LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(32-36)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	3	5	10	rVB	87970	89842	2.10%	0.443%
2	5.504	404	411	417	rBV	1249626	1836352	43.02%	9.046%
3	5.557	417	420	430	rVB	33089	70178	1.64%	0.346%
4	7.104	674	683	701	rBV	1104281	1789956	41.93%	8.818%
5	7.934	817	824	831	rBV	256319	404350	9.47%	1.992%
6	9.098	1014	1022	1035	rBV	668712	1115514	26.13%	5.495%
7	10.734	1292	1300	1313	rBV	298398	519942	12.18%	2.561%
8	13.186	1710	1717	1733	rBV	1728741	2601038	60.93%	12.813%
9	14.416	1917	1926	1939	rBV2	27561	98416	2.31%	0.485%
10	14.563	1944	1951	1965	rVB	450784	699900	16.39%	3.448%
11	15.969	2185	2190	2196	rBV	42912	56233	1.32%	0.277%
12	16.045	2196	2203	2224	rBV	1623697	2458118	57.58%	12.109%
13	17.304	2411	2417	2428	rBV	581908	845557	19.81%	4.165%
14	17.427	2432	2438	2444	rVB3	87567	121494	2.85%	0.599%
15	17.957	2523	2528	2536	rVB2	49767	76177	1.78%	0.375%
16	18.186	2563	2567	2573	rBV	77092	104643	2.45%	0.515%
17	19.415	2772	2776	2786	rBV2	39682	57044	1.34%	0.281%
18	19.851	2845	2850	2861	rBV	3548569	4269068	100.00%	21.030%
19	20.592	2972	2976	2979	rBV	68045	78053	1.83%	0.385%
20	21.080	3055	3059	3069	rBV	172234	267400	6.26%	1.317%
21	21.280	3090	3093	3098	rVB	77585	90136	2.11%	0.444%
22	21.374	3104	3109	3116	rBV	881079	1208586	28.31%	5.954%
23	23.792	3513	3520	3536	rVB2	694939	1441442	33.76%	7.101%

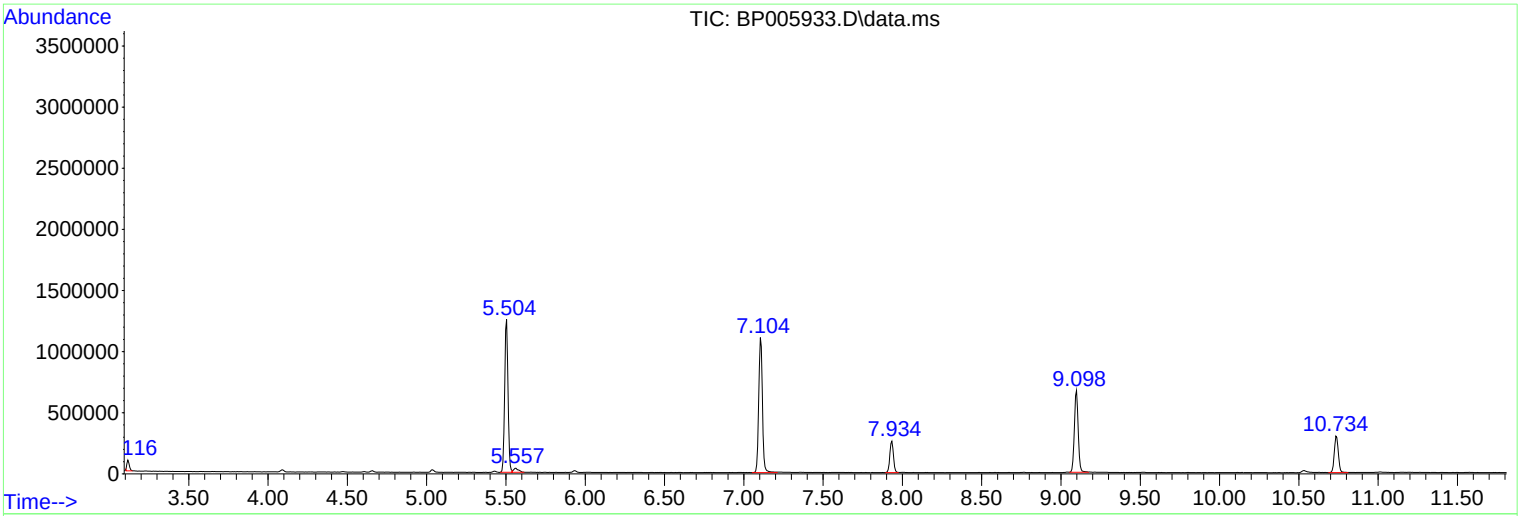
Sum of corrected areas: 20299439

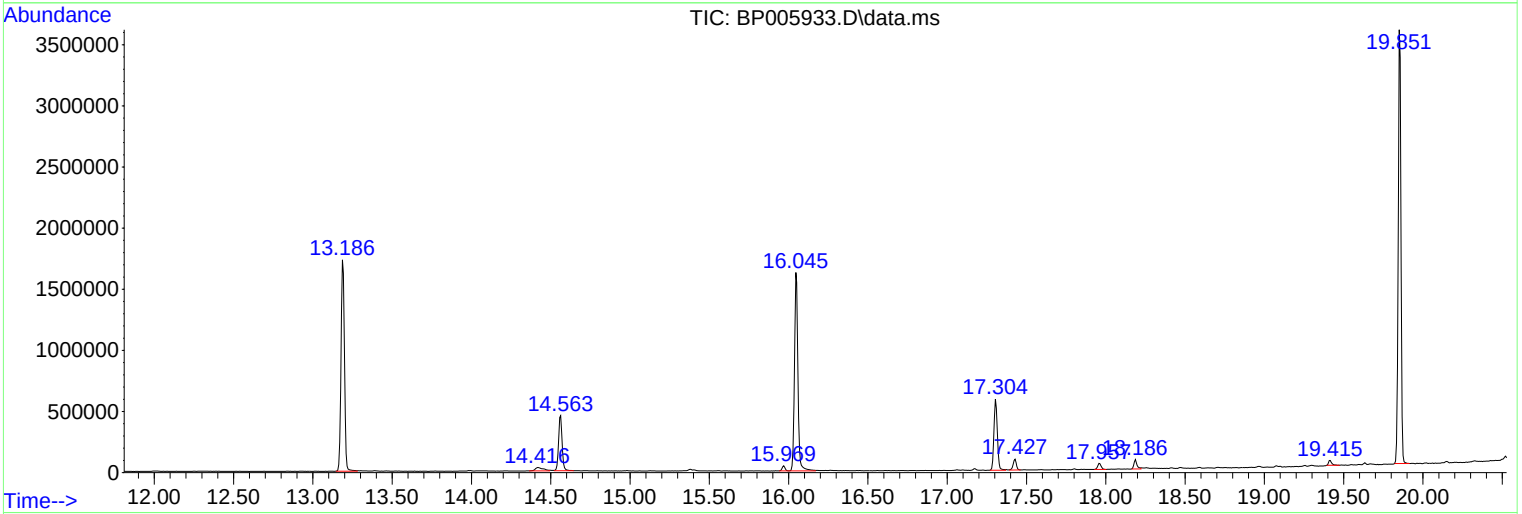
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

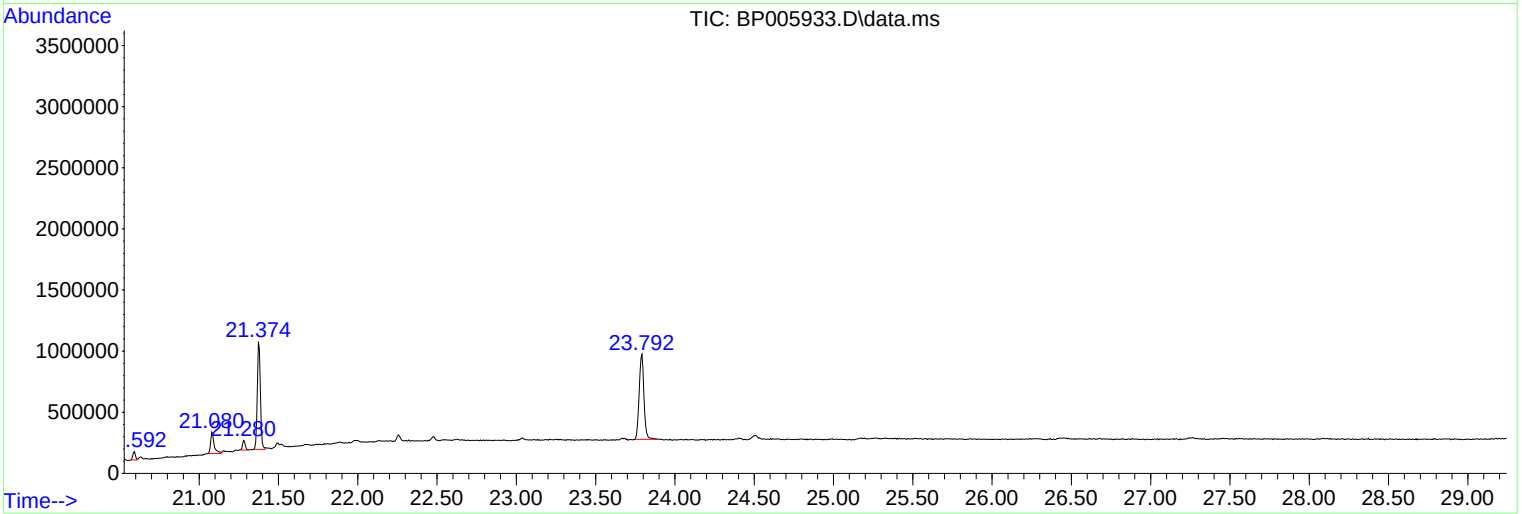
Instrument :
BNA_P
ClientSampleId :
17-B6(32-36)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(32-36)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

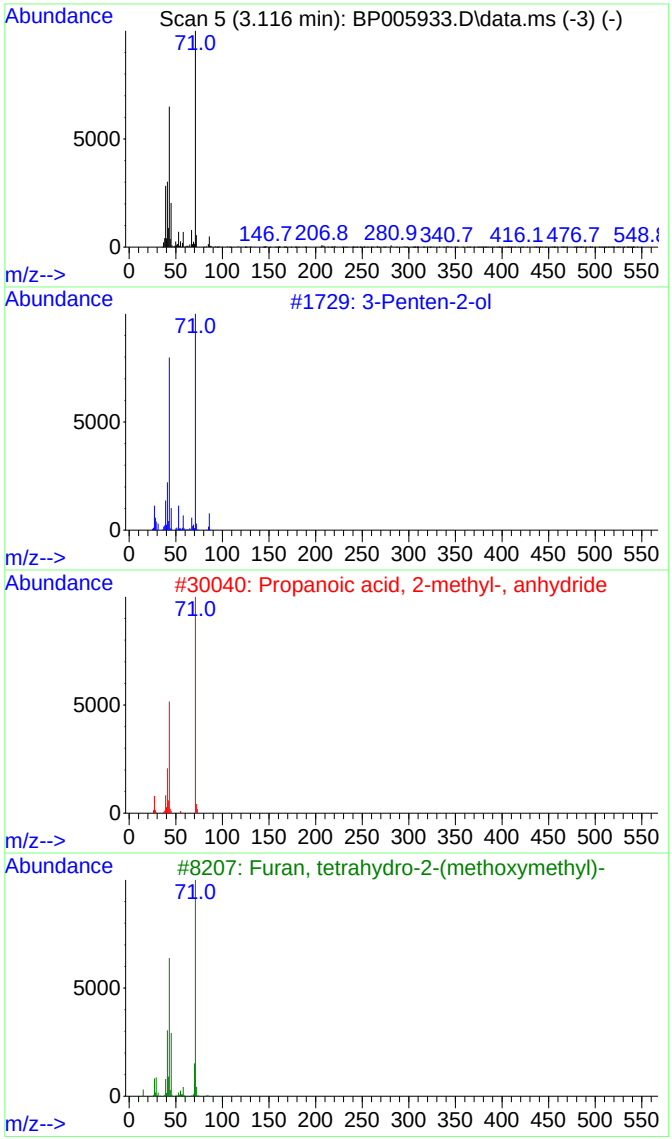
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

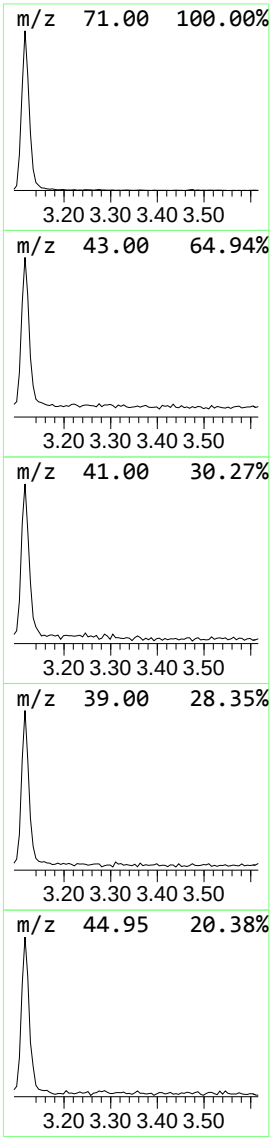
****

Peak Number 1 3-Penten-2-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	4.44 ng	89842	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	59
2	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	53
3	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	50
4	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	50
5	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(32-36)

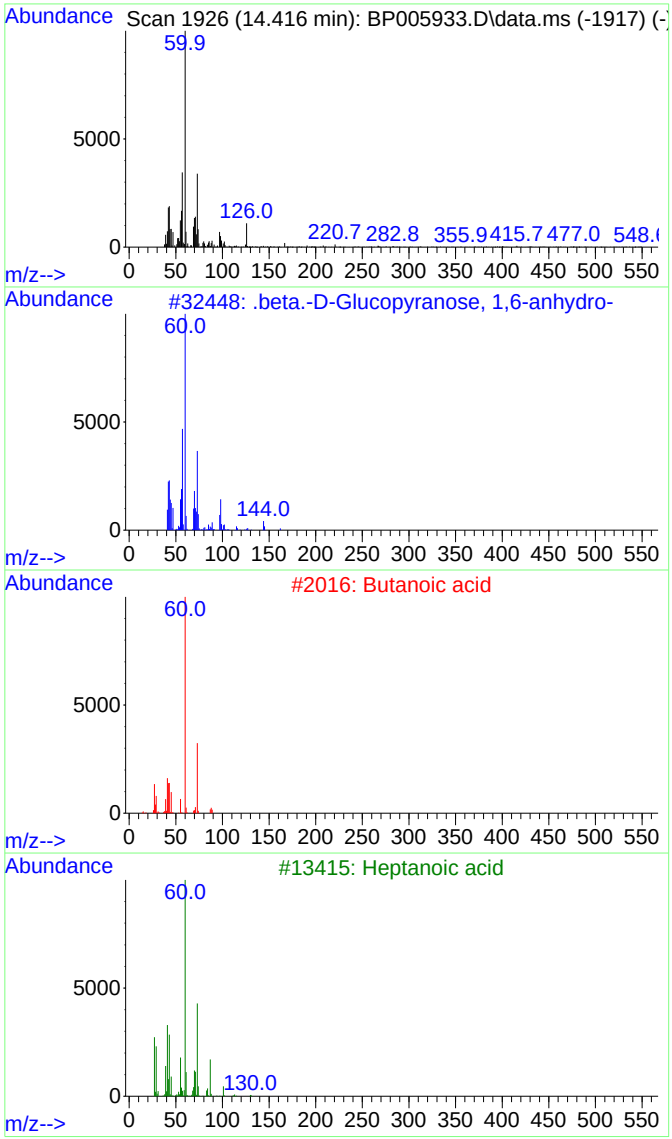
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

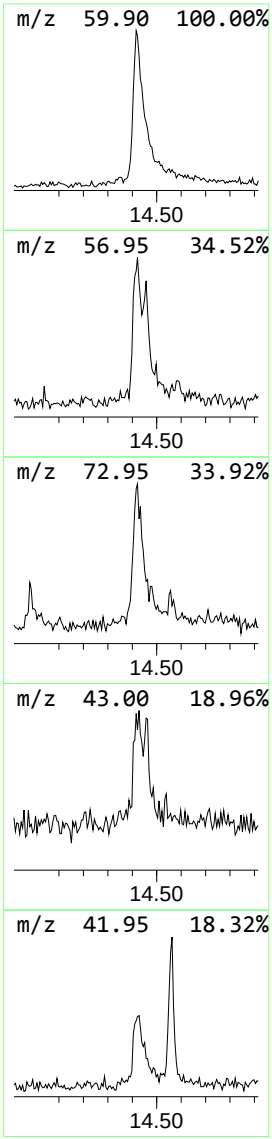
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 .beta.-D-Glucopyranose, 1,6... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	2.81 ng	98416	Acenaphthene-d10	14.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	72
2	Butanoic acid	88	C4H8O2	000107-92-6	64
3	Heptanoic acid	130	C7H14O2	000111-14-8	59
4	Pentanoic acid	102	C5H10O2	000109-52-4	45
5	Hexanoic acid	116	C6H12O2	000142-62-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(32-36)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

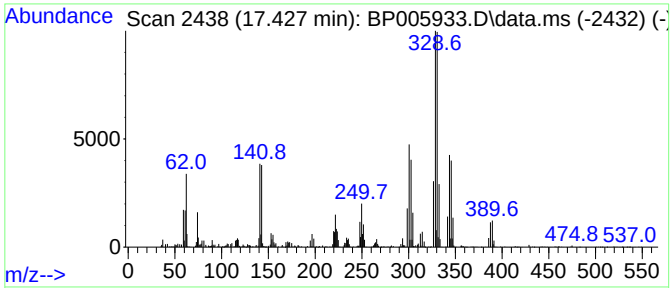
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

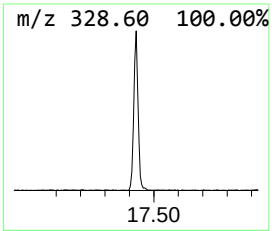
****

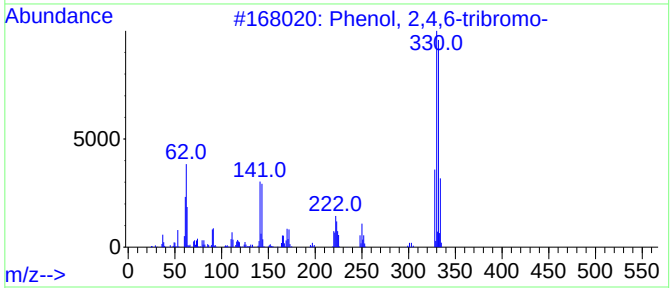
Peak Number 4 unknown17.427 Concentration Rank 4

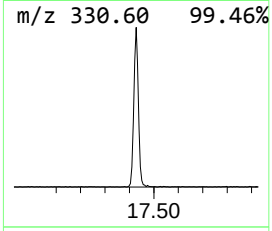
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.427	2.87 ng	121494	Phenanthrene-d10	17.304

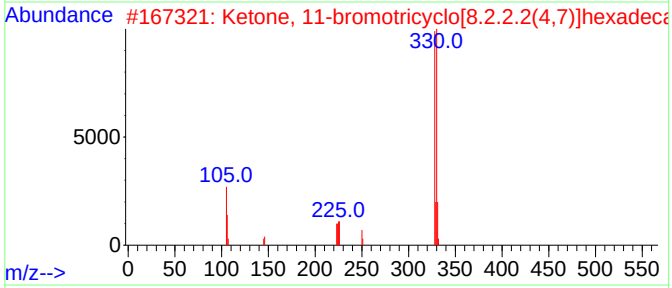
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	30
2	Ketone, 11-bromotricyclo[8.2.2.2...	328	C18H17BrO	018931-44-7	25
3	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	18
4	p-(6-Chloro-4-phenyl-2-quinolyl)...	330	C21H15ClN2	021923-52-4	10
5	6-Chloro-2-(6-methyl-3-pyridyl)-...	330	C21H15ClN2	021911-95-5	10

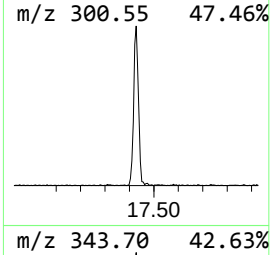


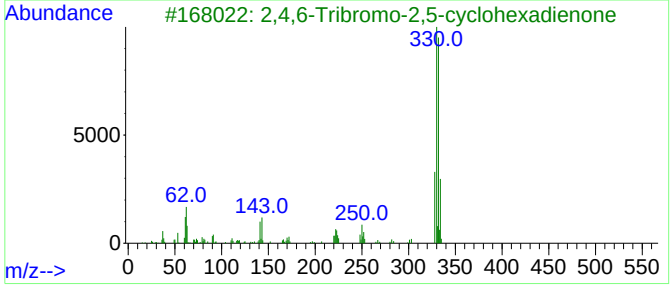


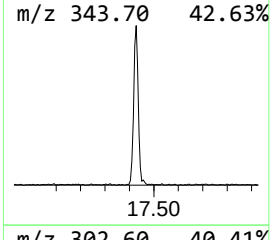


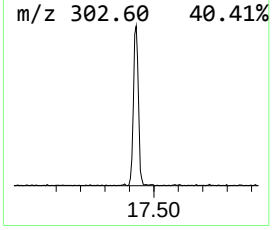












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(32-36)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

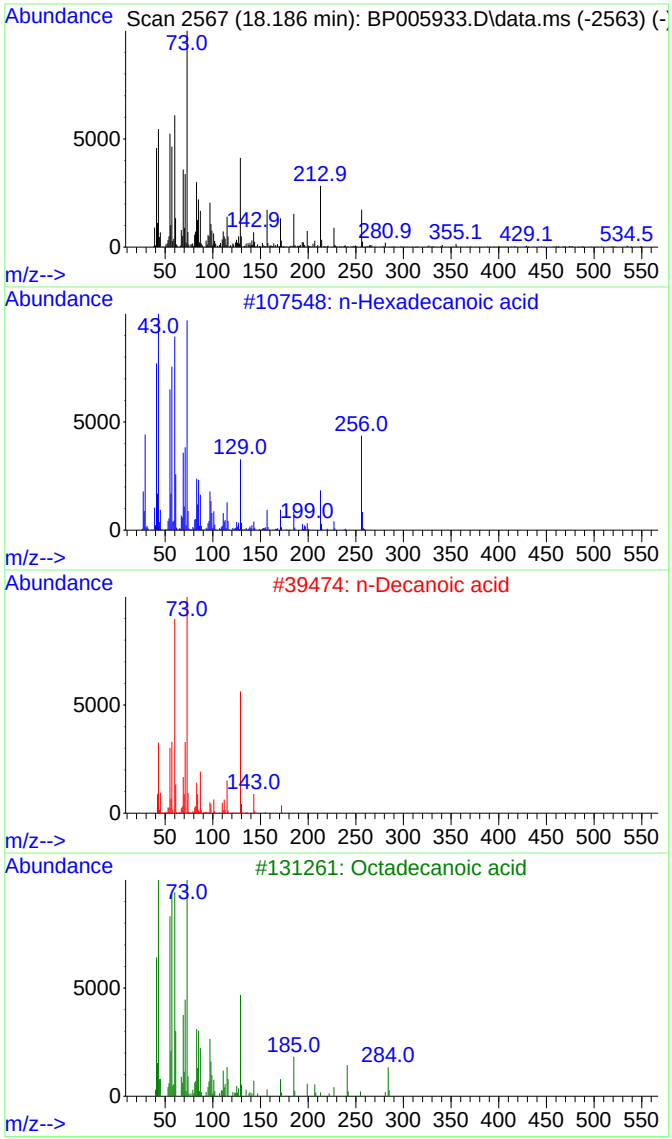
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

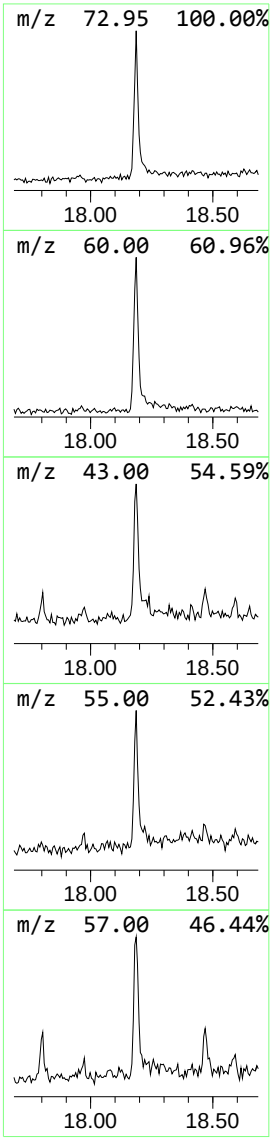
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	2.48 ng	104643	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	n-Decanoic acid	172	C10H20O2	000334-48-5	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
17-B6(32-36)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

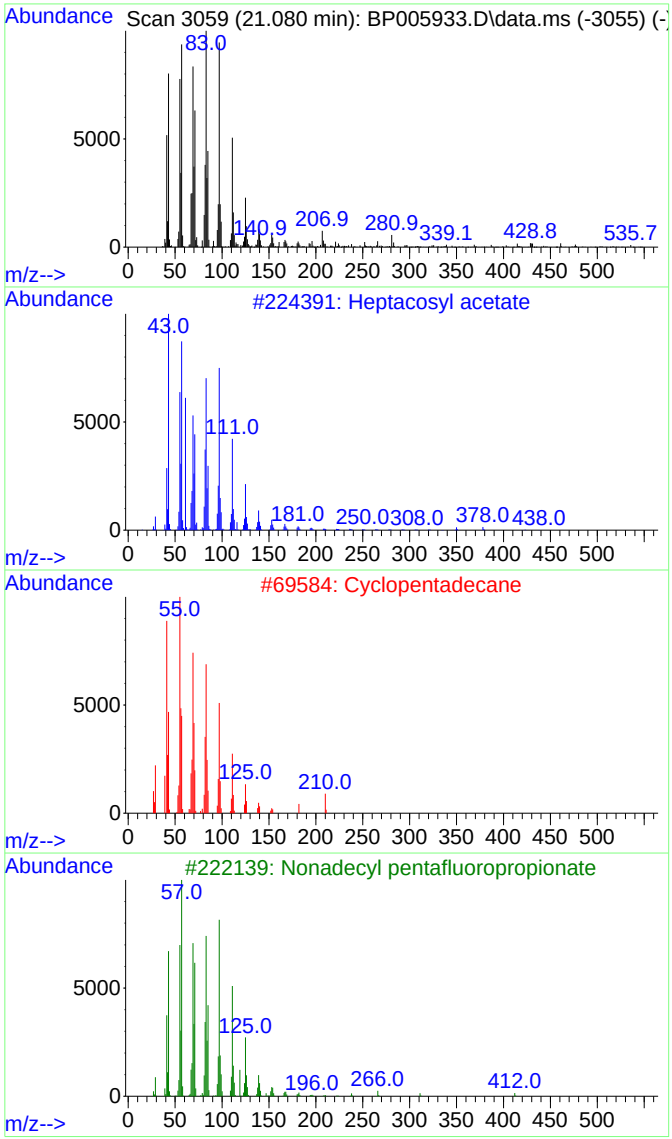
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

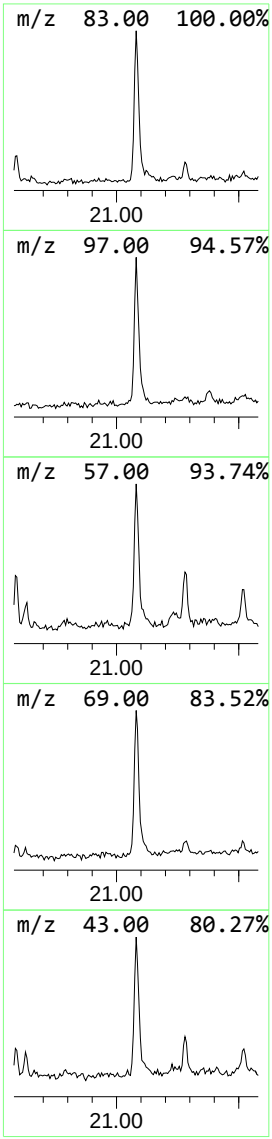
****

Peak Number 6 Heptacosyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	4.43 ng	267400	Chrysene-d12	21.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	95
2	Cyclopentadecane	210	C15H30	000295-48-7	94
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Triacontanol	438	C30H62O	000593-50-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061521\
Data File : BP005933.D
Acq On : 15 Jun 2021 16:37
Operator : CG/JU
Sample : M2672-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 17-B6(32-36)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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
3-Penten-2-ol	3.116	4.4	ng	89842	1	7.934	404350	20.0
.beta.-D-Glucop...	14.416	2.8	ng	98416	3	14.563	699900	20.0
unknown17.427	17.427	2.9	ng	121494	4	17.304	845557	20.0
n-Hexadecanoic ...	18.186	2.5	ng	104643	4	17.304	845557	20.0
Heptacosyl acetate	21.080	4.4	ng	267400	5	21.374	1208590	20.0