LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008756.D
Acq On : 10 Jan 2022 18:40
Operator : CG/JU
Sample : N1054-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

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-BP010622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008756.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.069	9	14	29	rVB	5484998	7396524	64.42%	11.486%
2	4.975	332	338	348	rVB3	70446	157296	1.37%	0.244%
3	5.452	412	419	429	rBV	1628357	2477509	21.58%	3.847%
4	7.040	682	689	706	rBV	1404402	2461834	21.44%	3.823%
5	7.869	822	830	837	rBV	1189924	1941493	16.91%	3.015%
6	9.028	1014	1027	1045	rBV	2818978	5089509	44.33%	7.903%
7	10.451	1261	1269	1287	rBV	410953	791983	6.90%	1.230%
8	10.669	1298	1306	1316	rBV	1190526	2060041	17.94%	3.199%
9	13.128	1717	1724	1752	rBV	6515497	10392965	90.52%	16.139%
10	14.504	1951	1958	1979	rBV	1629774	2675178	23.30%	4.154%
11	15.998	2205	2212	2230	rBV	2669429	4489998	39.10%	6.972%
12	17.257	2419	2426	2440	rBV	2052047	3110539	27.09%	4.830%
13	17.380	2443	2447	2455	rVB3	70757	119601	1.04%	0.186%
14	17.939	2537	2542	2548	rBV	131847	179604	1.56%	0.279%
15	18.151	2573	2578	2587	rBV	321006	515996	4.49%	0.801%
16	19.386	2784	2788	2798	rBV2	244297	400468	3.49%	0.622%
17	19.816	2856	2861	2874	rBV	8973071	11481935	100.00%	17.830%
18	20.568	2986	2989	2992	rBV	153248	186566	1.62%	0.290%
19	20.610	2993	2996	2999	rVB2	141699	154173	1.34%	0.239%
20	21.057	3069	3072	3080	rBV2	666320	896457	7.81%	1.392%
21	21.345	3116	3121	3127	rBV	2508757	3442116	29.98%	5.345%
22	21.504	3146	3148	3152	rVB	210266	208650	1.82%	0.324%
23	23.768	3527	3533	3544	rVB2	1746935	3765388	32.79%	5.847%

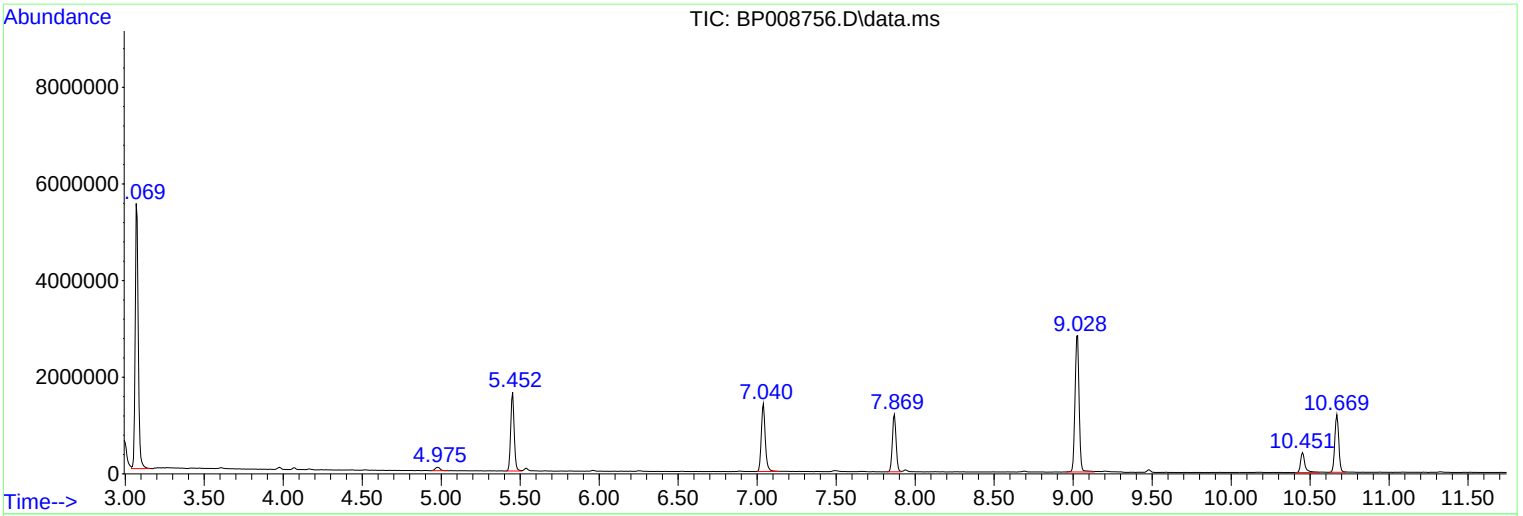
Sum of corrected areas: 64395823

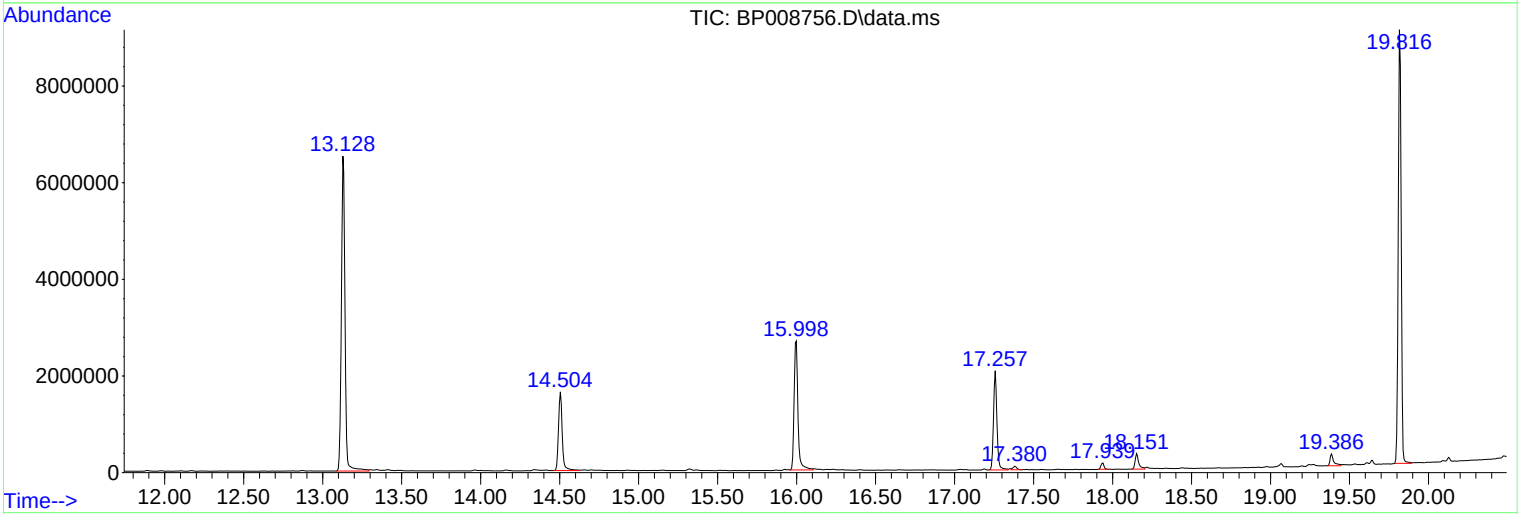
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008756.D
Acq On : 10 Jan 2022 18:40
Operator : CG/JU
Sample : N1054-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

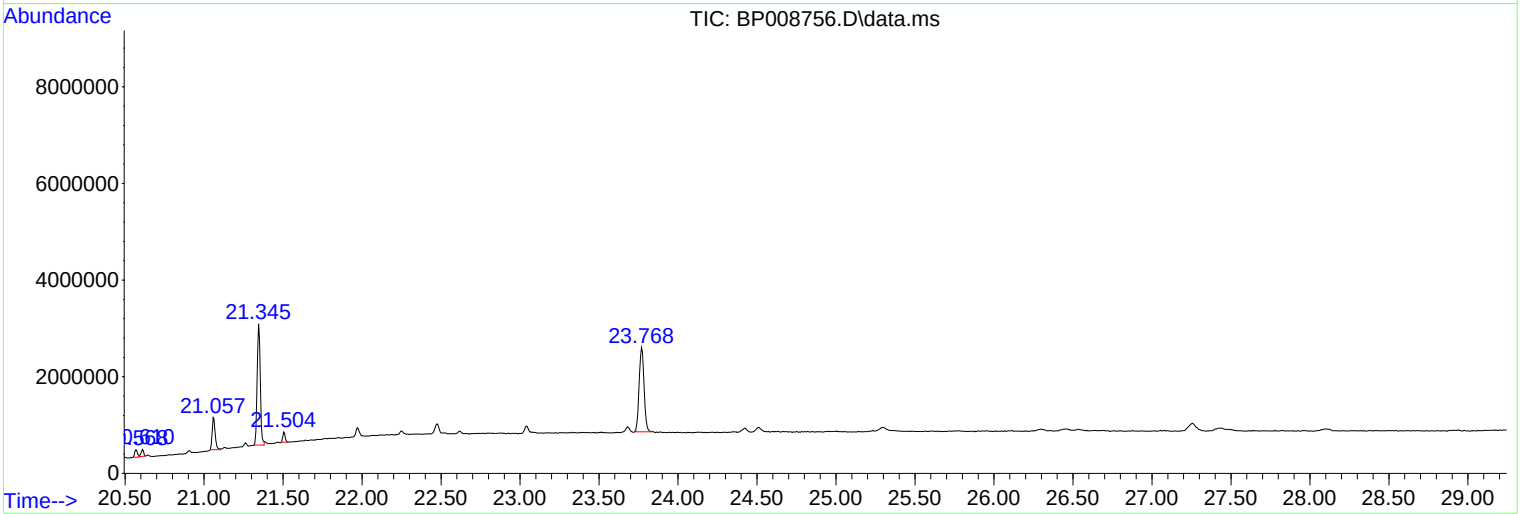
Instrument :
BNA_P
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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\BP011022\
Data File : BP008756.D
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Operator : CG/JU
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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

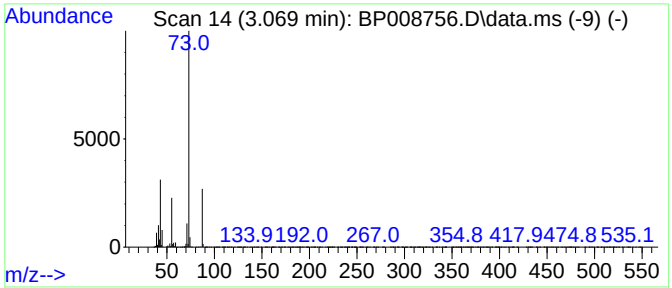
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

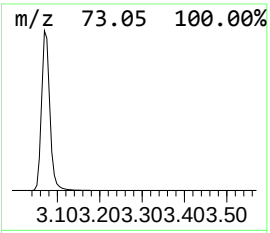
****

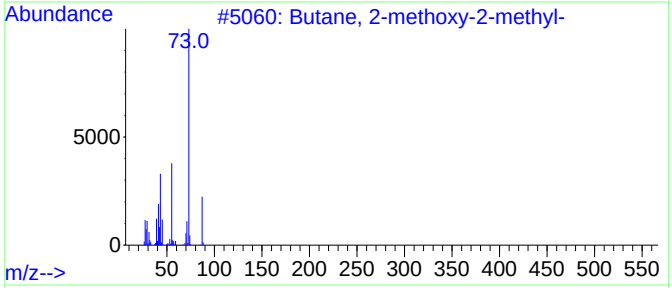
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

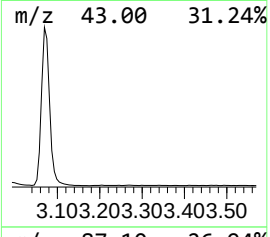
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.069	76.19 ng	7396520	1,4-Dichlorobenzene-d4	7.869

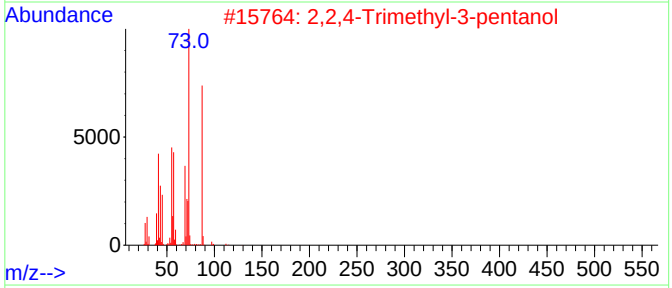
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9

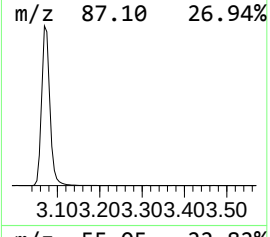


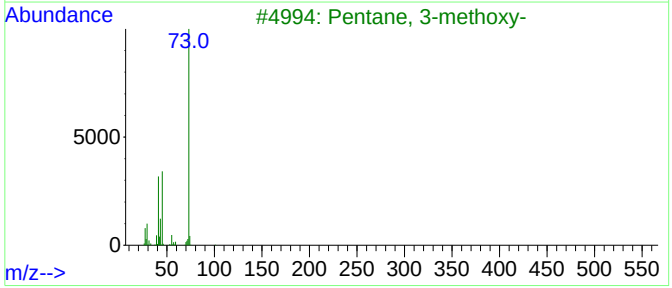


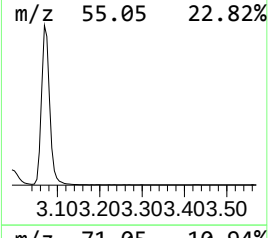


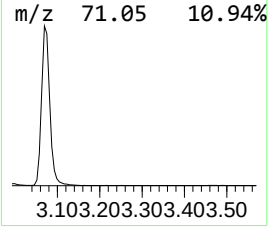












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008756.D
Acq On : 10 Jan 2022 18:40
Operator : CG/JU
Sample : N1054-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

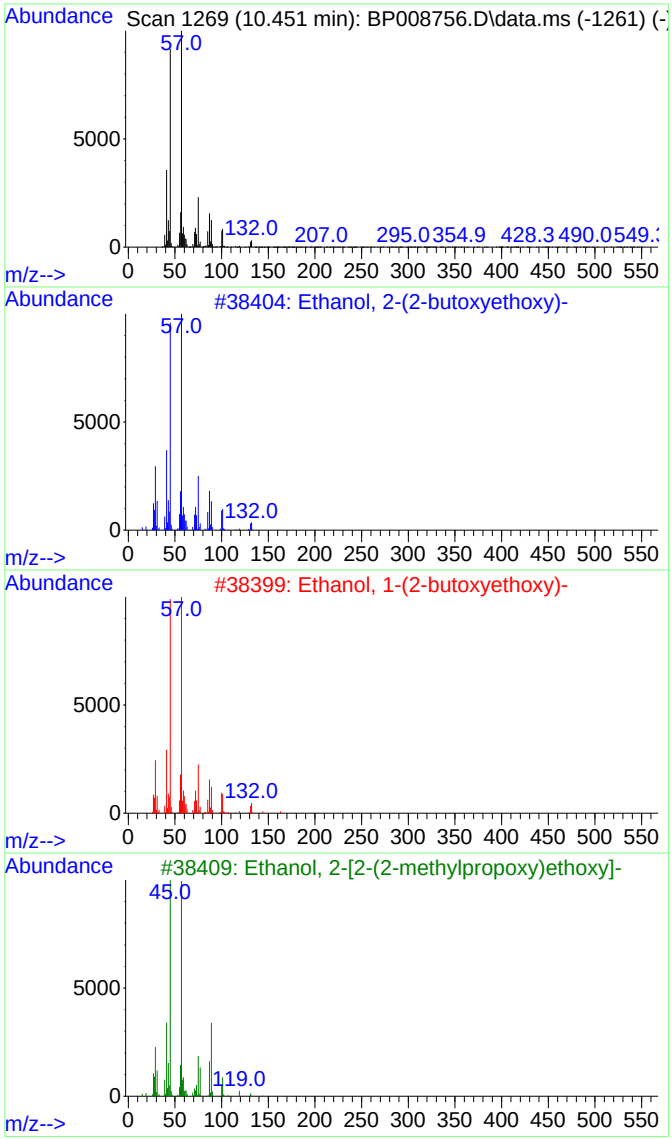
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

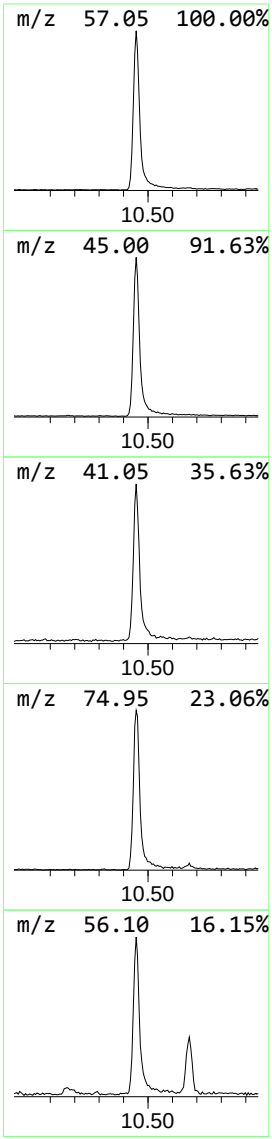
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	7.69 ng	791983	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008756.D
Acq On : 10 Jan 2022 18:40
Operator : CG/JU
Sample : N1054-11
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

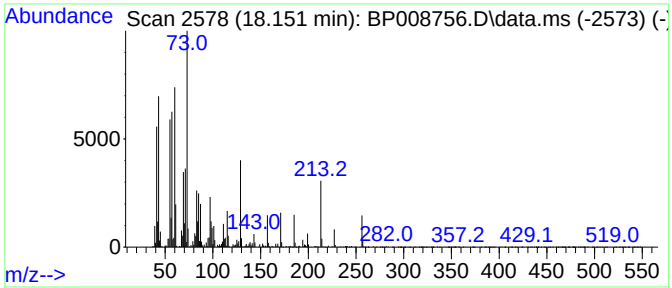
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

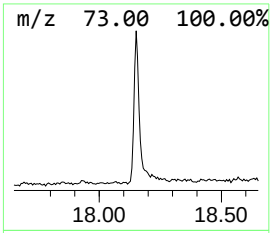
****

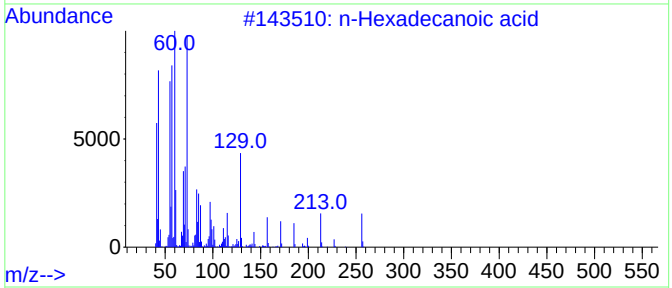
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

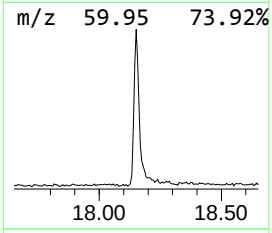
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	3.32 ng	515996	Phenanthrene-d10	17.257

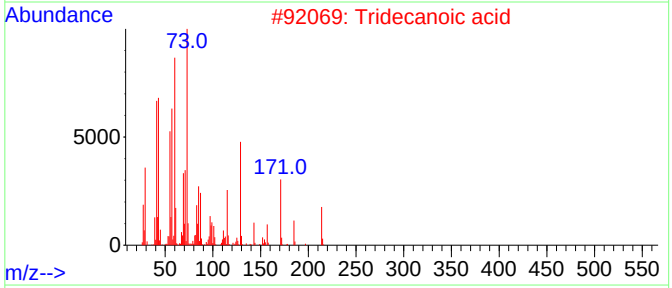
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81

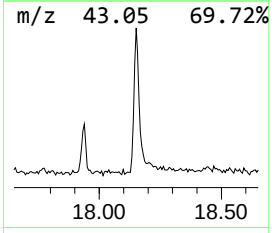


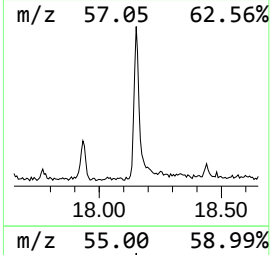


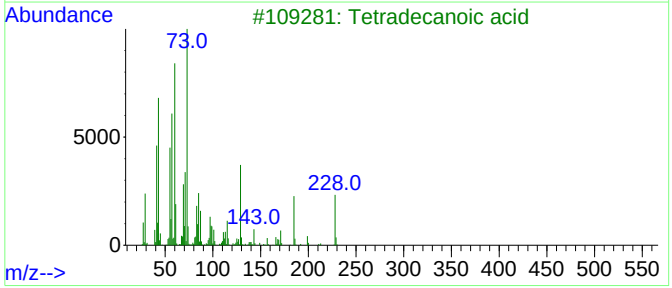


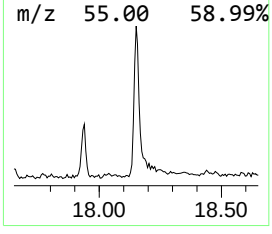












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008756.D
Acq On : 10 Jan 2022 18:40
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ClientSampleId :
20220021-CAPE-3-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

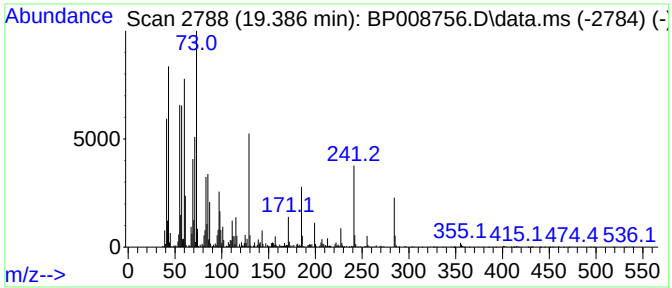
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

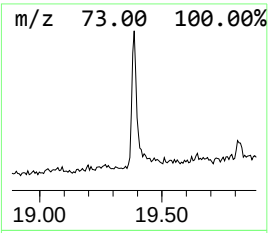
****

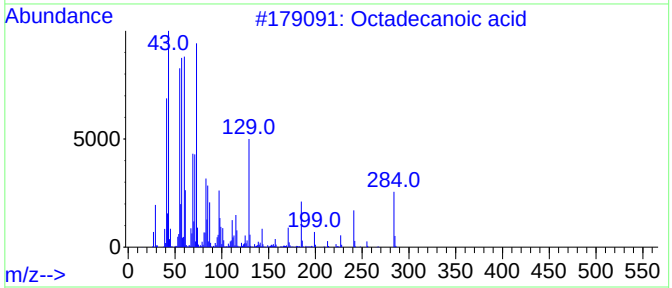
Peak Number 4 Octadecanoic acid Concentration Rank 5

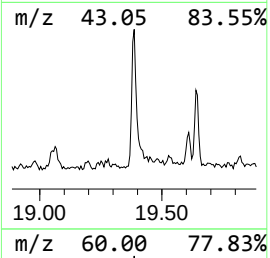
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	2.33 ng	400468	Chrysene-d12	21.345

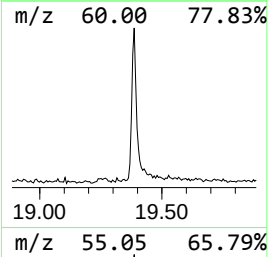
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50

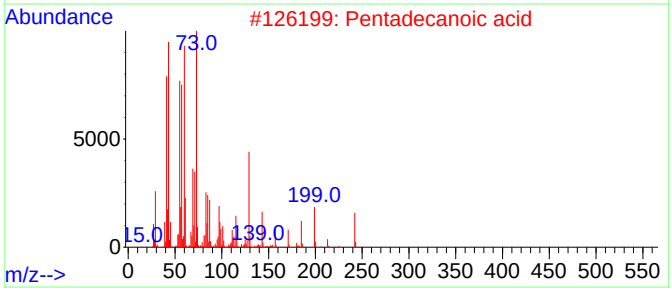


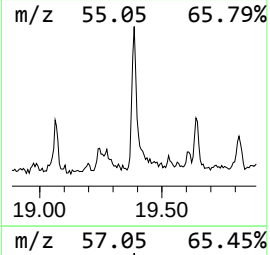


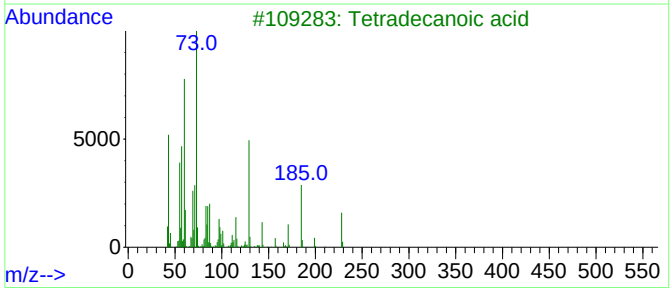


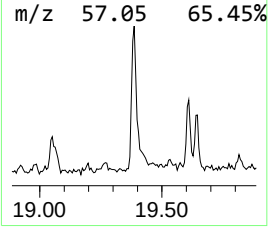












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

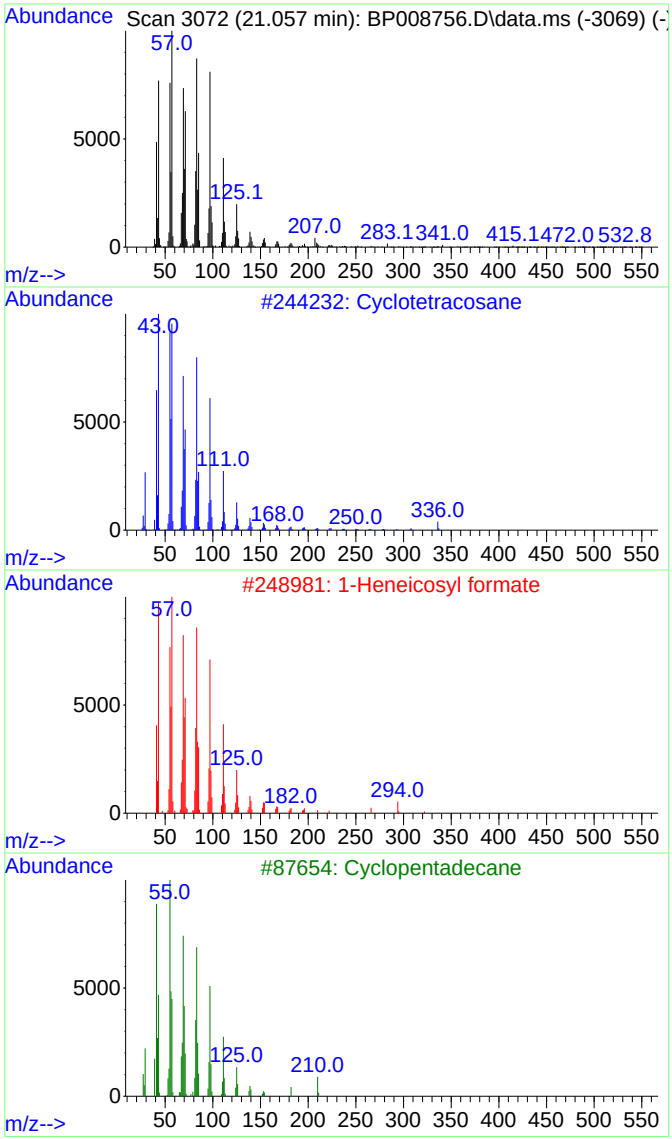
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

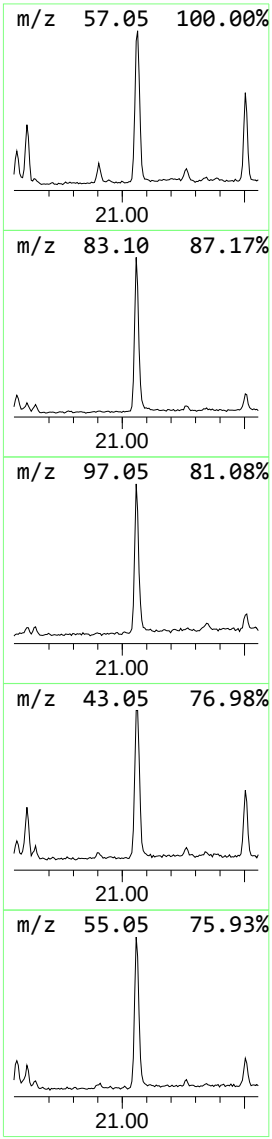
****

Peak Number 5 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	5.21 ng	896457	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	99
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3	Cyclopentadecane	210	C15H30	000295-48-7	94
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011022\
Data File : BP008756.D
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ALS Vial : 14 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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
Butane, 2-metho...	3.069	76.2	ng	7396520	1	7.869	1941490	20.0
Ethanol, 2-(2-b...	10.451	7.7	ng	791983	2	10.669	2060040	20.0
n-Hexadecanoic ...	18.151	3.3	ng	515996	4	17.257	3110540	20.0
Octadecanoic acid	19.386	2.3	ng	400468	5	21.345	3442120	20.0
Cyclotetracosane	21.057	5.2	ng	896457	5	21.345	3442120	20.0