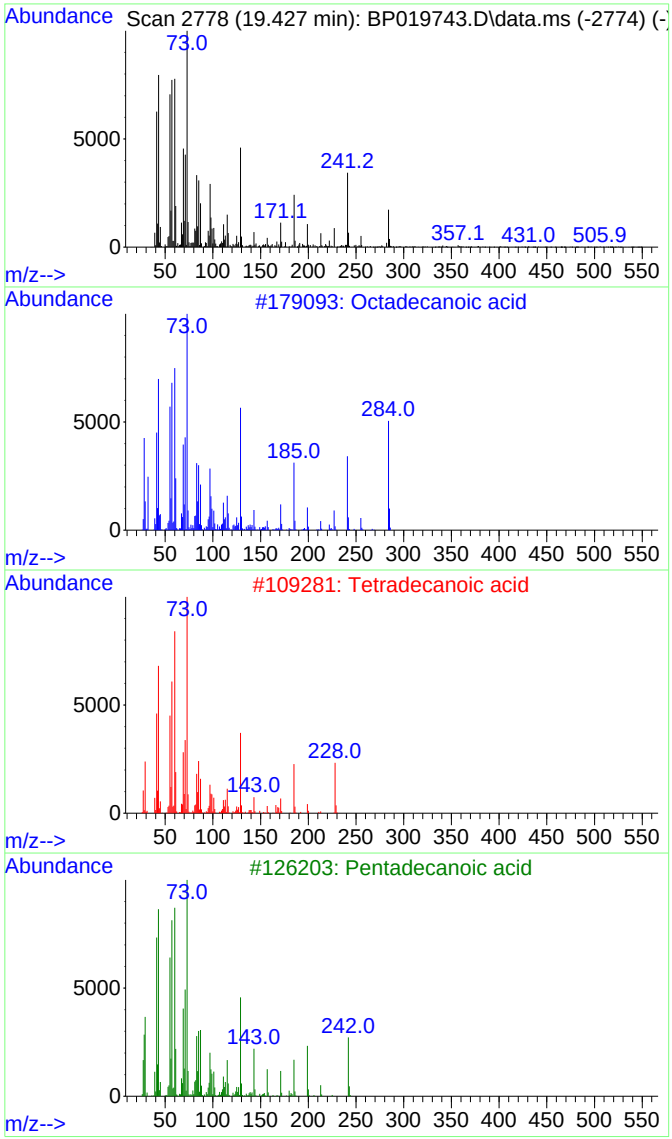
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

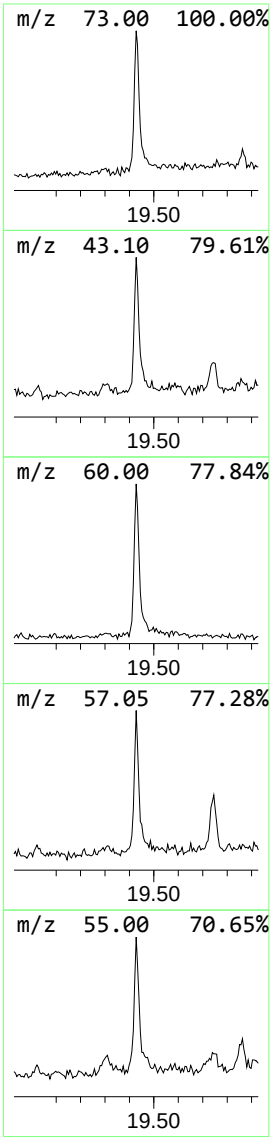
****

Peak Number 8 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.427	4.39 ng	255765	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
Data File : BP019743.D
Acq On : 16 Feb 2024 14:09
Operator : MA/JU
Sample : P1414-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB020724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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
2-Pentanone, 4-...	5.022	6.8	ng	128796	1	7.899	379458	20.0
10E,12Z-Octadec...	14.963	5.0	ng	179730	3	14.539	719433	20.0
Octadecanoic acid	15.563	171.2	ng	6157570	3	14.539	719433	20.0
(E)-4-(3-Hydrox...	16.698	2.6	ng	125710	4	17.298	951637	20.0
n-Hexadecanoic ...	18.192	11.0	ng	523200	4	17.298	951637	20.0
trans-Sinapalde...	18.463	3.9	ng	183272	4	17.298	951637	20.0
trans-Sinapyl a...	18.504	4.8	ng	226599	4	17.298	951637	20.0
Tetradecanoic acid	19.427	4.4	ng	255765	5	21.392	1164640	20.0