LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008192.D
Acq On : 02 Dec 2021 15:28
Operator : CG/JU
Sample : M4891-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MINEBROOK-1-COMP

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: BP008192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	323	329	338	rVB	179457	245840	6.75%	1.245%
2	5.387	400	408	425	rBV	1252756	1843436	50.64%	9.333%
3	6.981	670	679	696	rBV	1127785	1929635	53.01%	9.770%
4	7.793	811	817	826	rVB	270601	425515	11.69%	2.154%
5	8.957	1006	1015	1023	rBV	726647	1220732	33.54%	6.181%
6	10.393	1254	1259	1271	rBV2	38786	87345	2.40%	0.442%
7	10.593	1283	1293	1301	rBV	324593	554125	15.22%	2.806%
8	13.063	1705	1713	1729	rBV	1565109	2375144	65.25%	12.025%
9	14.104	1885	1890	1900	rBV3	23421	46183	1.27%	0.234%
10	14.445	1941	1948	1956	rBV	471879	721252	19.81%	3.652%
11	15.275	2081	2089	2098	rBV2	101218	213240	5.86%	1.080%
12	15.945	2196	2203	2211	rBV	1364289	2080804	57.16%	10.535%
13	17.133	2399	2405	2410	rBV2	47815	64186	1.76%	0.325%
14	17.204	2411	2417	2423	rBV	601278	893311	24.54%	4.523%
15	17.328	2435	2438	2444	rVB6	23653	39346	1.08%	0.199%
16	17.498	2463	2467	2472	rBV2	23442	42876	1.18%	0.217%
17	17.886	2529	2533	2537	rVB3	31229	39601	1.09%	0.200%
18	18.104	2565	2570	2578	rBV	213680	322155	8.85%	1.631%
19	18.169	2578	2581	2586	rVB	53418	71104	1.95%	0.360%
20	18.516	2637	2640	2646	rVB5	30795	39139	1.08%	0.198%
21	19.227	2758	2761	2769	rVB4	22353	37858	1.04%	0.192%
22	19.345	2776	2781	2789	rBV	106635	178668	4.91%	0.905%
23	19.774	2849	2854	2862	rBV	2868269	3640135	100.00%	18.430%
24	21.027	3063	3067	3074	rBV2	231505	343098	9.43%	1.737%
25	21.310	3110	3115	3120	rBV	892227	1114654	30.62%	5.643%
26	23.704	3516	3522	3536	rVB2	562266	1181894	32.47%	5.984%

Sum of corrected areas: 19751276

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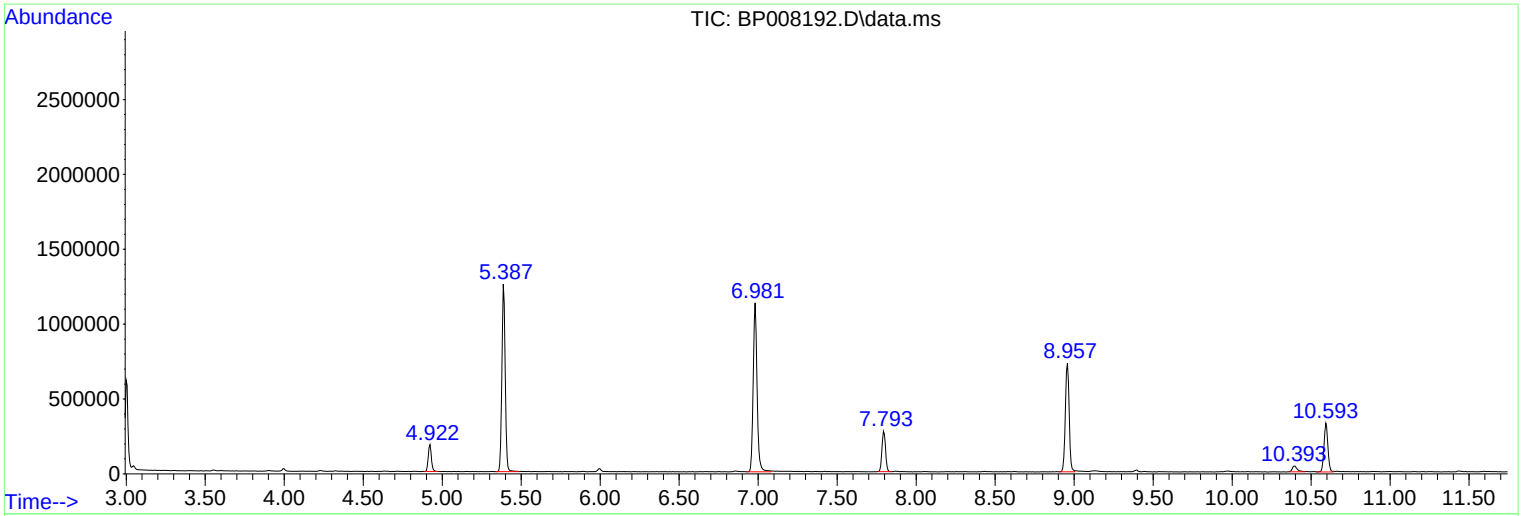
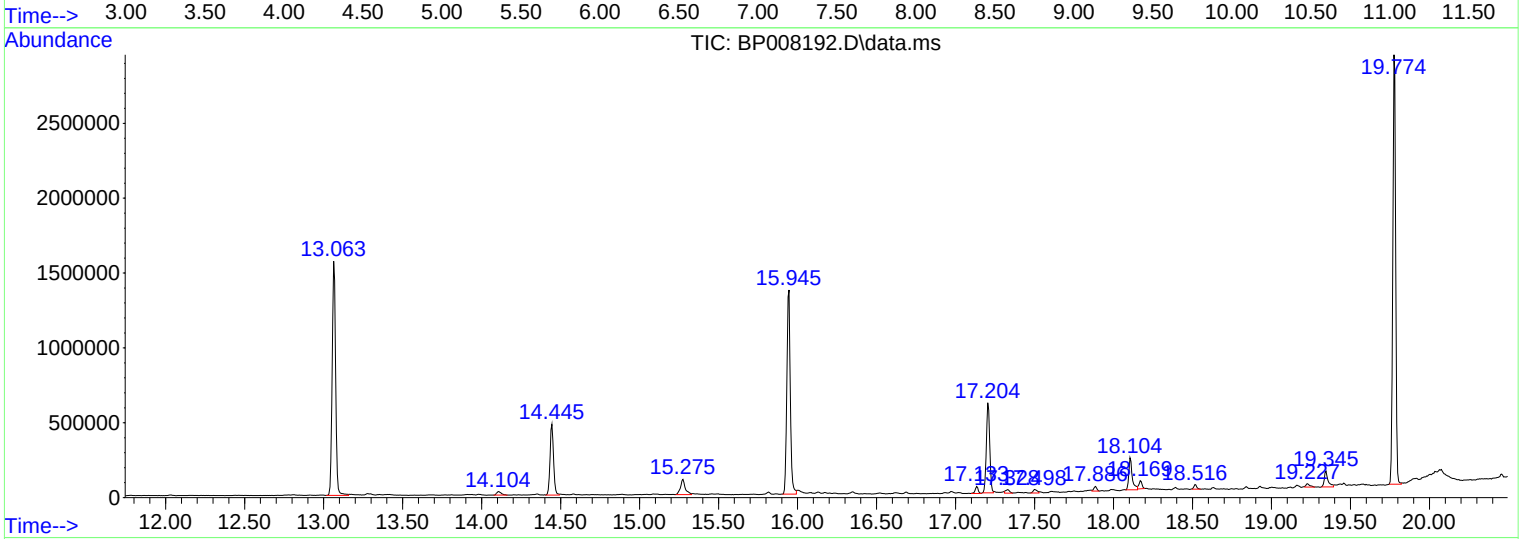
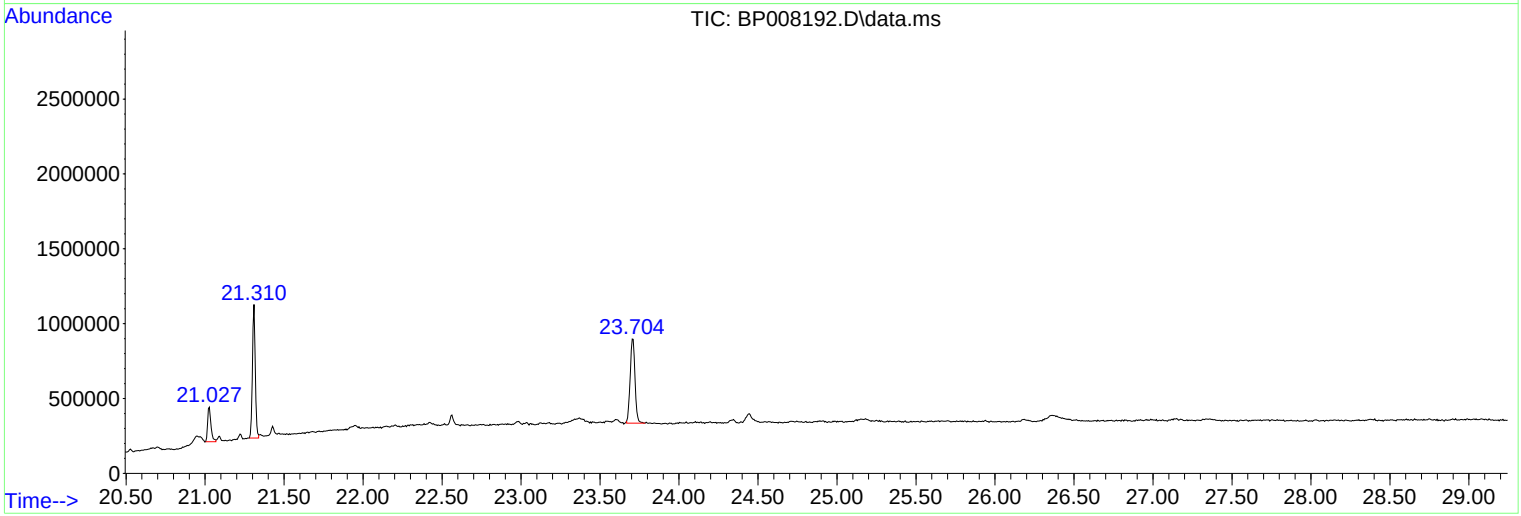
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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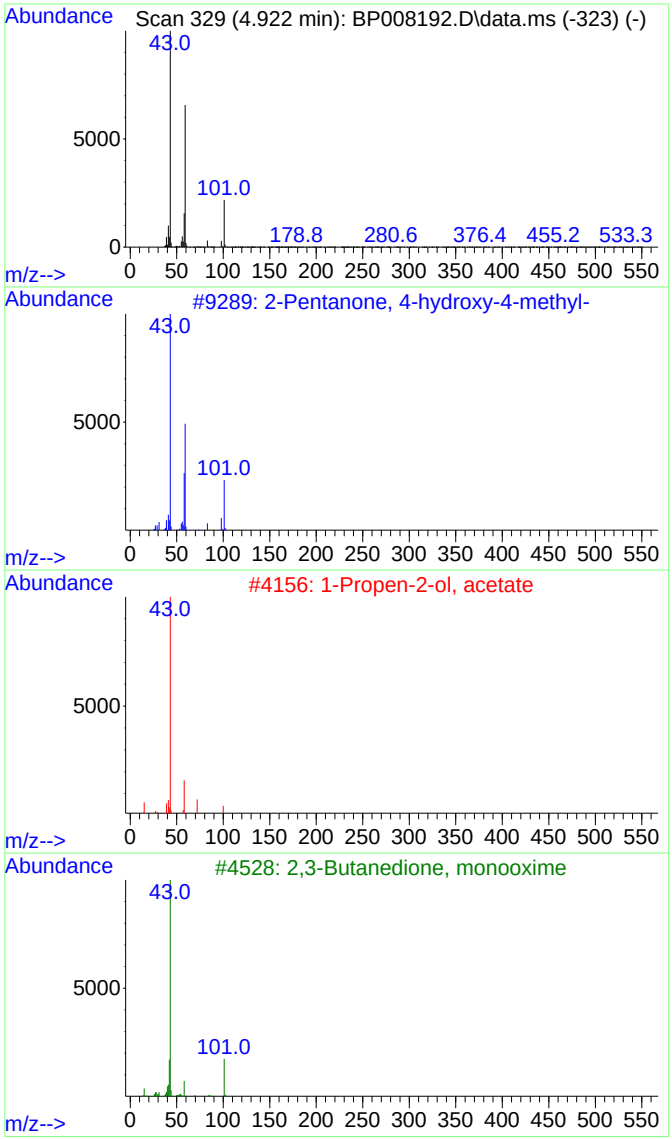
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

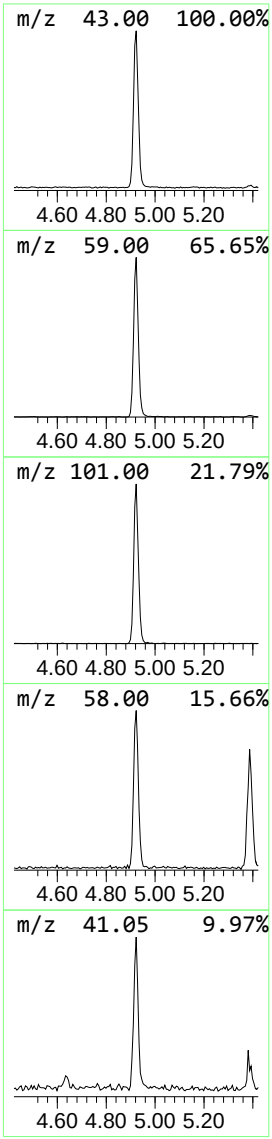
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	11.55 ng	245840	1,4-Dichlorobenzene-d4	7.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument :
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ClientSampleId :
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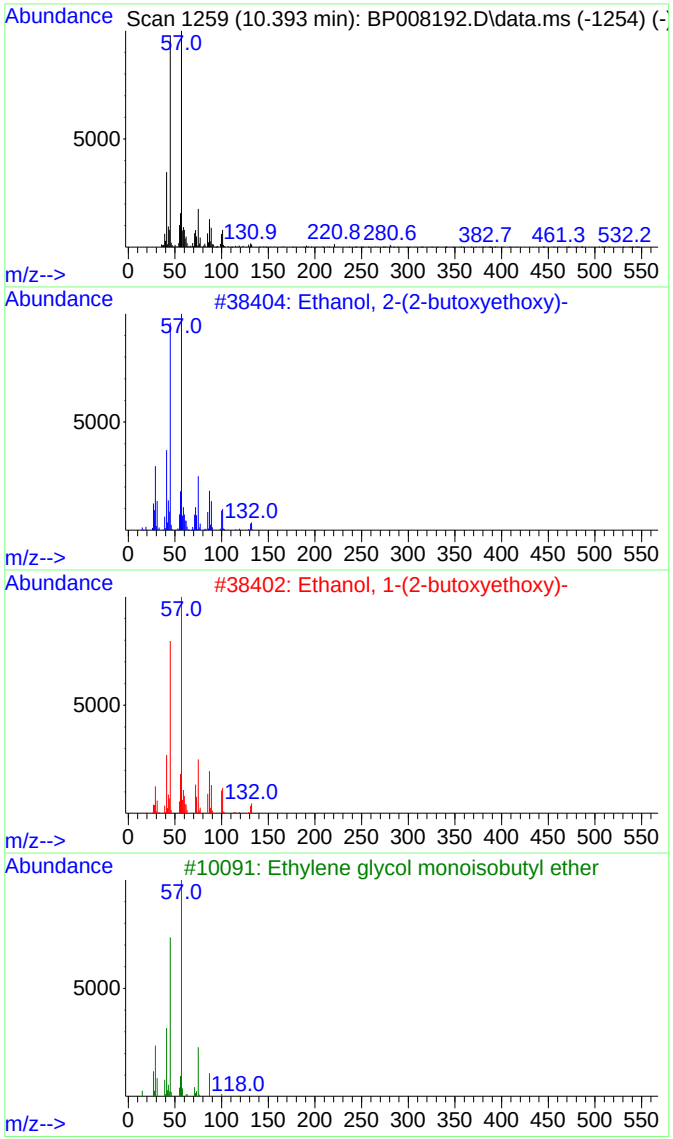
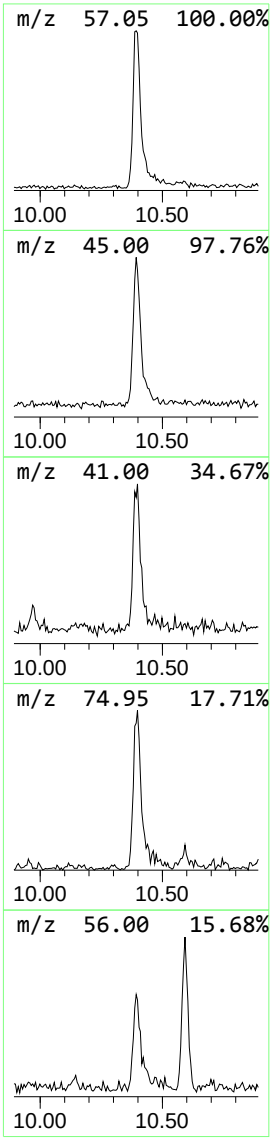
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.393	3.15 ng	87345	Naphthalene-d8	10.593

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MINEBROOK-1-COMP

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
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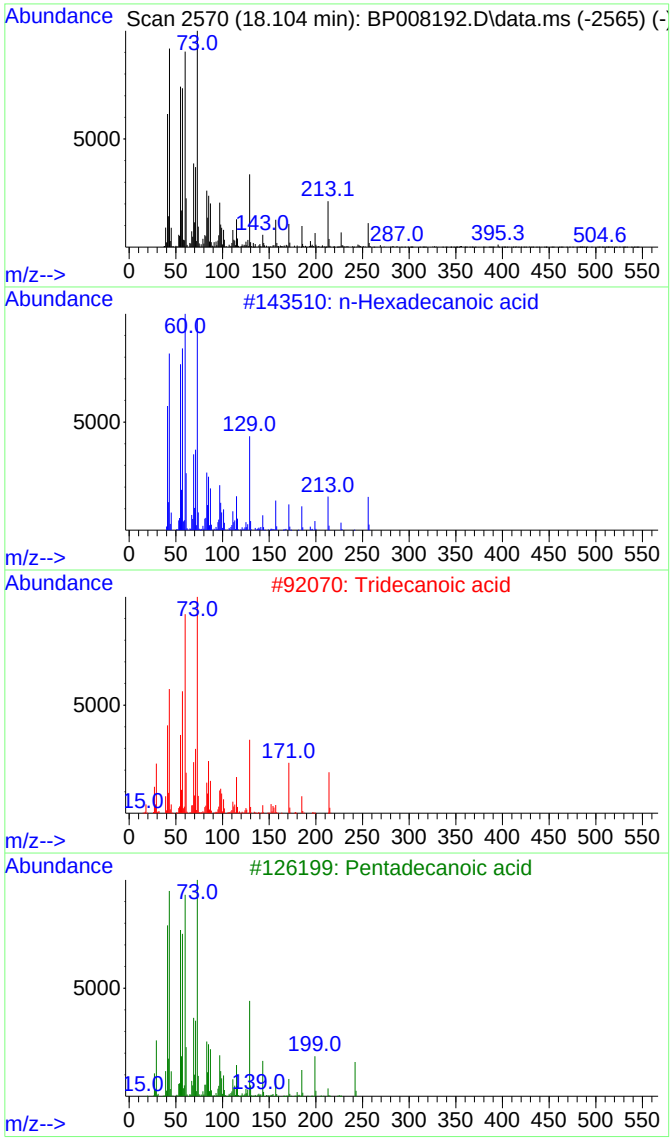
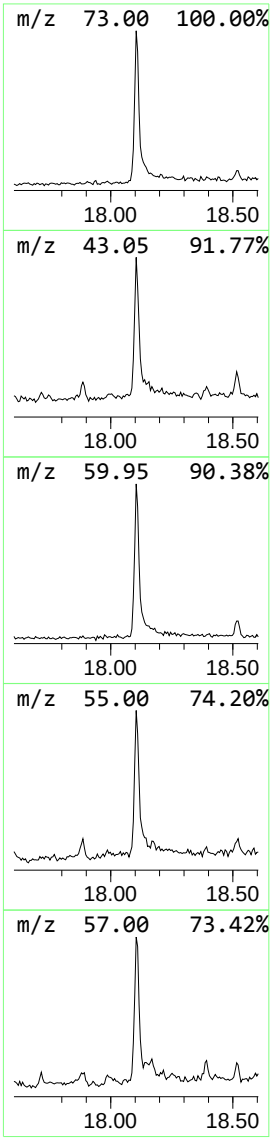
****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	7.21 ng	322155	Phenanthrene-d10	17.204

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MINEBROOK-1-COMP

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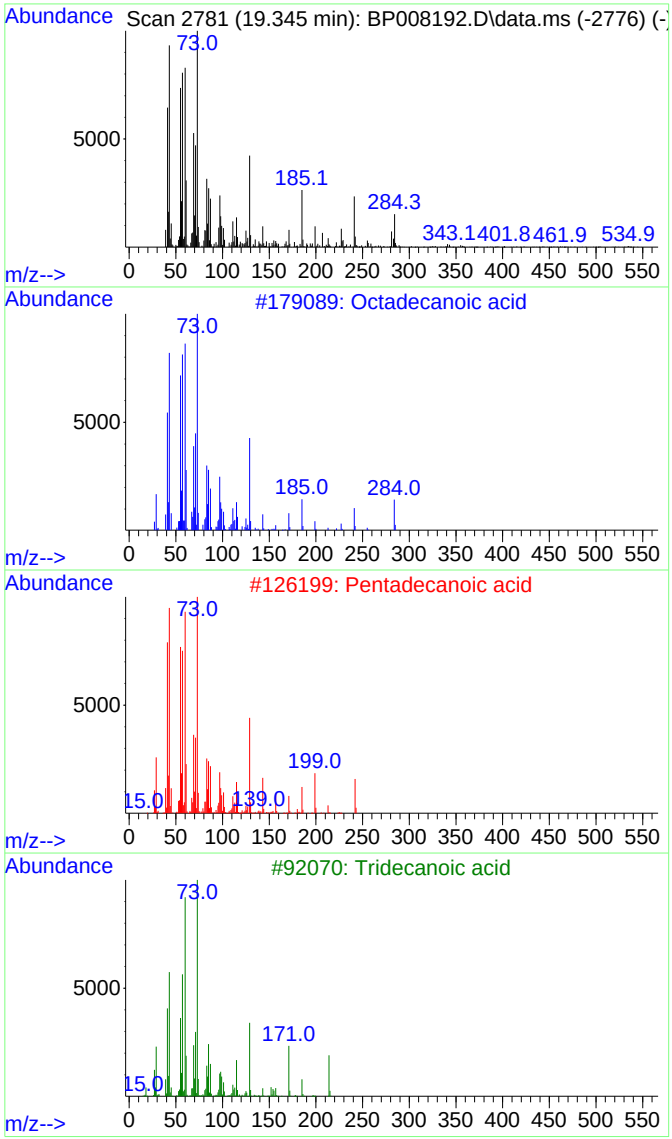
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

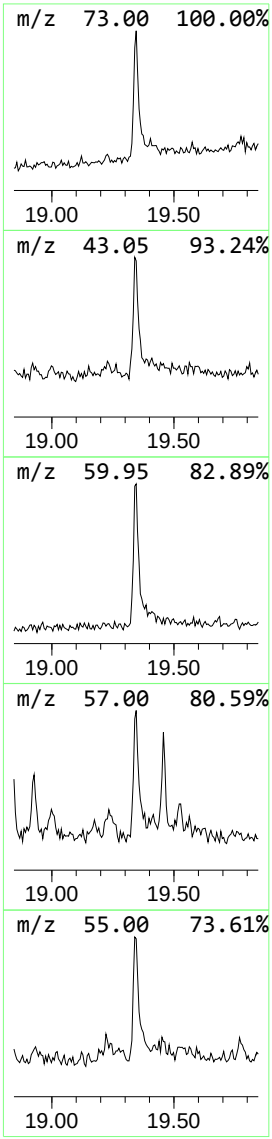
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	3.21 ng	178668	Chrysene-d12	21.310

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	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





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Sample : M4891-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MINEBROOK-1-COMP

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

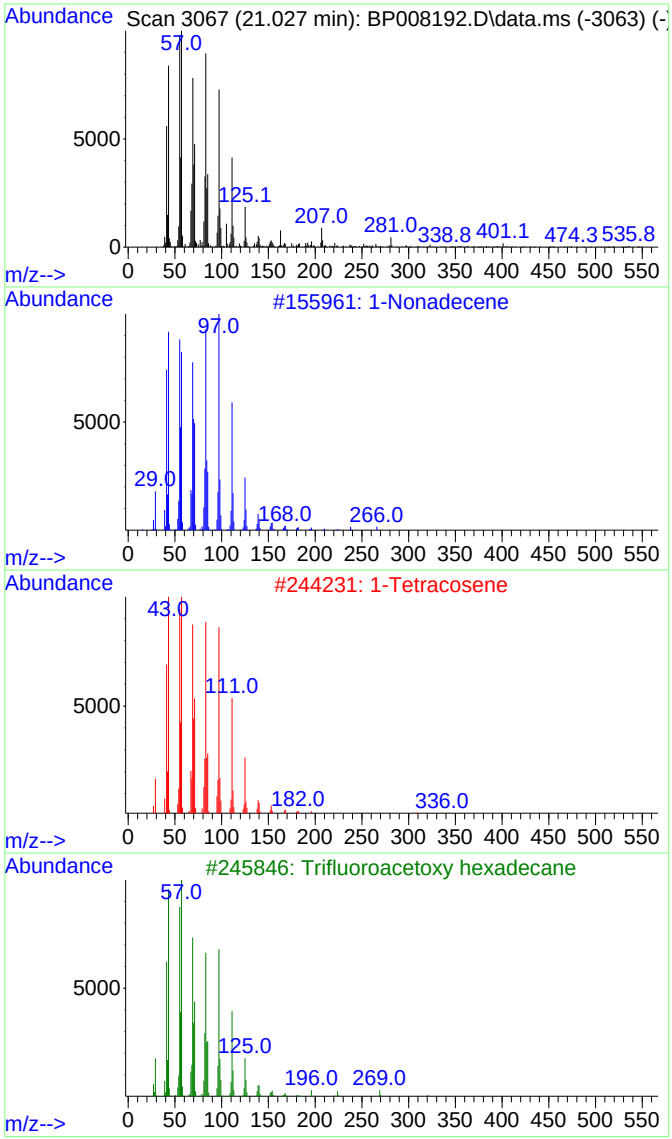
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

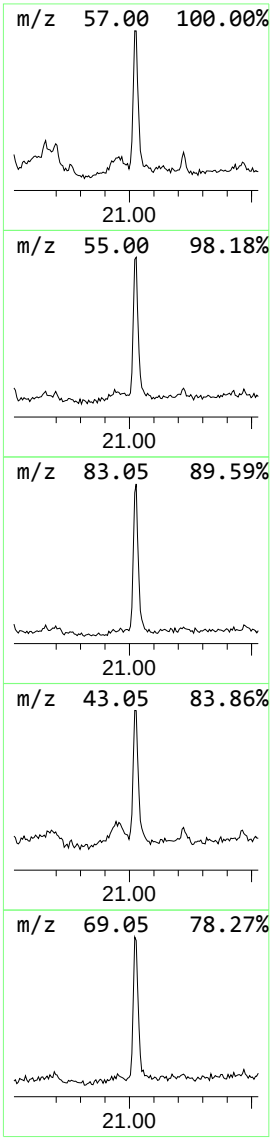
****

Peak Number 5 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	6.16 ng	343098	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	1-Tetracosene	336	C24H48	010192-32-2	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-...	4.922	11.6	ng	245840	1	7.793	425515	20.0
Ethanol, 2-(2-b...	10.393	3.1	ng	87345	2	10.593	554125	20.0
n-Hexadecanoic ...	18.104	7.2	ng	322155	4	17.204	893311	20.0
Octadecanoic acid	19.345	3.2	ng	178668	5	21.310	1114650	20.0
1-Nonadecene	21.027	6.2	ng	343098	5	21.310	1114650	20.0