LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013446.D
Acq On : 11 Jan 2023 16:29
Operator : CG/JU
Sample : 01064-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-13-01

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-BP121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.011	304	310	320	rVB	1606069	2324733	7.51%	0.971%
2	5.481	383	390	404	rVB	10243143	15517353	50.13%	6.480%
3	7.087	656	663	678	rVV	9916923	16349032	52.81%	6.827%
4	7.217	678	685	693	rVB	216795	376995	1.22%	0.157%
5	7.922	797	805	811	rBV	2259378	3536345	11.42%	1.477%
6	9.093	995	1004	1012	rBV	6138829	9965409	32.19%	4.161%
7	10.734	1276	1283	1292	rBV	3166210	5214153	16.84%	2.177%
8	13.193	1692	1701	1709	rBV	15439153	23167114	74.84%	9.674%
9	14.569	1929	1935	1942	rVB	5151780	7461456	24.10%	3.116%
10	15.851	2149	2153	2159	rBV	275781	372271	1.20%	0.155%
11	15.928	2161	2166	2173	rVV	1058750	1426182	4.61%	0.596%
12	16.063	2183	2189	2205	rBV	15010526	22108291	71.42%	9.232%
13	17.328	2398	2404	2413	rBV	6720102	9507575	30.71%	3.970%
14	18.198	2547	2552	2563	rBV	5049738	8360068	27.01%	3.491%
15	19.292	2734	2738	2740	rBV	1934020	2681177	8.66%	1.120%
16	19.322	2740	2743	2750	rVV2	3511123	7451082	24.07%	3.111%
17	19.381	2750	2753	2757	rVV	3473327	4779975	15.44%	1.996%
18	19.439	2758	2763	2782	rVB	17945575	29047051	93.83%	12.129%
19	19.881	2833	2838	2844	rBV	24912072	30955839	100.00%	12.926%
20	21.104	3043	3046	3053	rBV	4028320	6268200	20.25%	2.617%
21	21.422	3093	3100	3102	rBV	12996099	24863618	80.32%	10.382%
22	23.886	3514	3519	3528	rVB2	3810149	7749553	25.03%	3.236%

Sum of corrected areas: 239483472

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Misc :
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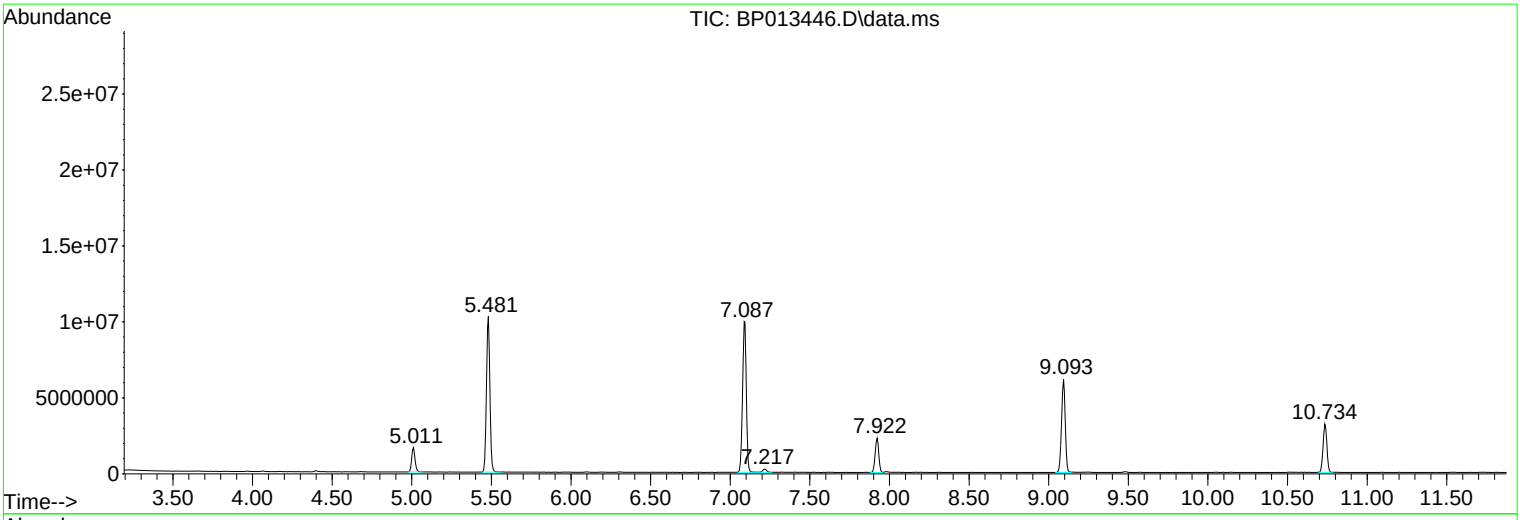
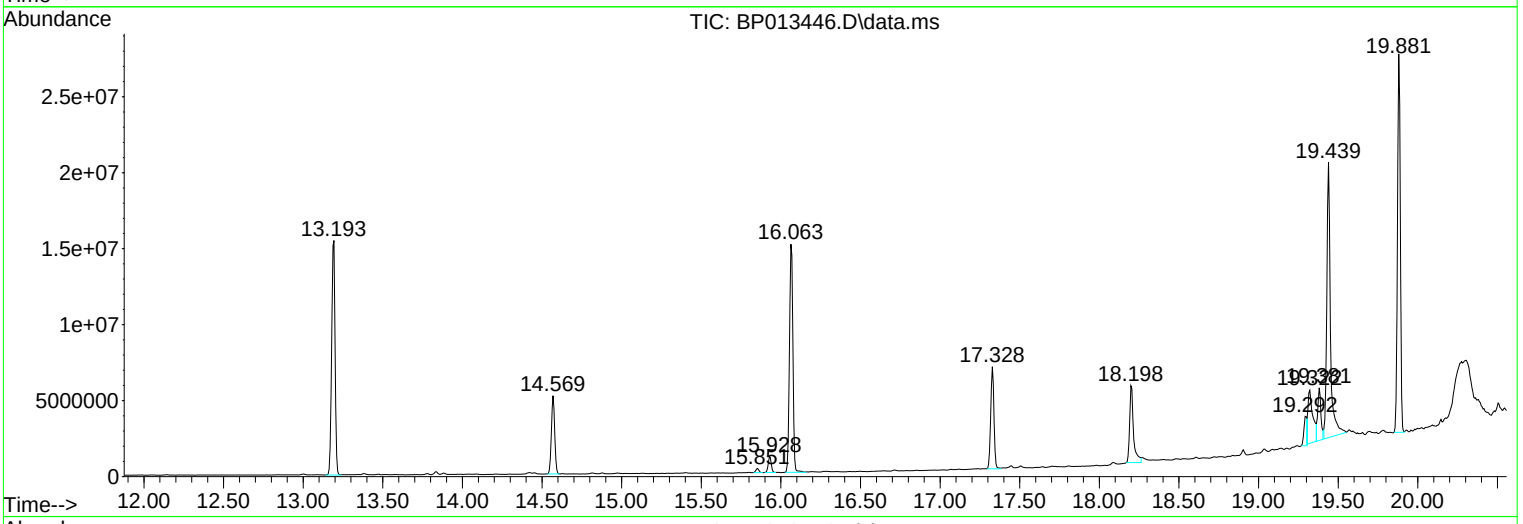
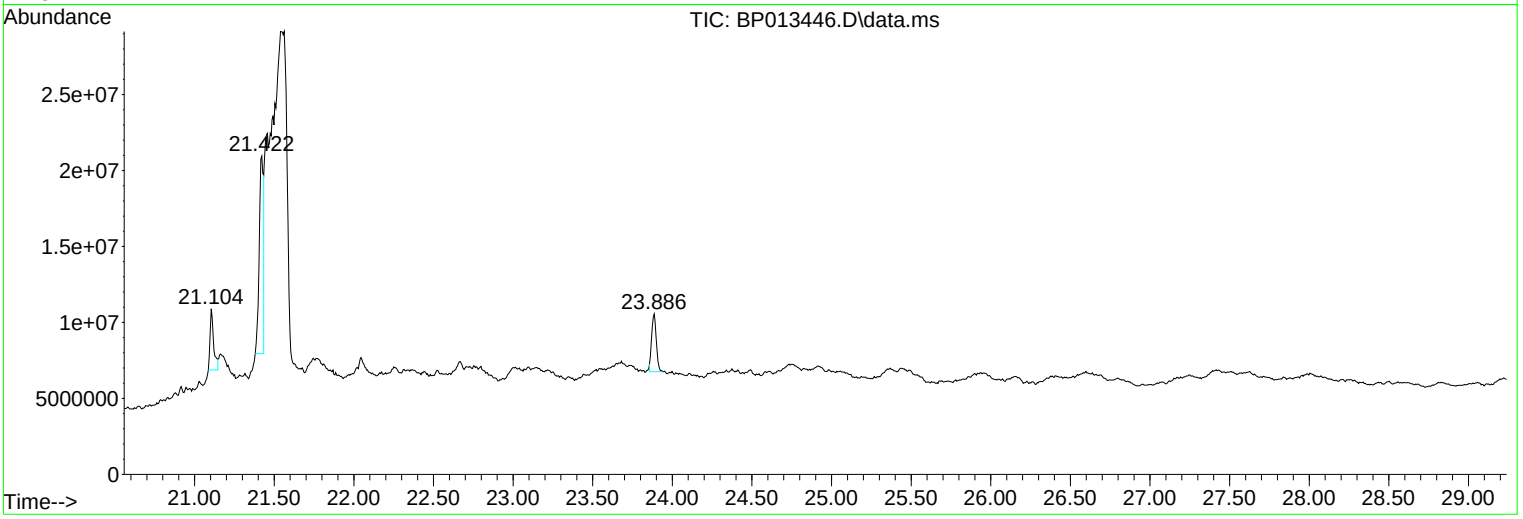
Instrument :
BNA_P
ClientSampleId :
S-13-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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TIC Library : C:\Database\NIST20.L
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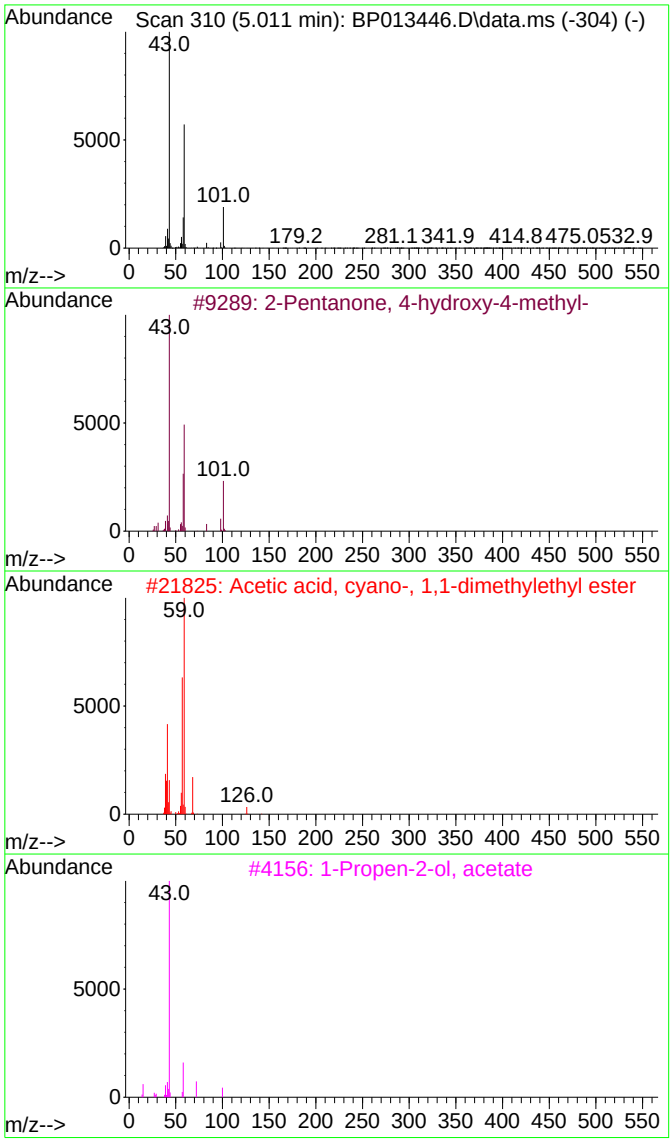
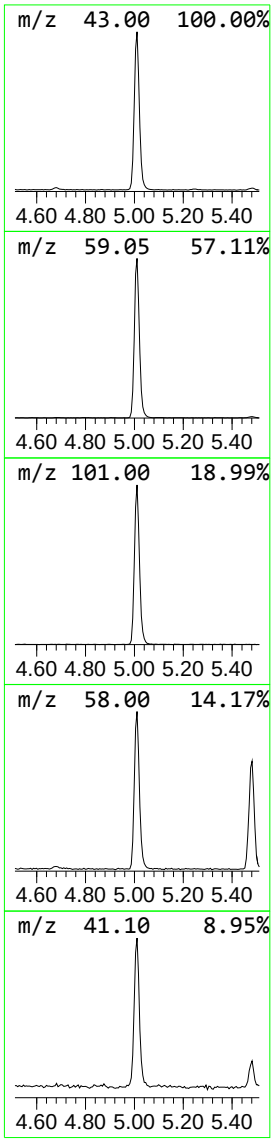
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	13.15 ng	2324730	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





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Sample : 01064-04
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Instrument :
BNA_P
ClientSampleId :
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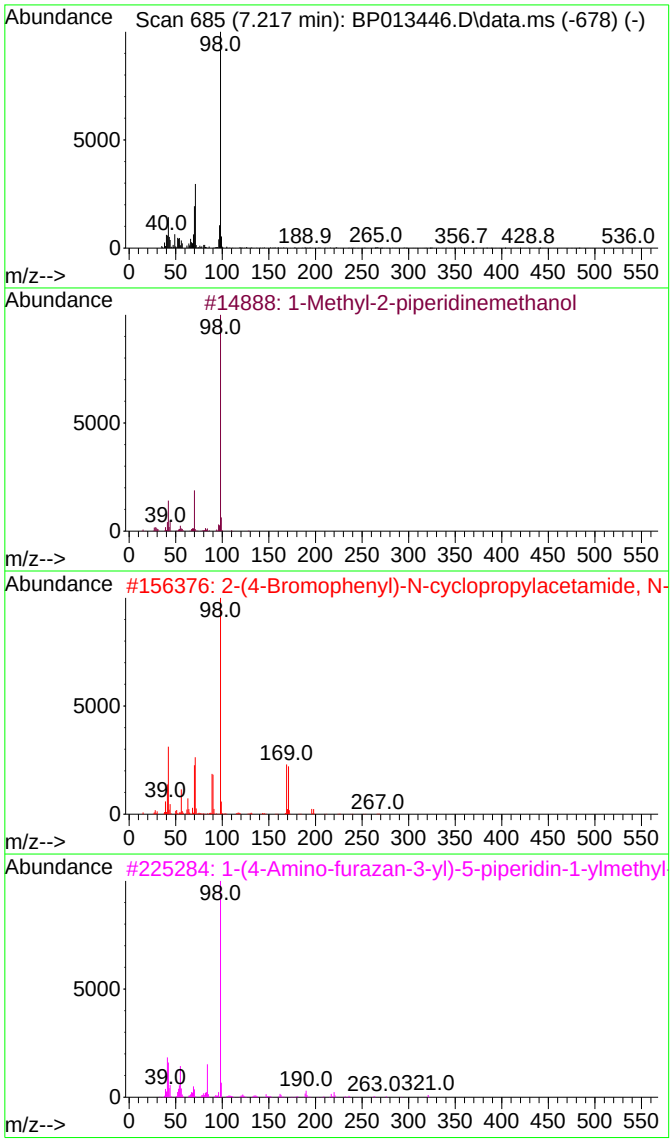
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

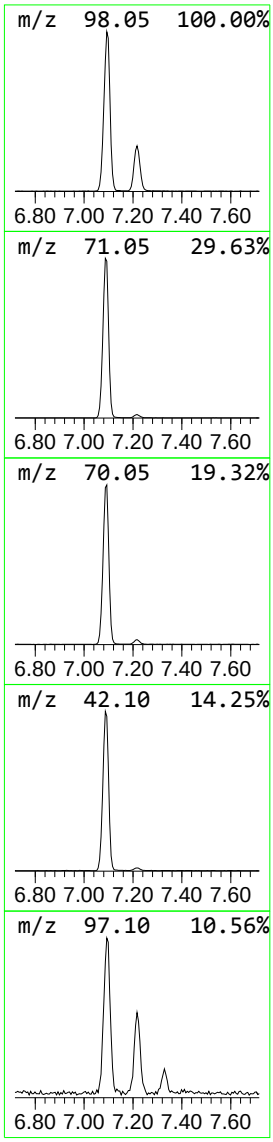
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Methyl-2-piperidinemethanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.217	2.13 ng	376995	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-piperidinemethanol	129	C7H15NO	020845-34-5	53
2	2-(4-Bromophenyl)-N-cyclopropyla...	267	C12H14BrNO	1791024-37-7	50
3	1-(4-Amino-furazan-3-yl)-5-piper...	321	C13H19N7O3	311314-85-9	47
4	Propan-2-ol, 1-(2-methyl-4-nitro...	300	C12H20N4O3S	306326-24-9	47
5	4H-1,2,4-Triazol-3-amine, 4-methyl-	98	C3H6N4	016681-76-8	47





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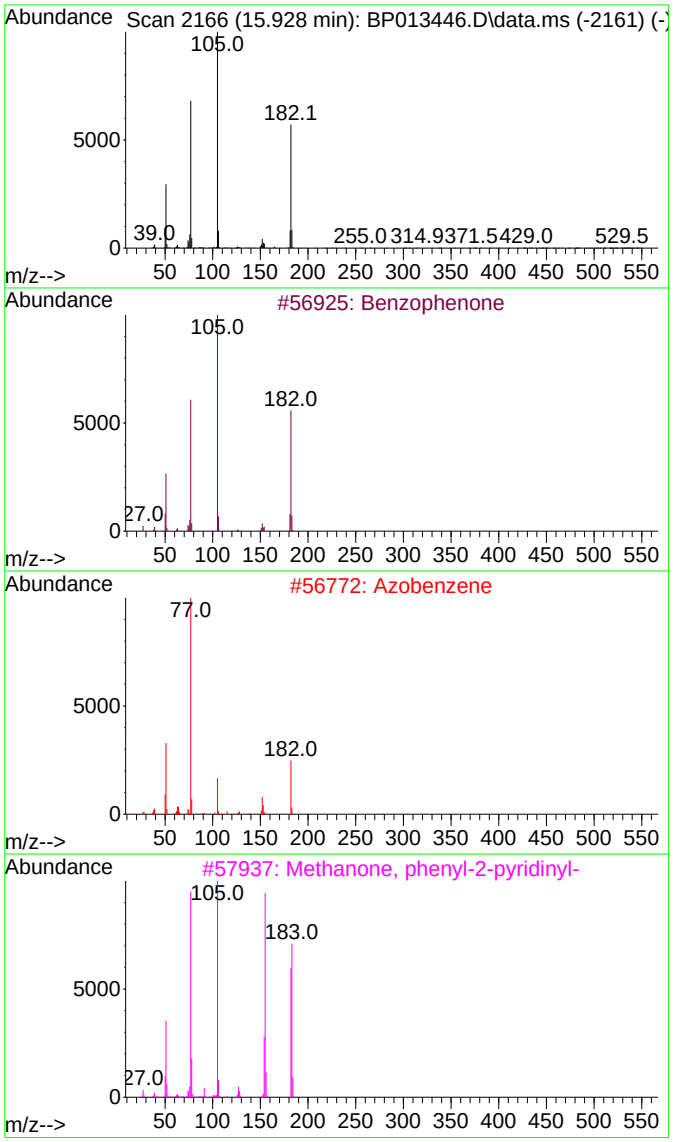
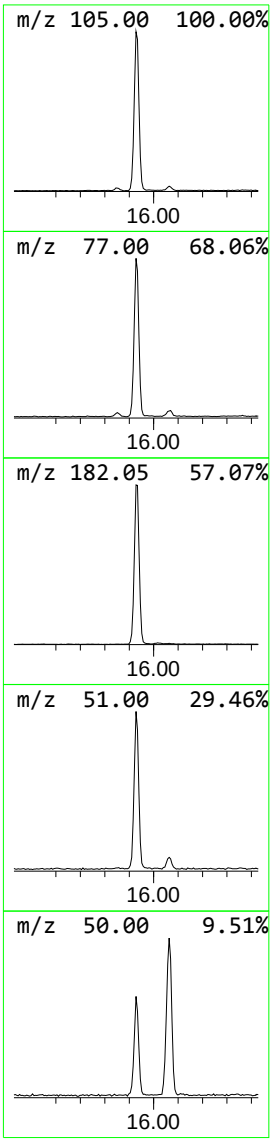
****

Peak Number 3 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.928	3.82 ng	1426180	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
4	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	50
5	Azobenzene, (E)-	182	C12H10N2	017082-12-1	50





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Misc :
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Instrument :
BNA_P
ClientSampleId :
S-13-01

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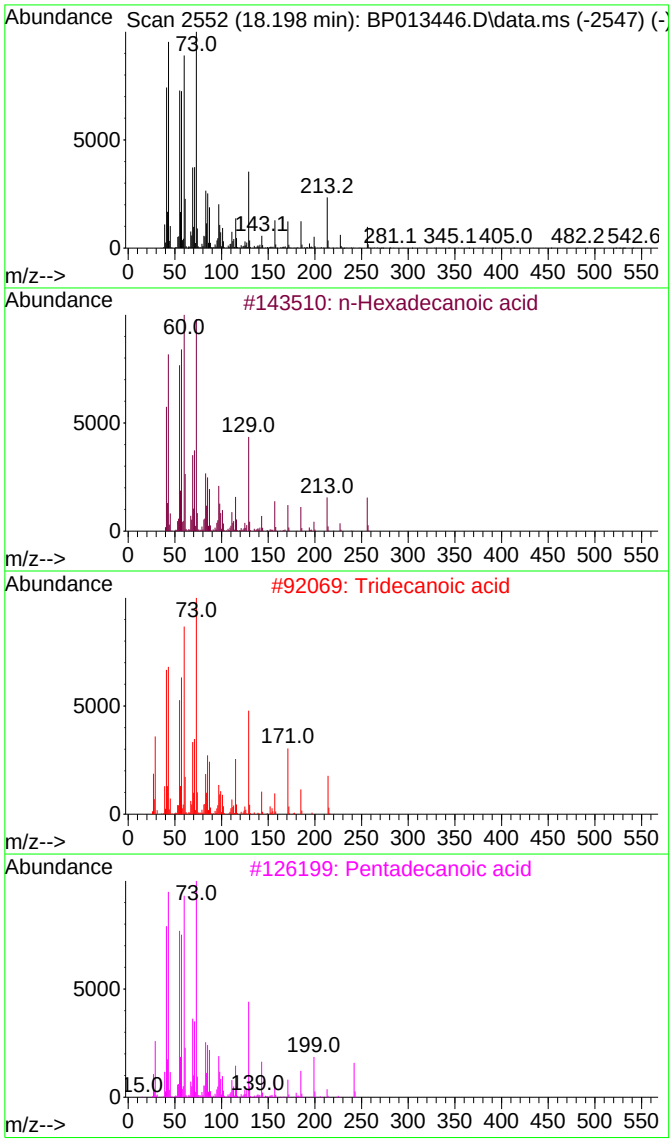
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

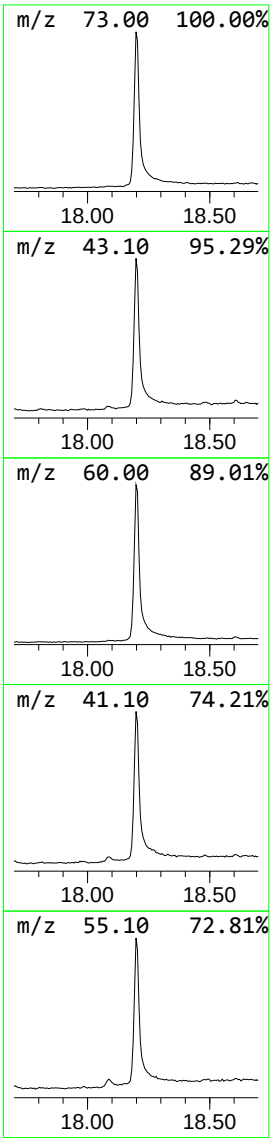
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	17.59 ng	8360070	Phenanthrene-d10	17.328

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Sample : 01064-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-13-01

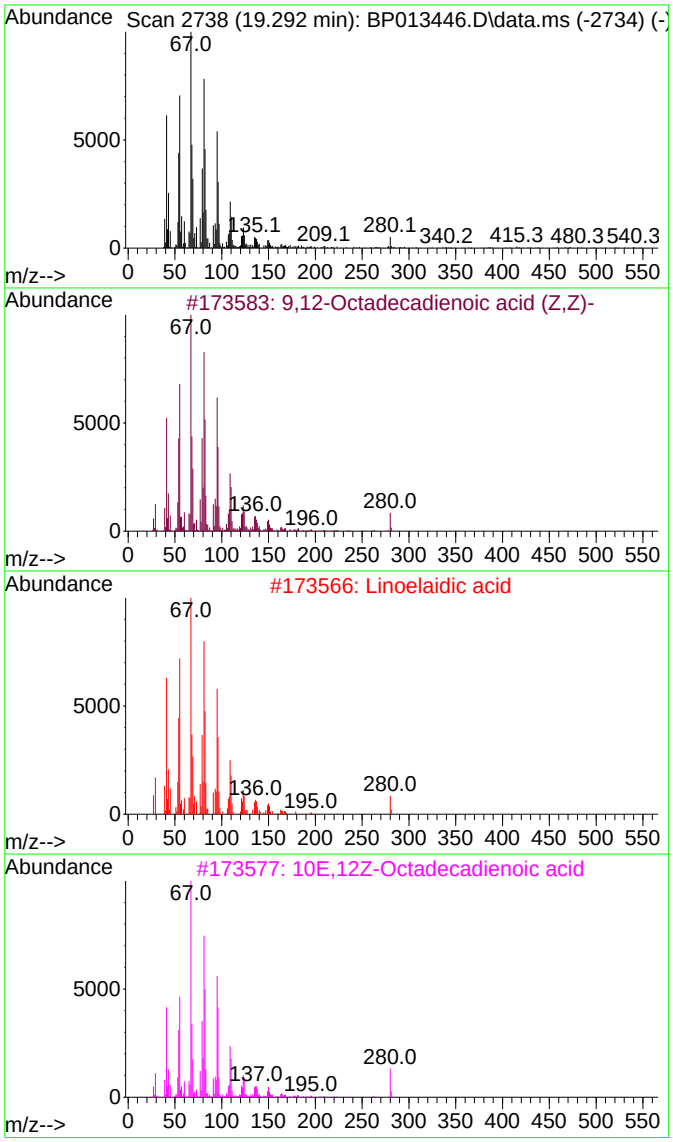
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

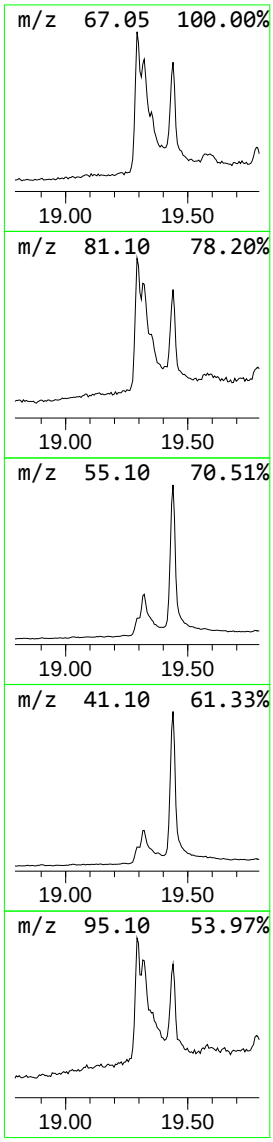
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.292	5.64 ng	2681180	Phenanthrene-d10	17.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	Linoelaidic acid	280	C18H32O2	000506-21-8	99
3	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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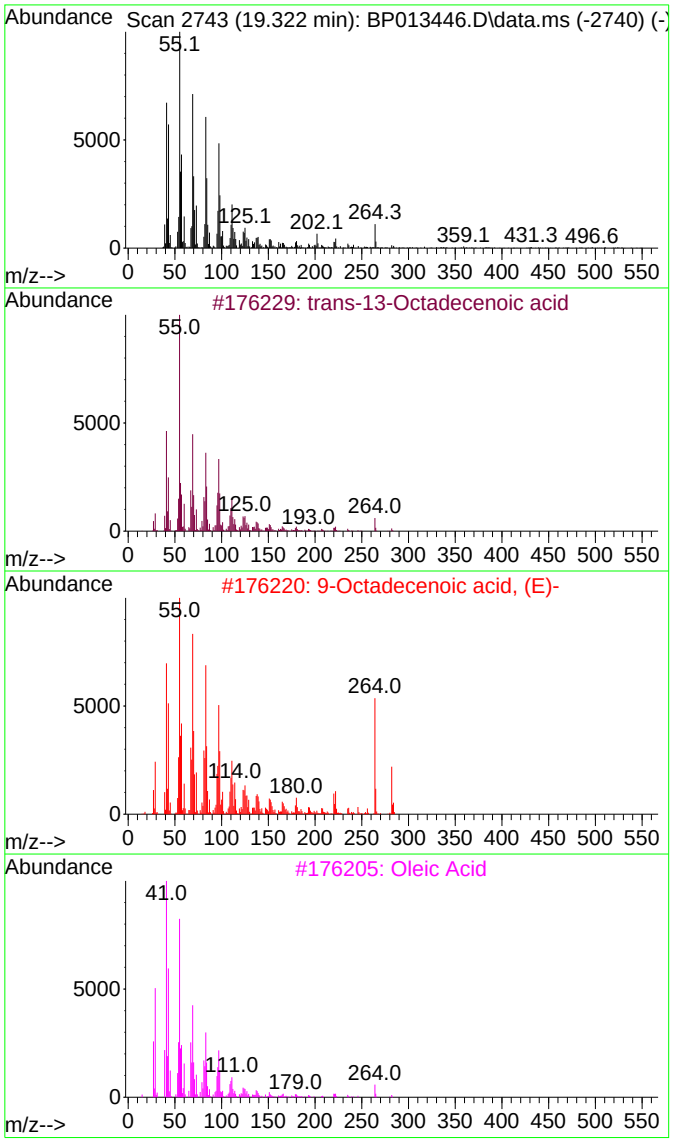
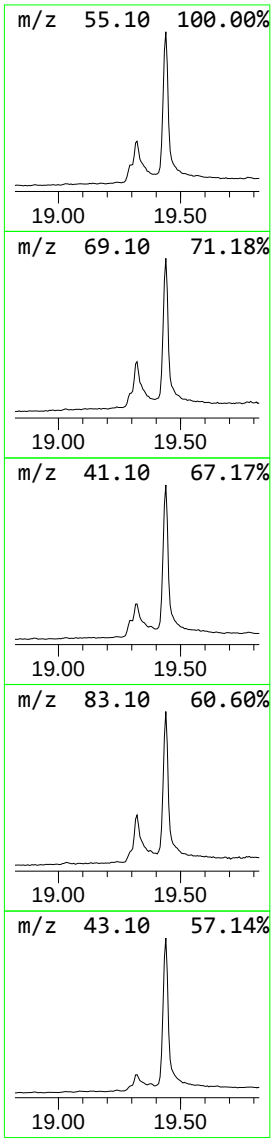
****

Peak Number 6 trans-13-Octadecenoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.322	15.67 ng	7451080	Phenanthrene-d10	17.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	93
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91
3	Oleic Acid	282	C18H34O2	000112-80-1	91
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	83
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	83





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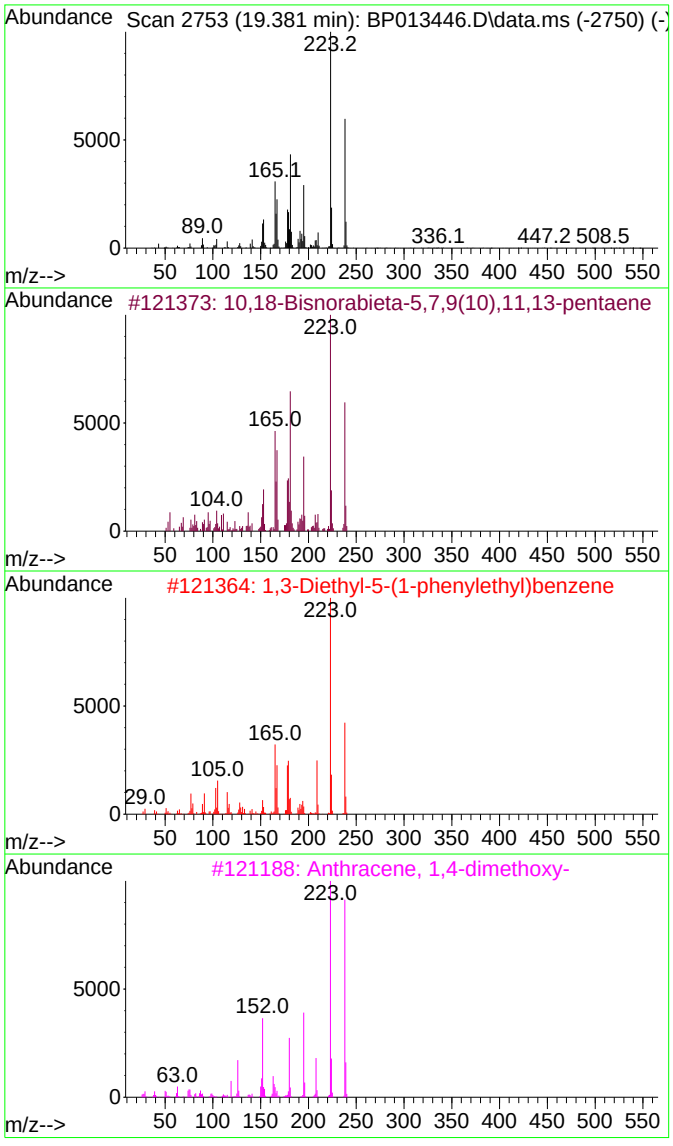
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

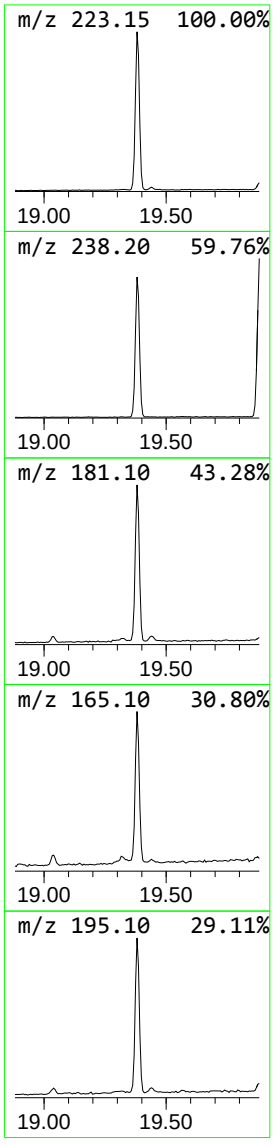
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.381	3.84 ng	4779980	Chrysene-d12	21.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	89
3	Anthracene, 1,4-dimethoxy-	238	C16H14O2	013076-29-4	64
4	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	60
5	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	53





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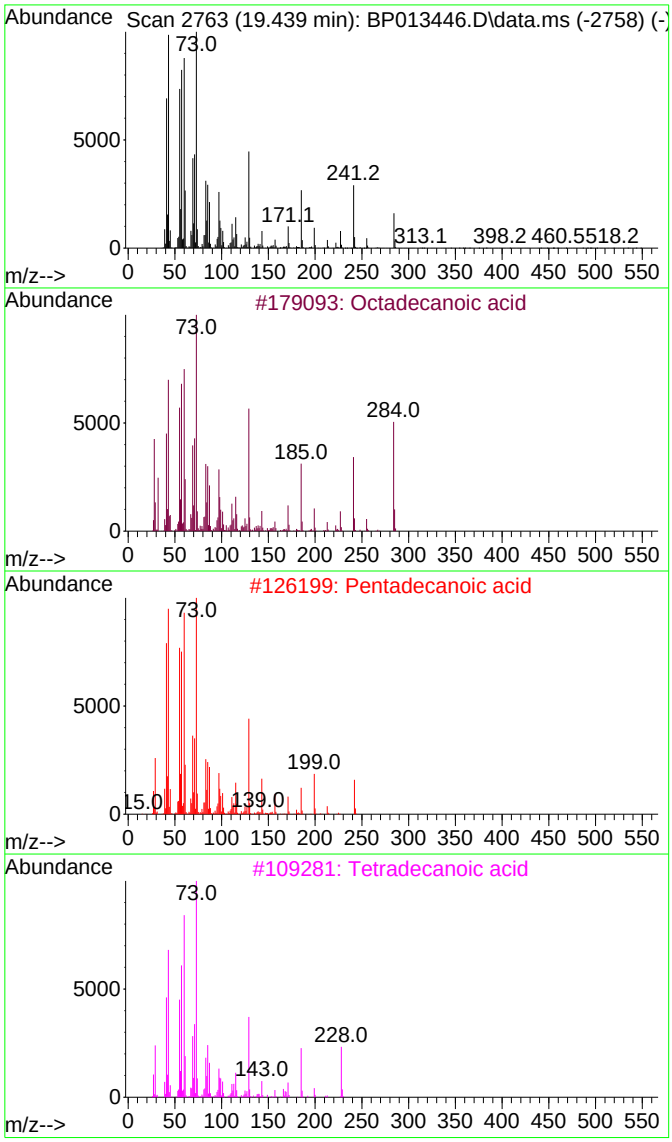
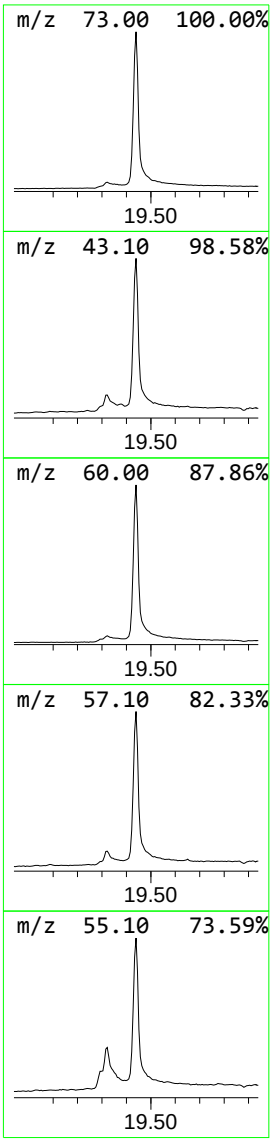
****

Peak Number 8 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	23.37 ng	29047100	Chrysene-d12	21.416

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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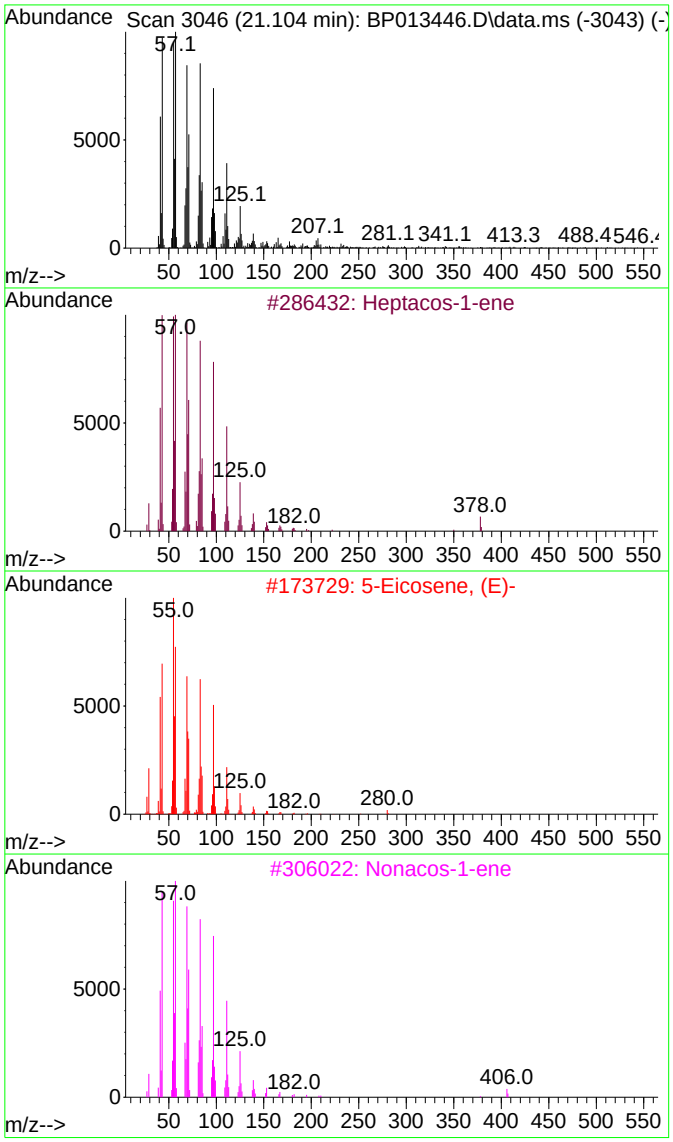
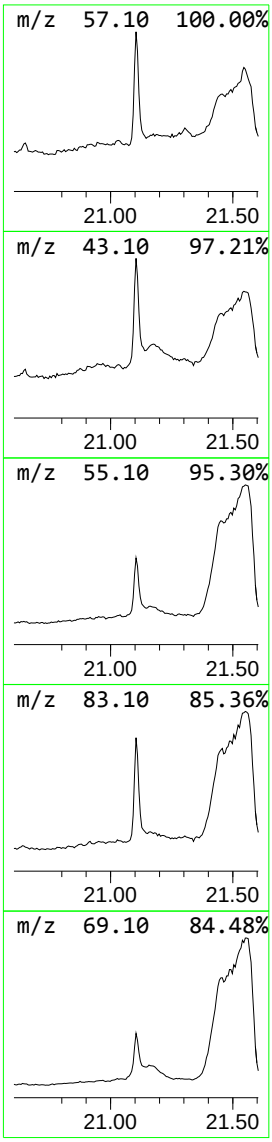
****

Peak Number 9 Heptacos-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	5.04 ng	6268200	Chrysene-d12	21.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	Nonacos-1-ene	406	C29H58	018835-35-3	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013446.D
Acq On : 11 Jan 2023 16:29
Operator : CG/JU
Sample : 01064-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-13-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.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-...	5.011	13.2	ng	2324730	1	7.922	3536350	20.0
1-Methyl-2-pipe...	7.217	2.1	ng	376995	1	7.922	3536350	20.0
Benzophenone	15.928	3.8	ng	1426180	3	14.569	7461460	20.0
n-Hexadecanoic ...	18.198	17.6	ng	8360070	4	17.328	9507580	20.0
9,12-Octadecadi...	19.292	5.6	ng	2681180	4	17.328	9507580	20.0
trans-13-Octade...	19.322	15.7	ng	7451080	4	17.328	9507580	20.0
10,18-Bisnorabi...	19.381	3.8	ng	4779980	5	21.416	24863600	20.0
Octadecanoic acid	19.439	23.4	ng	29047100	5	21.416	24863600	20.0
Heptacos-1-ene	21.104	5.0	ng	6268200	5	21.416	24863600	20.0