LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-30-9.5-10.0-DUP

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-BP042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	358	365	380	rBV	474106	687109	43.23%	8.647%
2	6.822	628	635	650	rBV	427813	694317	43.68%	8.737%
3	7.634	767	773	782	rBV	116173	174946	11.01%	2.202%
4	8.799	963	971	981	rBV	271055	440926	27.74%	5.549%
5	10.422	1238	1247	1259	rBV	119824	209154	13.16%	2.632%
6	12.916	1663	1671	1682	rBV	546226	810724	51.01%	10.202%
7	13.769	1811	1816	1824	rVB2	16150	25963	1.63%	0.327%
8	14.187	1876	1887	1897	rBV7	8202	28764	1.81%	0.362%
9	14.304	1900	1907	1916	rVB	177450	267352	16.82%	3.364%
10	15.704	2135	2145	2151	rBV2	19390	37520	2.36%	0.472%
11	15.810	2156	2163	2175	rBV	573645	818181	51.48%	10.296%
12	17.069	2369	2377	2388	rBV	244329	360544	22.68%	4.537%
13	17.192	2392	2398	2403	rVB10	10692	17998	1.13%	0.226%
14	17.975	2526	2531	2539	rBV	134865	194624	12.24%	2.449%
15	18.039	2539	2542	2549	rVB4	10795	19732	1.24%	0.248%
16	19.216	2738	2742	2748	rBV	55420	72599	4.57%	0.914%
17	19.651	2810	2816	2823	rBV	1403120	1589436	100.00%	20.002%
18	20.433	2946	2949	2953	rVB5	19324	23606	1.49%	0.297%
19	20.857	3017	3021	3023	rBV2	24715	35828	2.25%	0.451%
20	20.892	3023	3027	3035	rVV2	110056	179885	11.32%	2.264%
21	20.963	3035	3039	3048	rVV	72542	104464	6.57%	1.315%
22	21.174	3070	3075	3080	rBV	418841	542860	34.15%	6.831%
23	22.351	3271	3275	3279	rVB	46776	65531	4.12%	0.825%
24	23.433	3453	3459	3467	rBV2	290124	544515	34.26%	6.852%

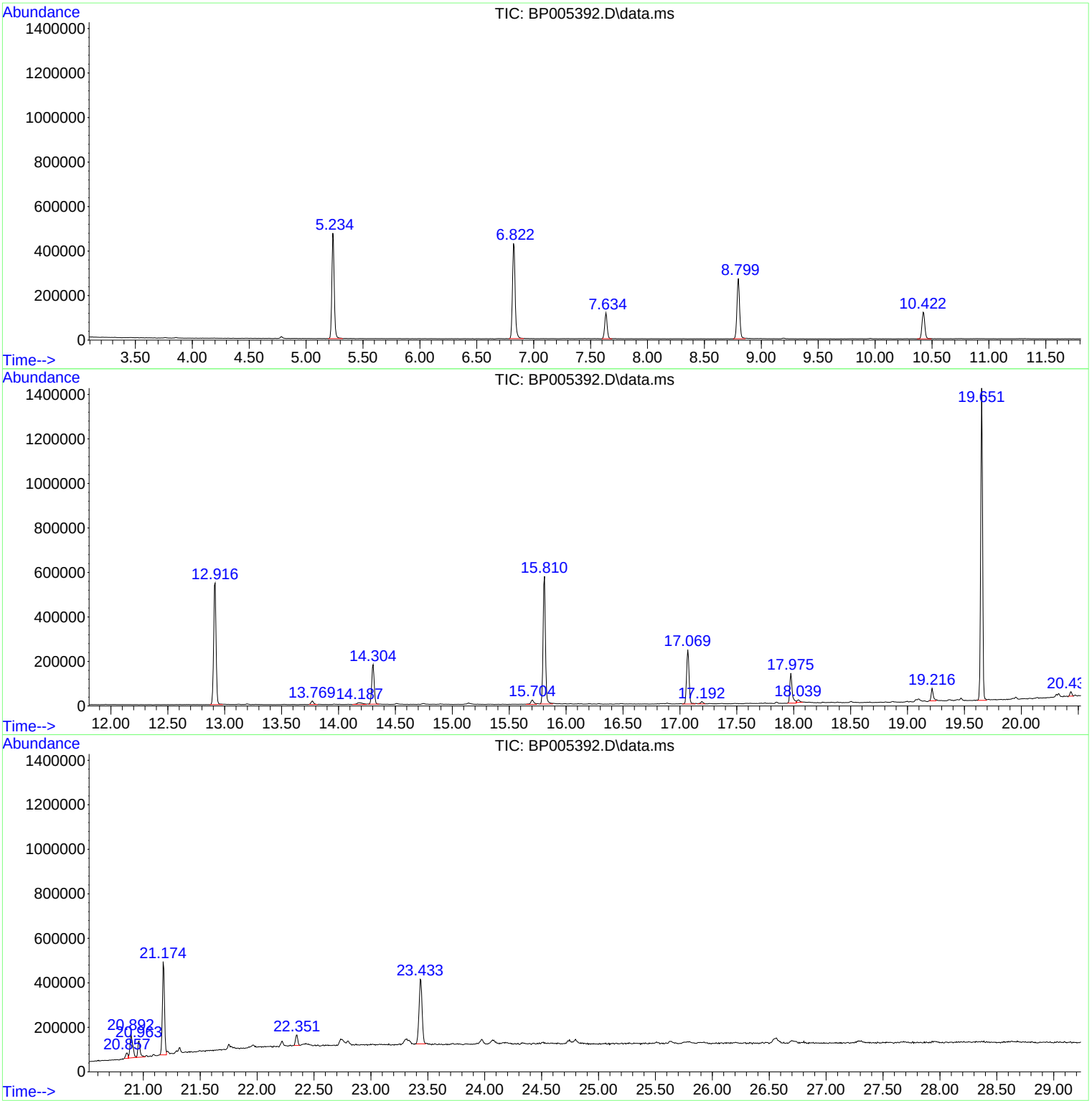
Sum of corrected areas: 7946578

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

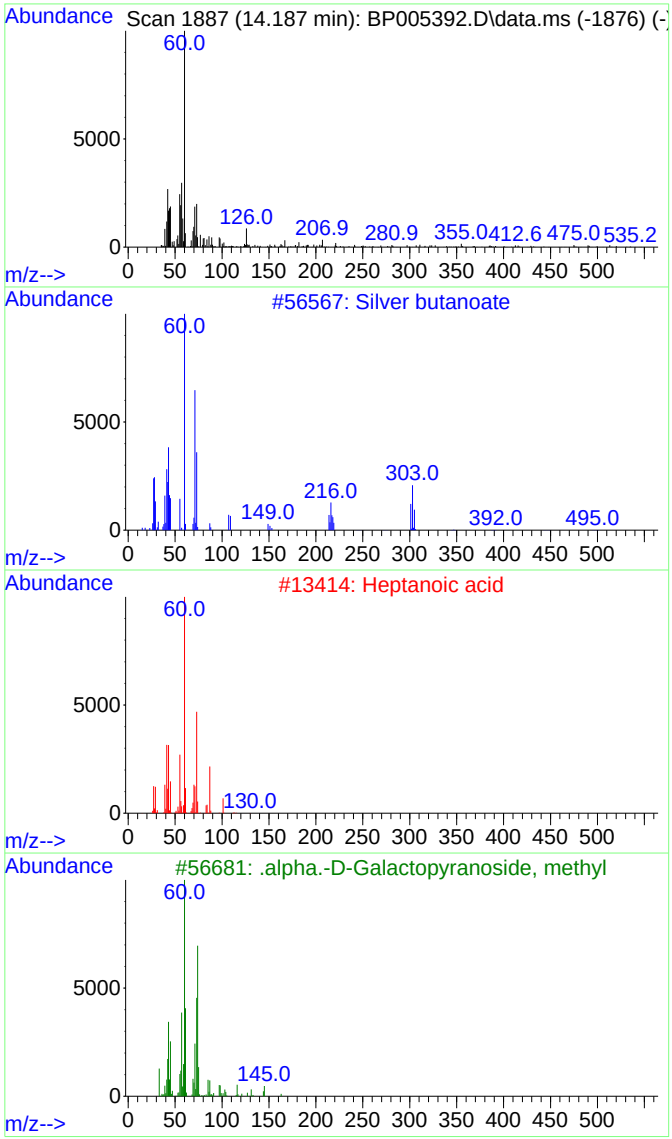
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

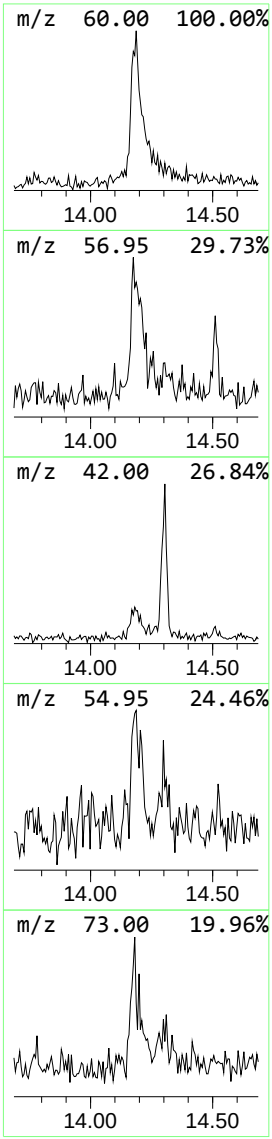
****

Peak Number 1 unknown14.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.187	2.15 ng	28764	Acenaphthene-d10	14.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silver butanoate	194	C4H7AgO2	005076-24-4	40
2	Heptanoic acid	130	C7H14O2	000111-14-8	37
3	.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	37
4	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	35
5	.alpha.-L-Galactopyranoside, met...	178	C7H14O5	014687-15-1	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

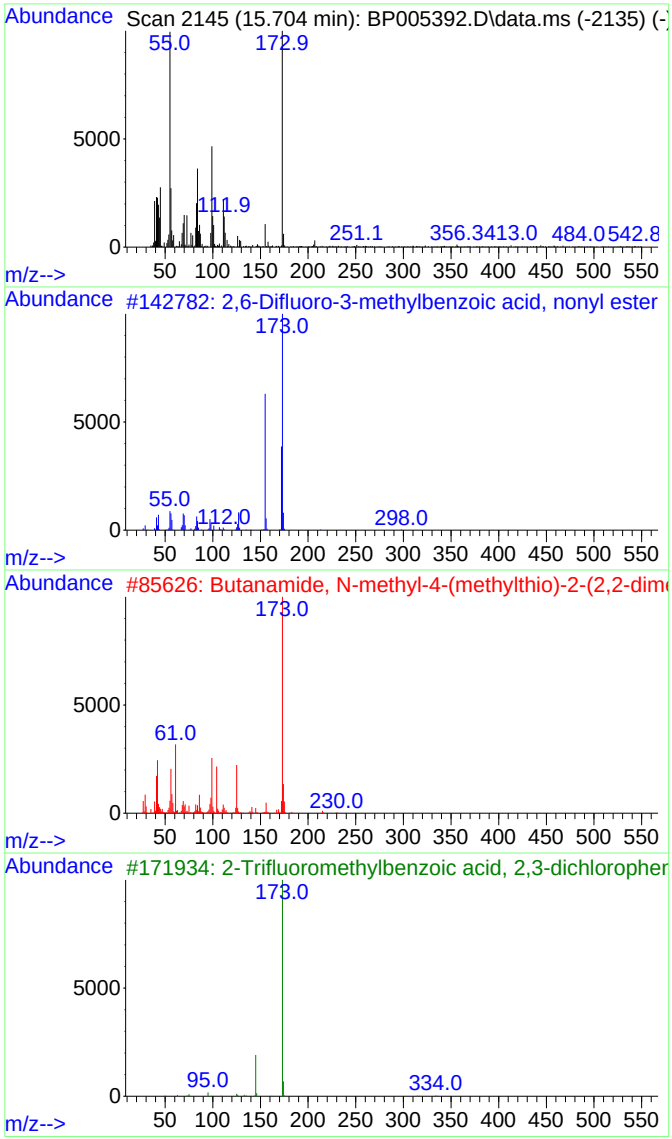
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

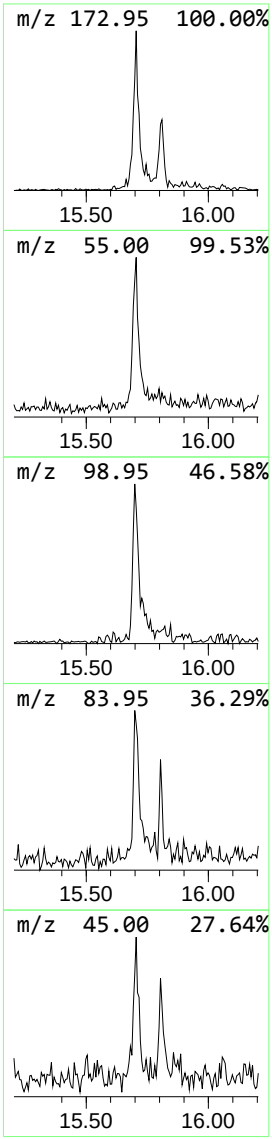
****

Peak Number 2 unknown15.70 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.704	2.08 ng	37520	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Difluoro-3-methylbenzoic aci...	298	C17H24F2O2	1000338-84-6	38
2	Butanamide, N-methyl-4-(methylth...	230	C11H22N2OS	097443-86-2	38
3	2-Trifluoromethylbenzoic acid, 2...	334	C14H7Cl2F3O2	1000331-16-8	35
4	4-Trifluoromethylbenzoic acid. 4...	414	C24H37F3O2	1000283-03-4	25
5	1-Dimethylthexylsilyloxyheptane	258	C15H34OSi	1000281-97-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

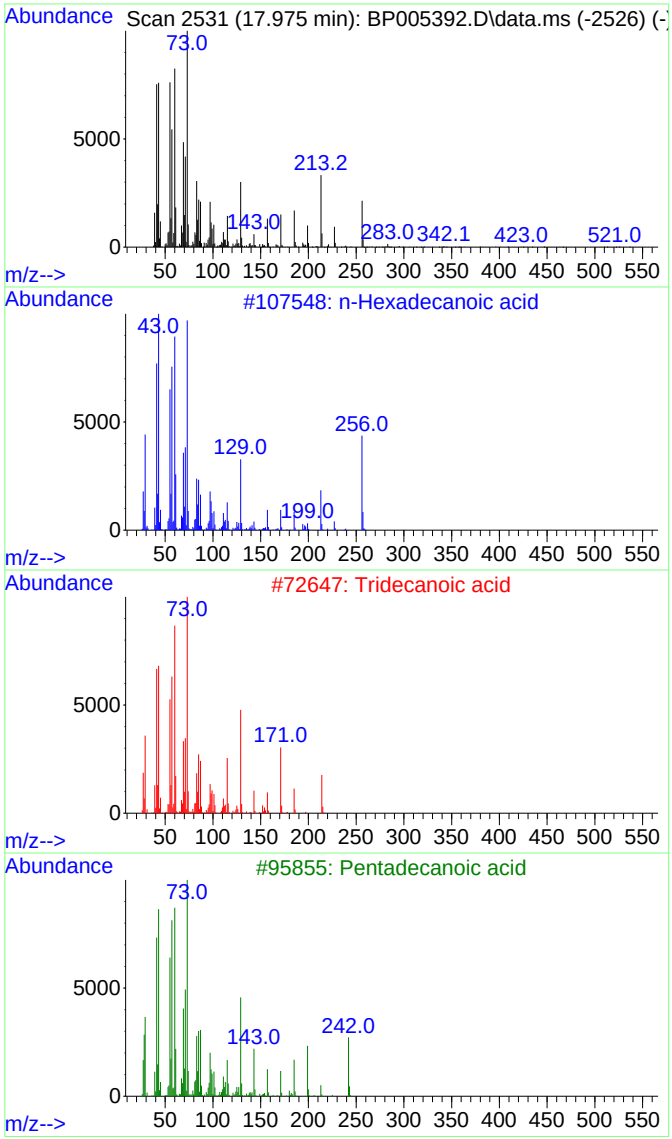
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

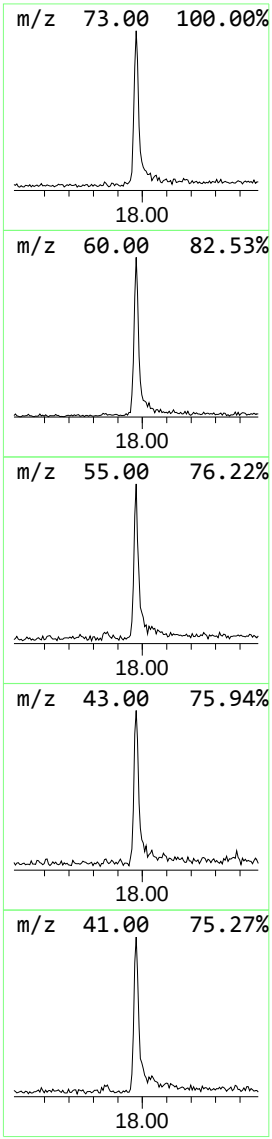
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.975	10.80 ng	194624	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
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	60
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

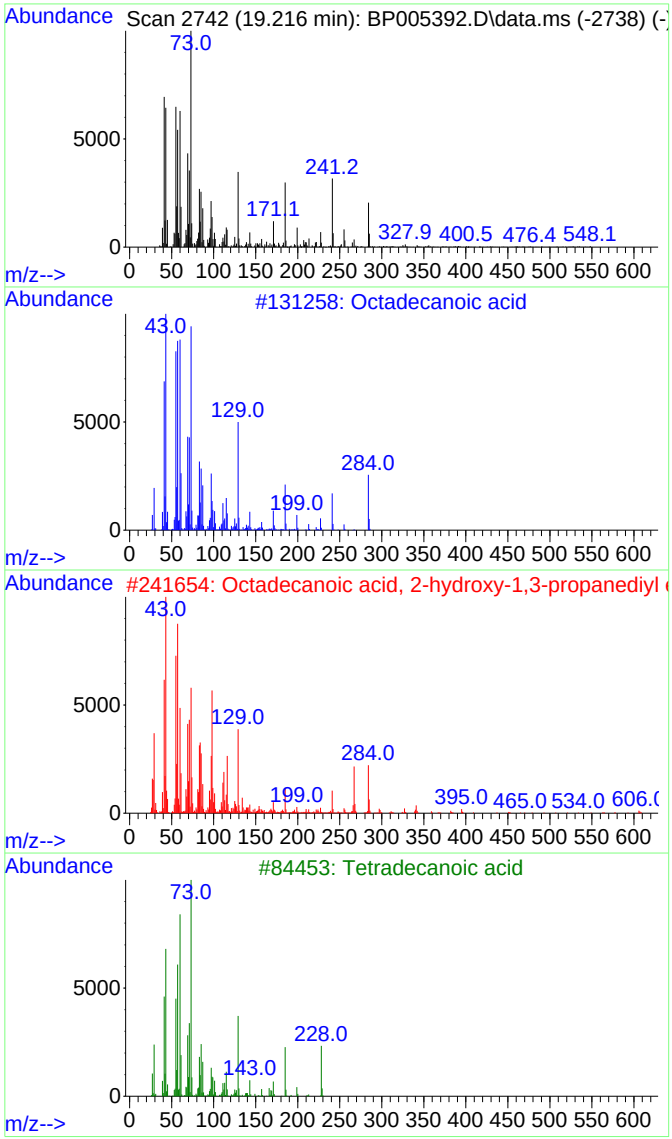
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

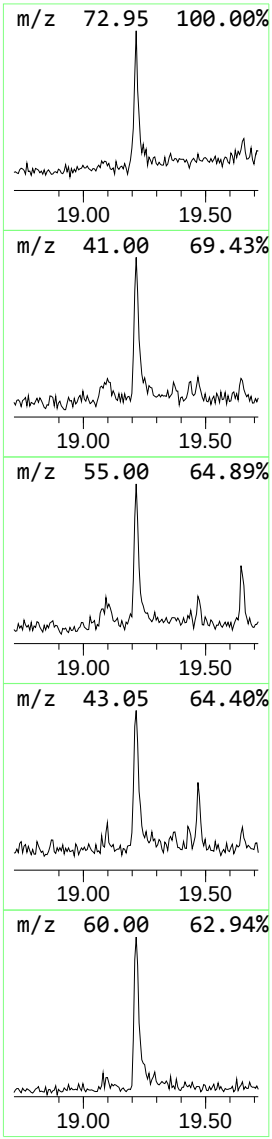
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.216	2.67 ng	72599	Chrysene-d12	21.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Octadecanoic acid, 2-hydroxy-1,3...	625	C39H76O5	000504-40-5	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

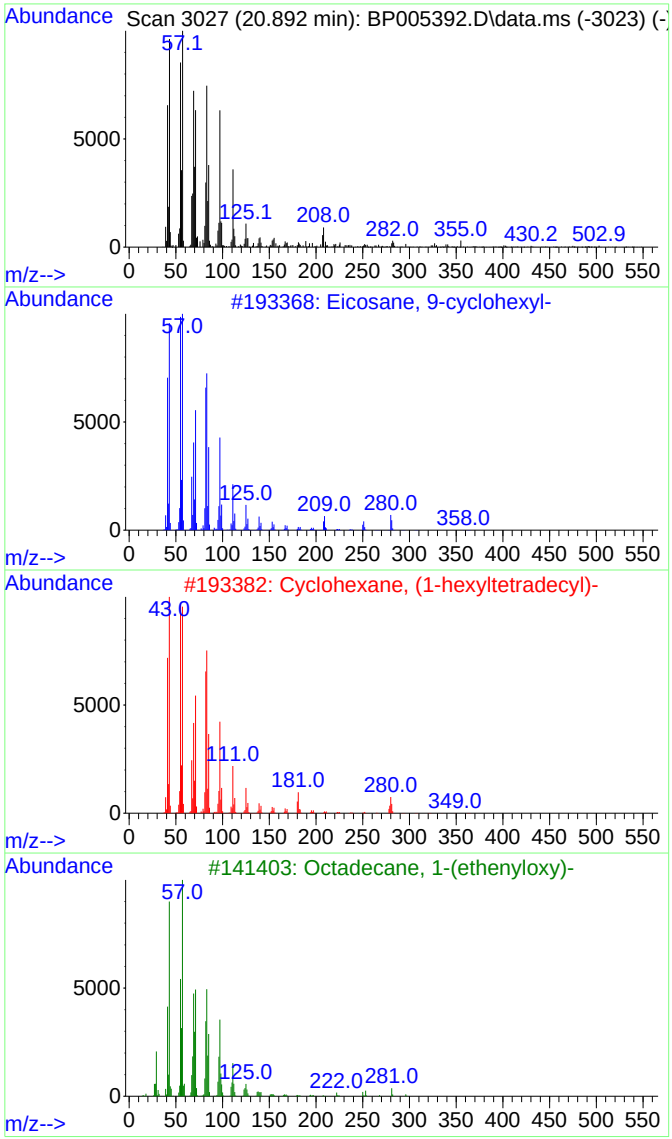
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

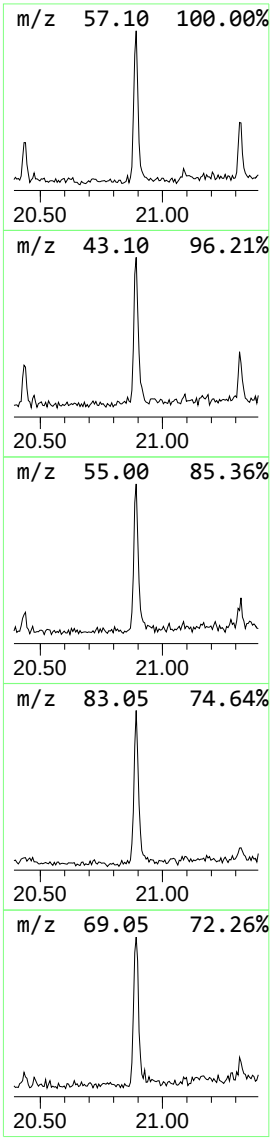
****

Peak Number 5 Eicosane, 9-cyclohexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	6.63 ng	179885	Chrysene-d12	21.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 9-cyclohexyl-	364	C26H52	004443-61-2	90
2	Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	90
3	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	90
4	Cyclooctacosane	392	C28H56	000297-24-5	90
5	1-Triacontanol	438	C30H62O	000593-50-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0-DUP

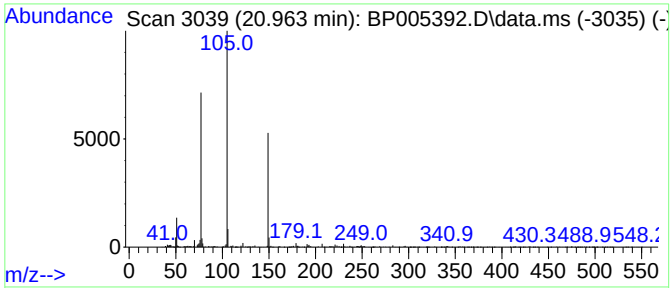
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

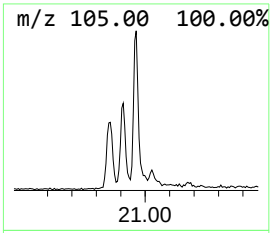
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

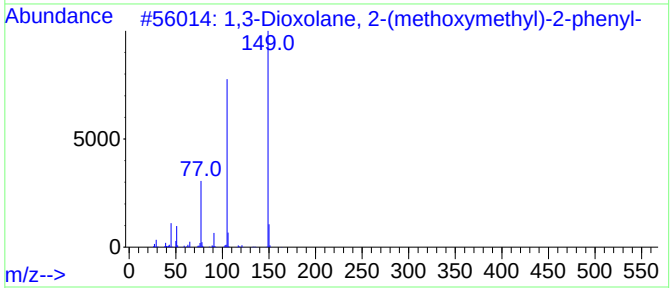
****
Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 3

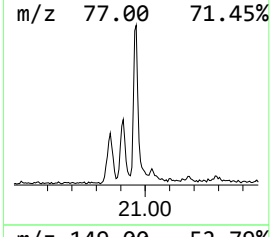
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	3.85 ng	104464	Chrysene-d12	21.174

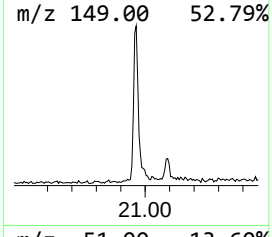
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
2	Pentanediamide, N,N'-di-benzoyloxy-	370	C19H18N2O6	1000253-26-3	38
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38
4	Pyrazine-2-carboxylic acid, 4,5-...	301	C15H15N3O4	1000259-49-5	38
5	Benzamide, N-(3-ethynylphenyl)-	221	C15H11NO	208943-24-2	38

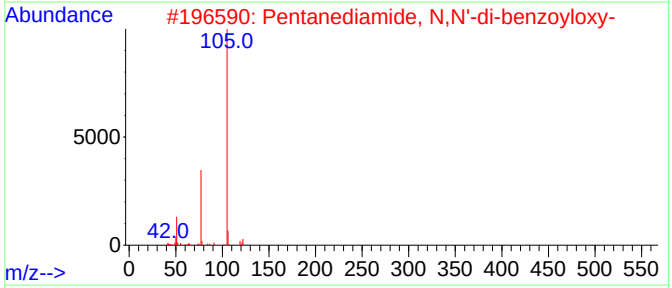


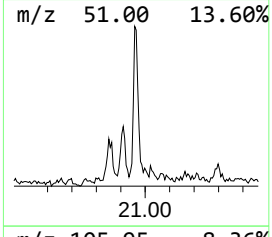


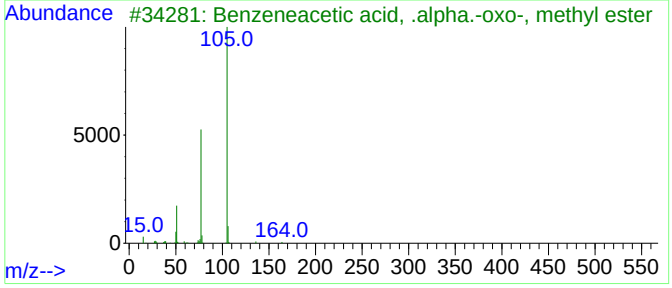


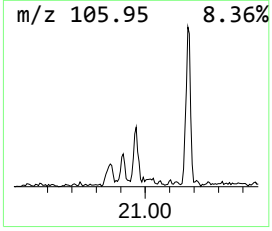












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

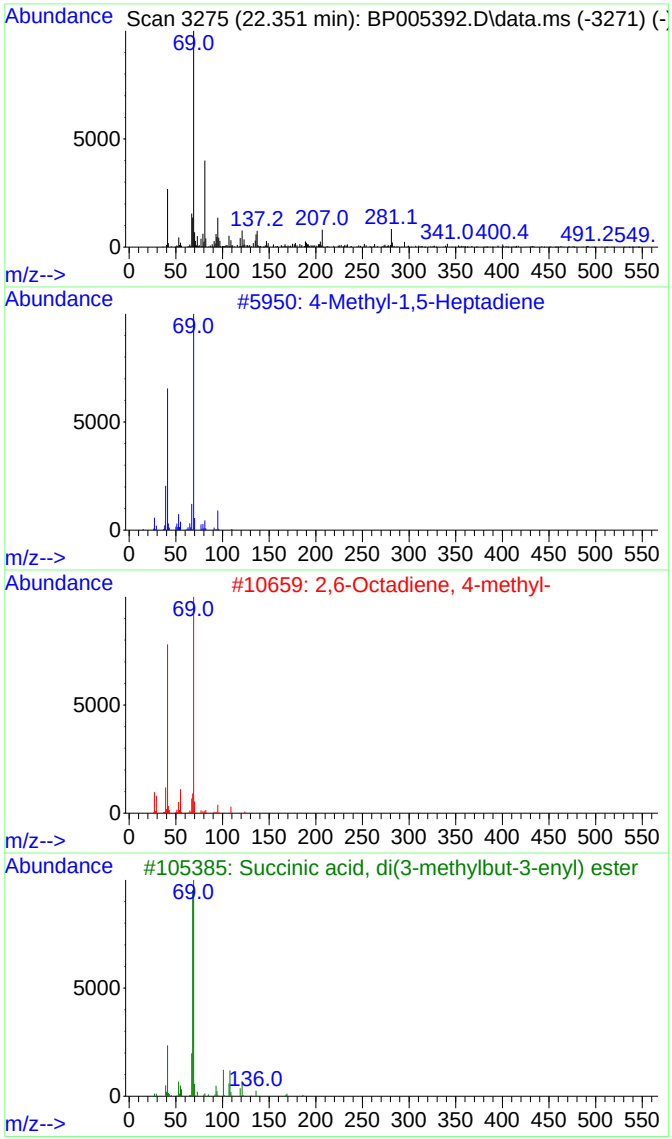
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

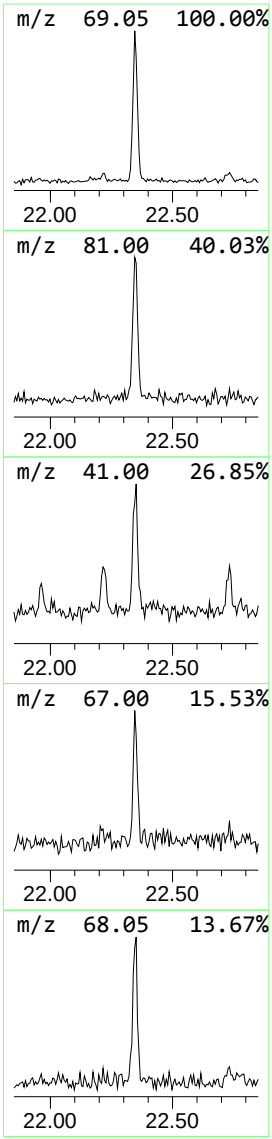
****

Peak Number 7 4-Methyl-1,5-Heptadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.351	2.41 ng	65531	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64
2	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	59
3	Succinic acid, di(3-methylbut-3-...	254	C14H22O4	1000353-45-6	53
4	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	53
5	Methacrylic acid, 3-ethylphenyl ...	190	C12H14O2	1000360-69-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005392.D
Acq On : 23 Apr 2021 14:17
Operator : CG/JU
Sample : M2107-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-30-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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
unknown14.18	14.187	2.1	ng	28764	3	14.304	267352	20.0
unknown15.70	15.704	2.1	ng	37520	4	17.069	360544	20.0
n-Hexadecanoic ...	17.975	10.8	ng	194624	4	17.069	360544	20.0
Octadecanoic acid	19.216	2.7	ng	72599	5	21.174	542860	20.0
Eicosane, 9-cyc...	20.892	6.6	ng	179885	5	21.174	542860	20.0
1,3-Dioxolane, ...	20.963	3.9	ng	104464	5	21.174	542860	20.0
4-Methyl-1,5-He...	22.351	2.4	ng	65531	6	23.433	544515	20.0