LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008140.D
Acq On : 29 Nov 2021 14:16
Operator : CG/JU
Sample : M4844-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K-1

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008140.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	324	330	340	rBV	199556	276776	5.71%	1.093%
2	5.393	402	409	418	rBV	1565381	2260568	46.62%	8.927%
3	6.987	671	680	693	rBV	1425016	2394719	49.39%	9.457%
4	7.805	810	819	827	rBV	330684	520847	10.74%	2.057%
5	8.963	1008	1016	1027	rBV	928953	1528940	31.53%	6.038%
6	10.393	1252	1259	1278	rBV	119930	244695	5.05%	0.966%
7	10.599	1286	1294	1303	rBV	410670	696390	14.36%	2.750%
8	13.069	1707	1714	1727	rBV	2192148	3247414	66.97%	12.824%
9	14.445	1940	1948	1955	rBV	606658	916436	18.90%	3.619%
10	15.945	2196	2203	2212	rBV	1809081	2627467	54.19%	10.376%
11	17.204	2411	2417	2422	rBV	776072	1124345	23.19%	4.440%
12	17.251	2422	2425	2430	rVB	65049	91228	1.88%	0.360%
13	18.110	2563	2571	2579	rBV2	209057	317250	6.54%	1.253%
14	19.228	2755	2761	2768	rBV	201605	295305	6.09%	1.166%
15	19.345	2777	2781	2790	rBV2	149962	222012	4.58%	0.877%
16	19.575	2816	2820	2830	rVB	167713	253904	5.24%	1.003%
17	19.780	2849	2855	2860	rBV	3745412	4848706	100.00%	19.148%
18	20.527	2979	2982	2986	rBV	142541	169678	3.50%	0.670%
19	20.869	3037	3040	3044	rBV2	52404	58300	1.20%	0.230%
20	21.027	3063	3067	3073	rVB2	213907	289109	5.96%	1.142%
21	21.086	3075	3077	3083	rVB2	64986	82150	1.69%	0.324%
22	21.304	3109	3114	3119	rBV	1047350	1508062	31.10%	5.956%
23	23.698	3515	3521	3529	rBV2	670699	1347768	27.80%	5.323%

Sum of corrected areas: 25322069

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
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Instrument :
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ClientSampleId :
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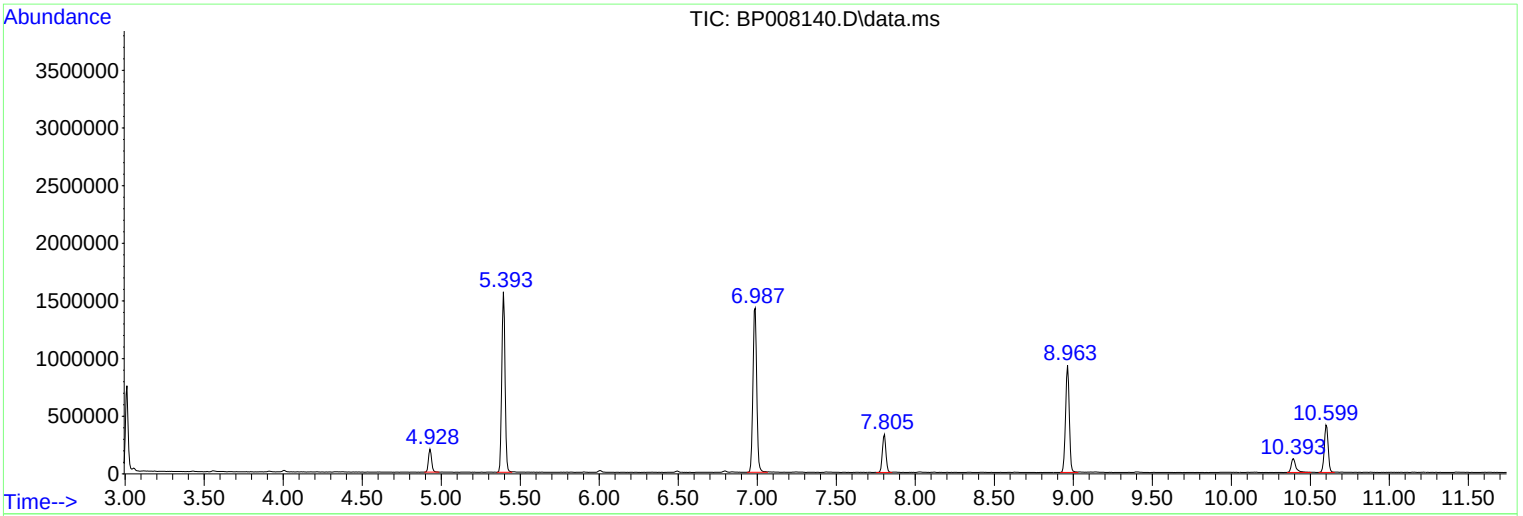
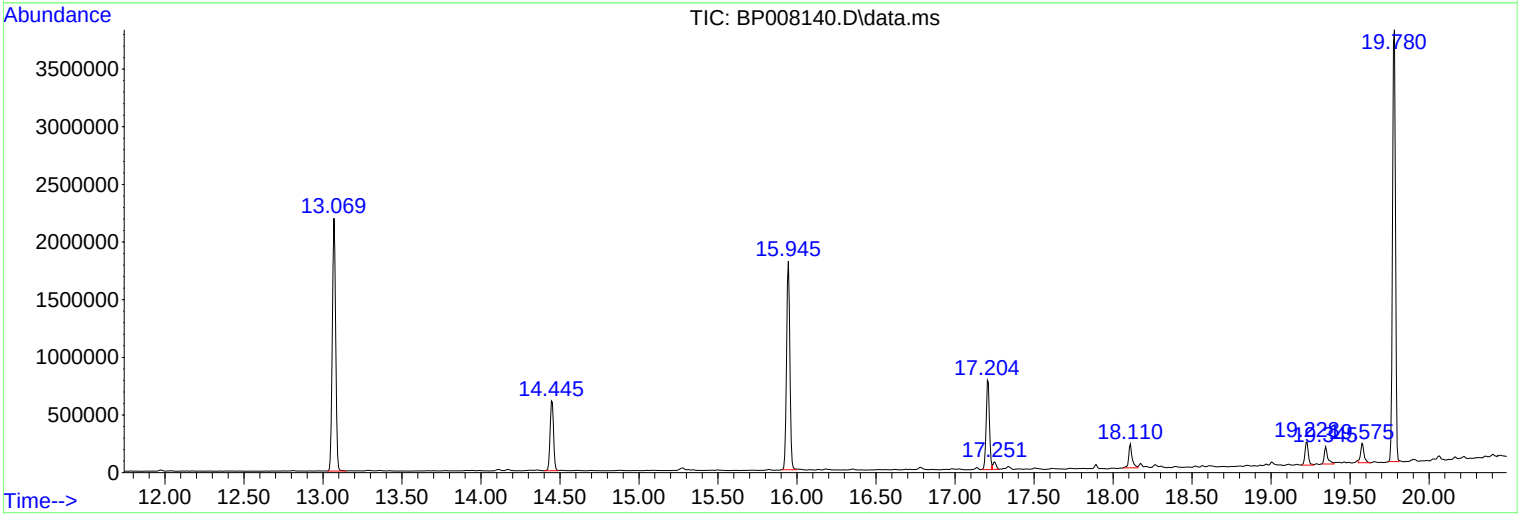
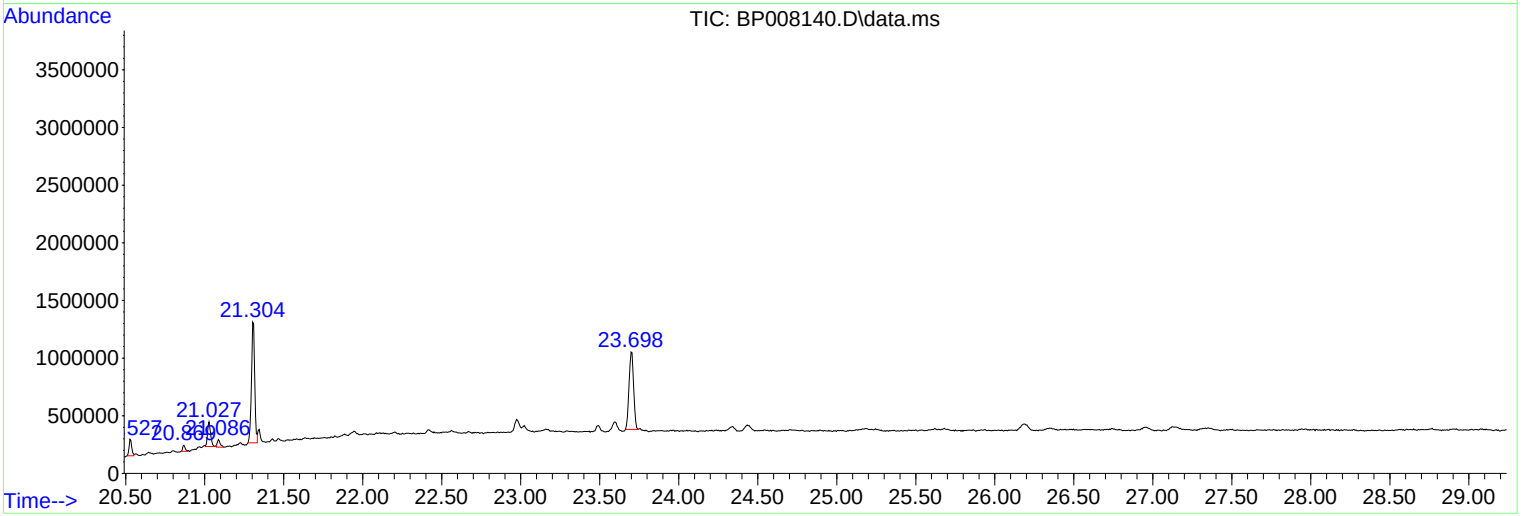
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BP008140.D
Acq On : 29 Nov 2021 14:16
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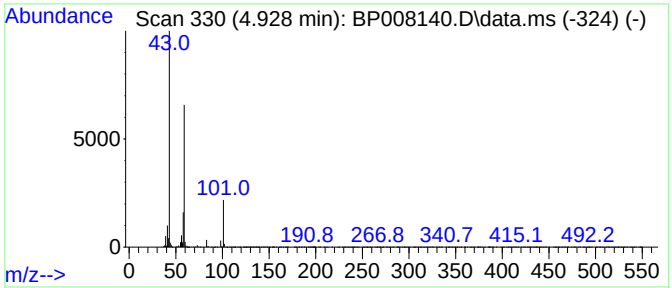
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

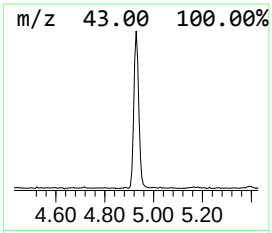
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

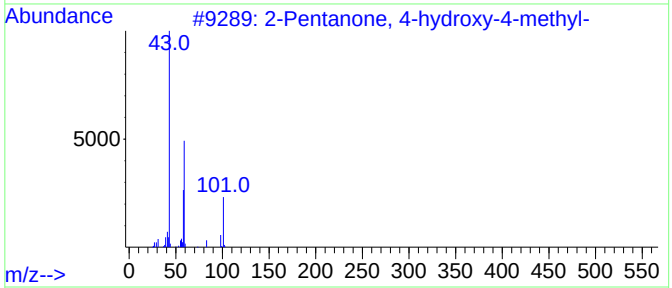
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

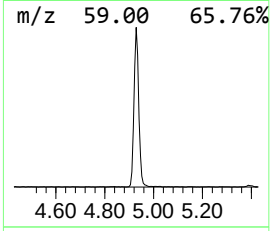
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	10.63 ng	276776	1,4-Dichlorobenzene-d4	7.805

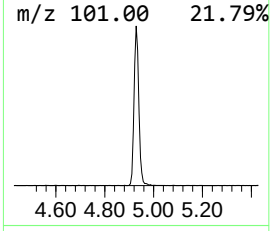
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Guanidine	59	CH5N3	000113-00-8	9

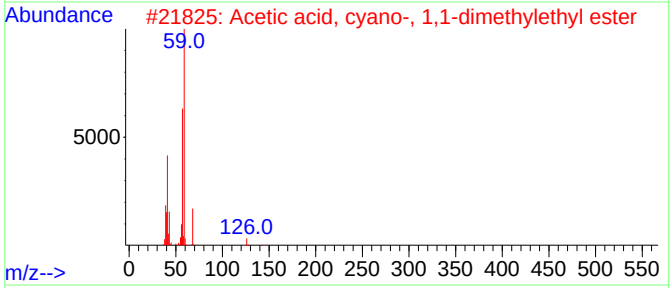


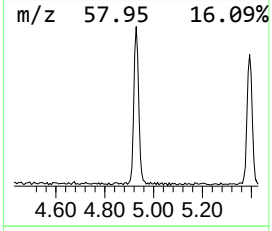


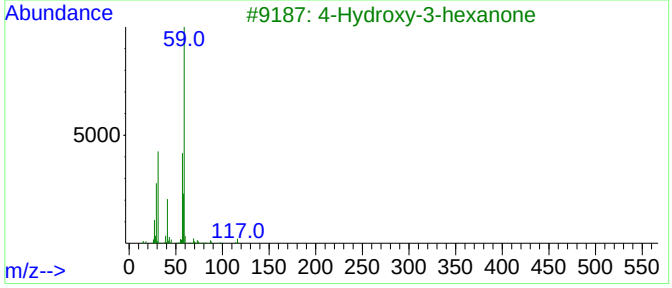


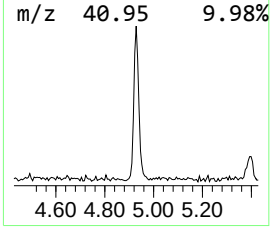












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008140.D
Acq On : 29 Nov 2021 14:16
Operator : CG/JU
Sample : M4844-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

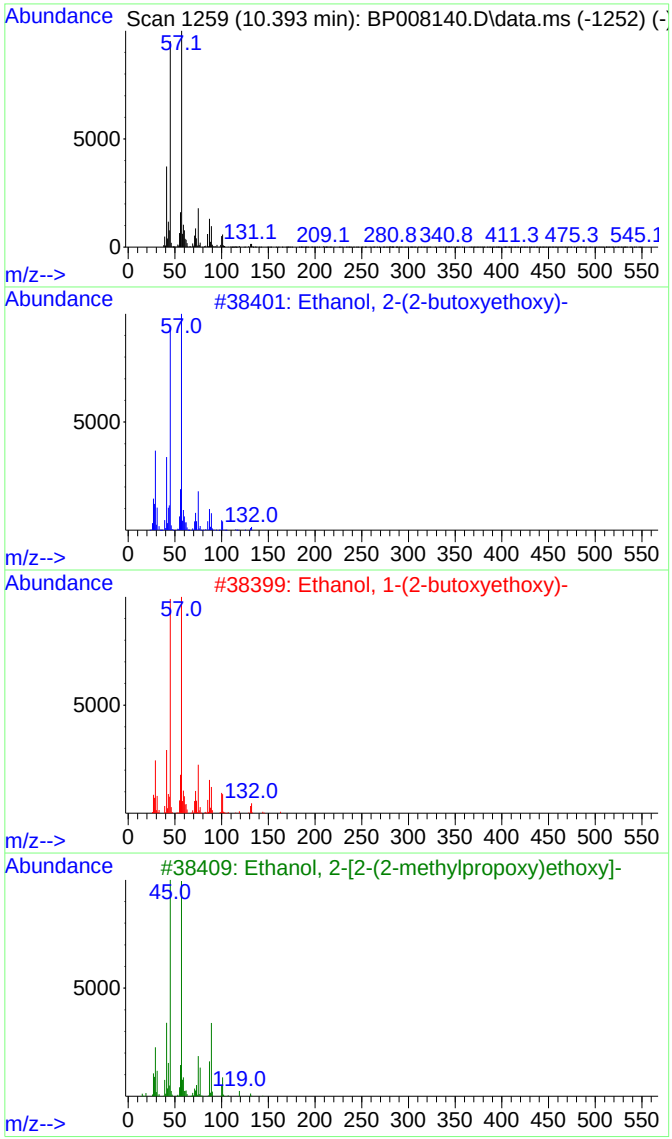
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

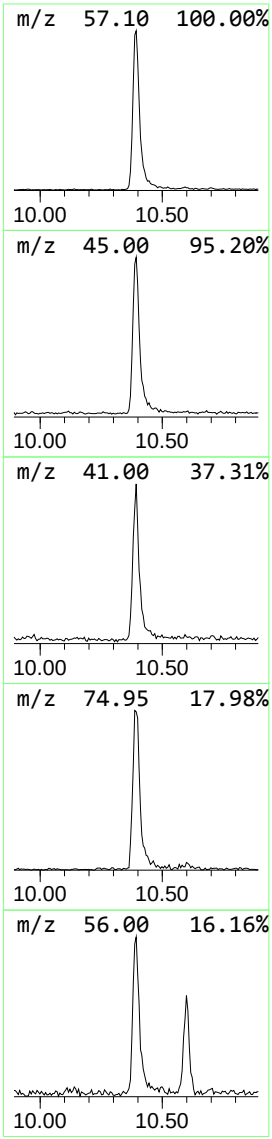
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.393	7.03 ng	244695	Naphthalene-d8	10.599

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Instrument :
BNA_P
ClientSampleId :
K-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

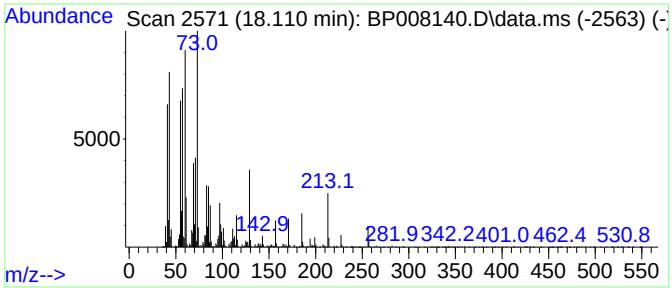
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

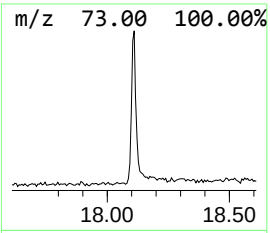
****

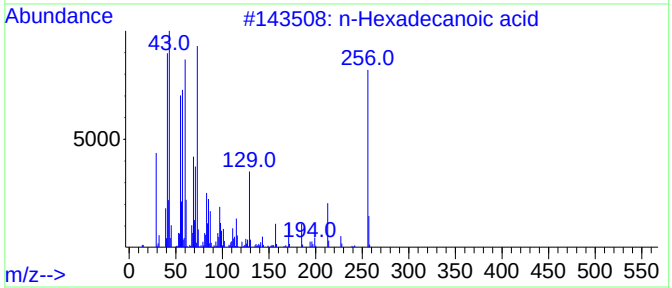
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

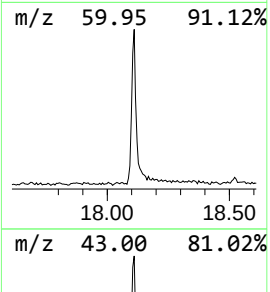
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.110	5.64 ng	317250	Phenanthrene-d10	17.204

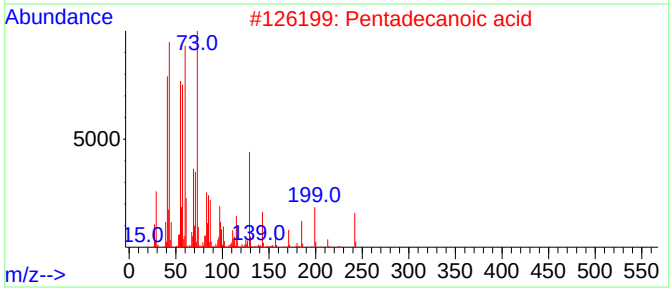
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64

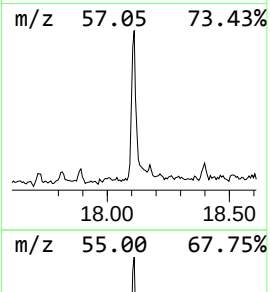


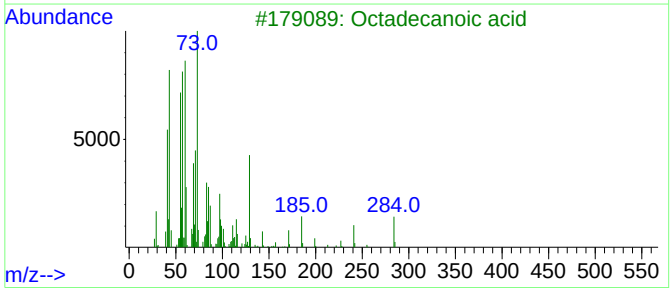












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008140.D
Acq On : 29 Nov 2021 14:16
Operator : CG/JU
Sample : M4844-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

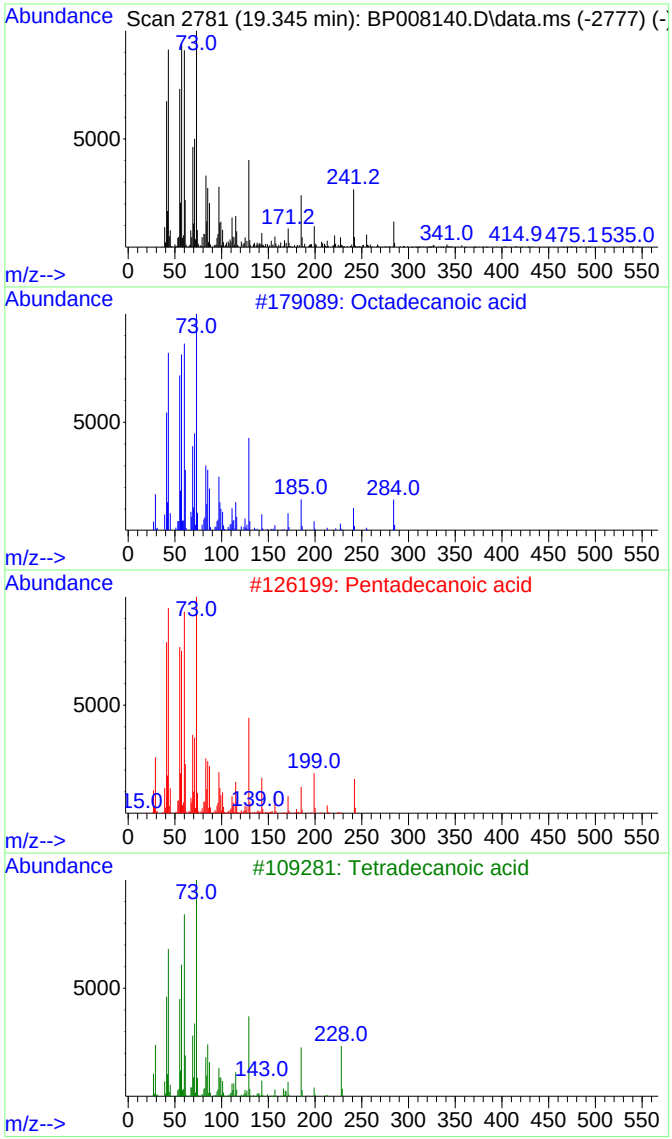
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

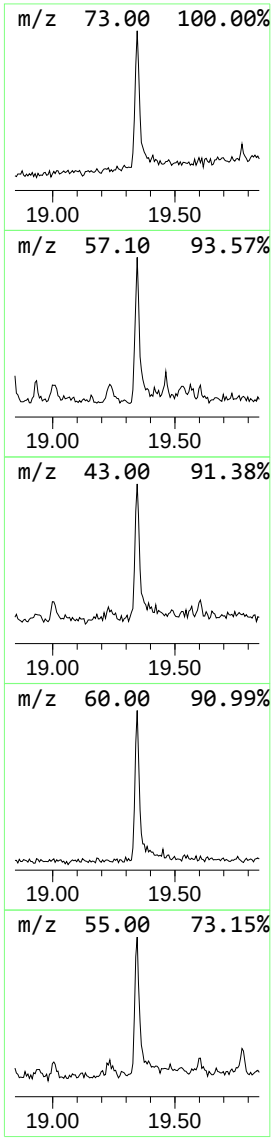
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	2.94 ng	222012	Chrysene-d12	21.304

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Operator : CG/JU
Sample : M4844-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

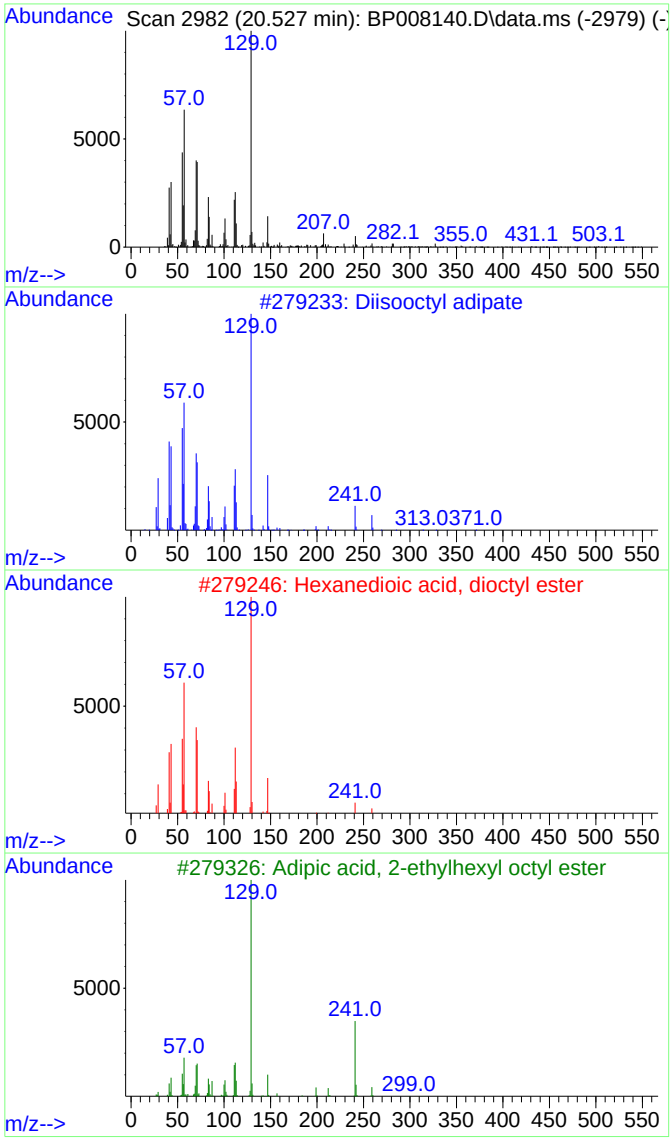
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

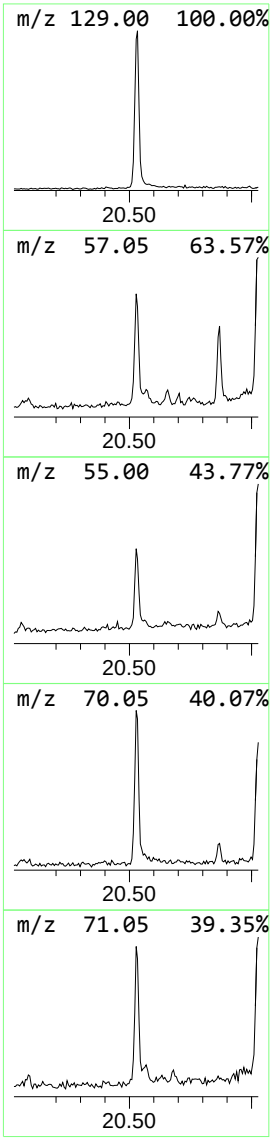
****

Peak Number 6 Diisooctyl adipate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.528	2.25 ng	169678	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisooctyl adipate	370	C22H42O4	001330-86-5	91
2	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
3	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
4	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	68
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	59





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

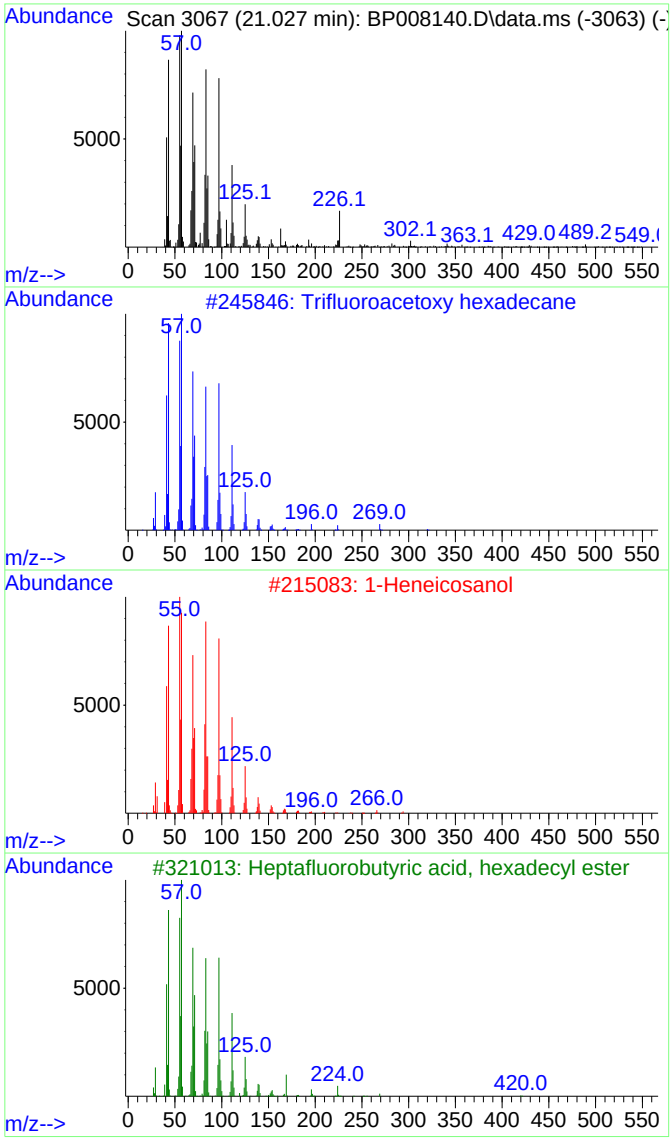
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

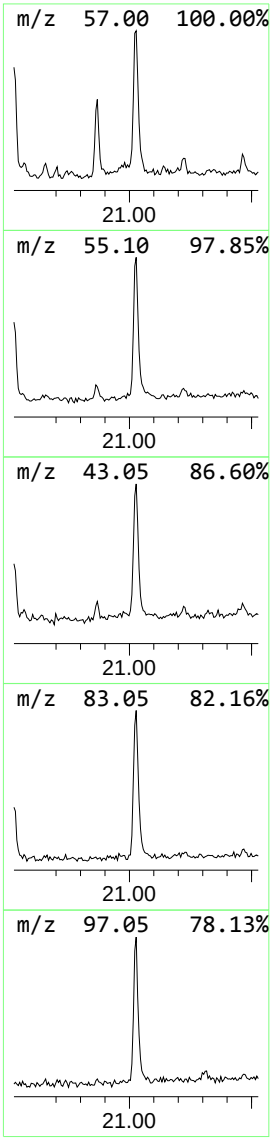
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.028	3.83 ng	289109	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	1-Tetracosene	336	C24H48	010192-32-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008140.D
Acq On : 29 Nov 2021 14:16
Operator : CG/JU
Sample : M4844-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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-...	4.928	10.6	ng	276776	1	7.805	520847	20.0
Ethanol, 2-(2-b...	10.393	7.0	ng	244695	2	10.599	696390	20.0
n-Hexadecanoic ...	18.110	5.6	ng	317250	4	17.204	1124350	20.0
Octadecanoic acid	19.345	2.9	ng	222012	5	21.304	1508060	20.0
Diisooctyl adipate	20.528	2.3	ng	169678	5	21.304	1508060	20.0
Trifluoroacetox...	21.028	3.8	ng	289109	5	21.304	1508060	20.0