LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041408.D
Acq On : 15 Aug 2023 16:27
Operator : MA/JU
Sample : 03985-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PNNL-APM2-0811-2

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_M\Methods\8270-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	360	366	382	rBV	1617329	2372843	49.49%	7.451%
2	6.945	633	639	661	rBV	1466358	2428906	50.66%	7.627%
3	7.763	771	778	787	rBV	632523	966051	20.15%	3.034%
4	8.939	971	978	998	rBV	885452	1508880	31.47%	4.738%
5	10.569	1245	1255	1269	rBV	723828	1261544	26.31%	3.961%
6	13.045	1669	1676	1693	rBV	2351360	3355128	69.98%	10.536%
7	13.316	1714	1722	1733	rBV	824463	1287758	26.86%	4.044%
8	14.427	1904	1911	1925	rBV	1086180	1553986	32.41%	4.880%
9	15.927	2160	2166	2181	rBV	1867498	2617989	54.60%	8.221%
10	17.186	2373	2380	2392	rBV	1308967	1832082	38.21%	5.753%
11	18.092	2528	2534	2551	rBV	891878	1560262	32.54%	4.899%
12	19.256	2729	2732	2739	rVB7	28472	48552	1.01%	0.152%
13	19.374	2747	2752	2771	rBV	527466	940085	19.61%	2.952%
14	19.827	2823	2829	2840	rBV	4224916	4794419	100.00%	15.055%
15	21.097	3041	3045	3052	rBV	231254	347021	7.24%	1.090%
16	21.303	3076	3080	3085	rBV	236379	265988	5.55%	0.835%
17	21.392	3091	3095	3106	rBV	1657271	2208392	46.06%	6.935%
18	23.756	3491	3497	3511	rVB	1276672	2495628	52.05%	7.837%

Sum of corrected areas: 31845514

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Instrument :
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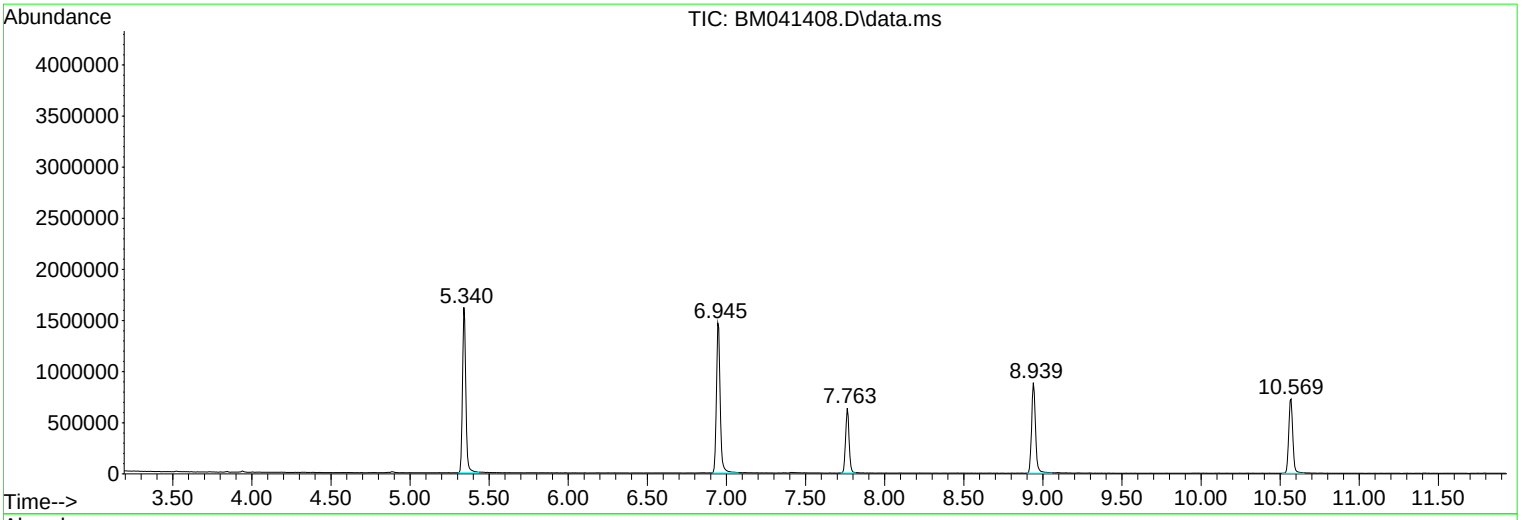
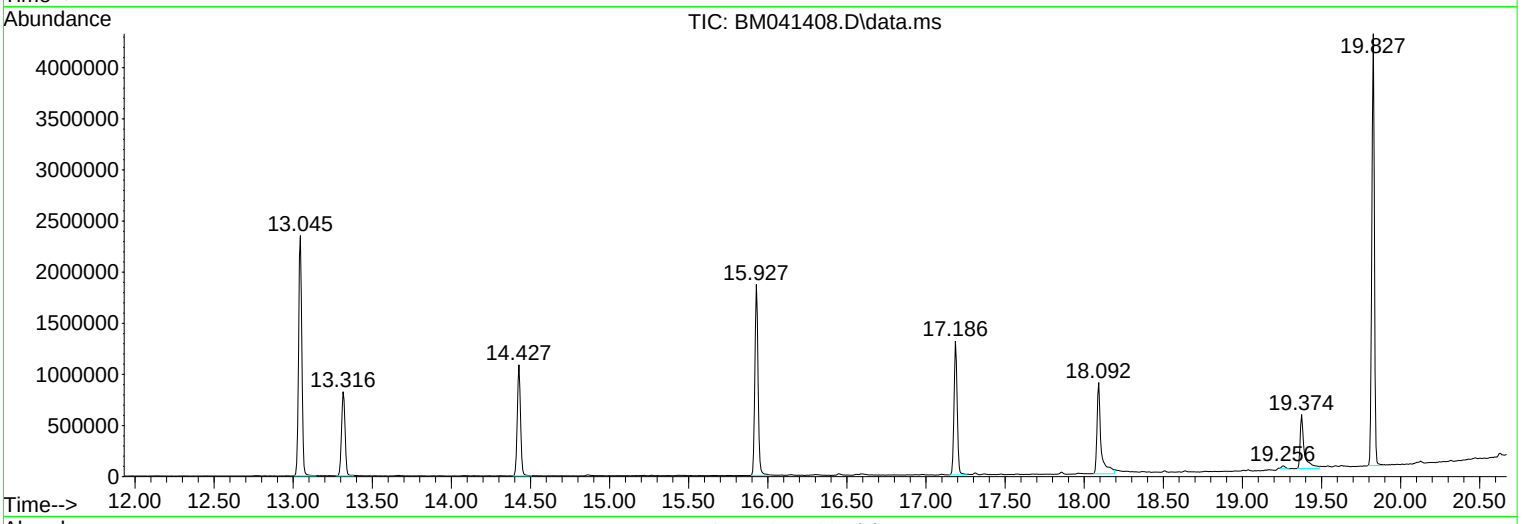
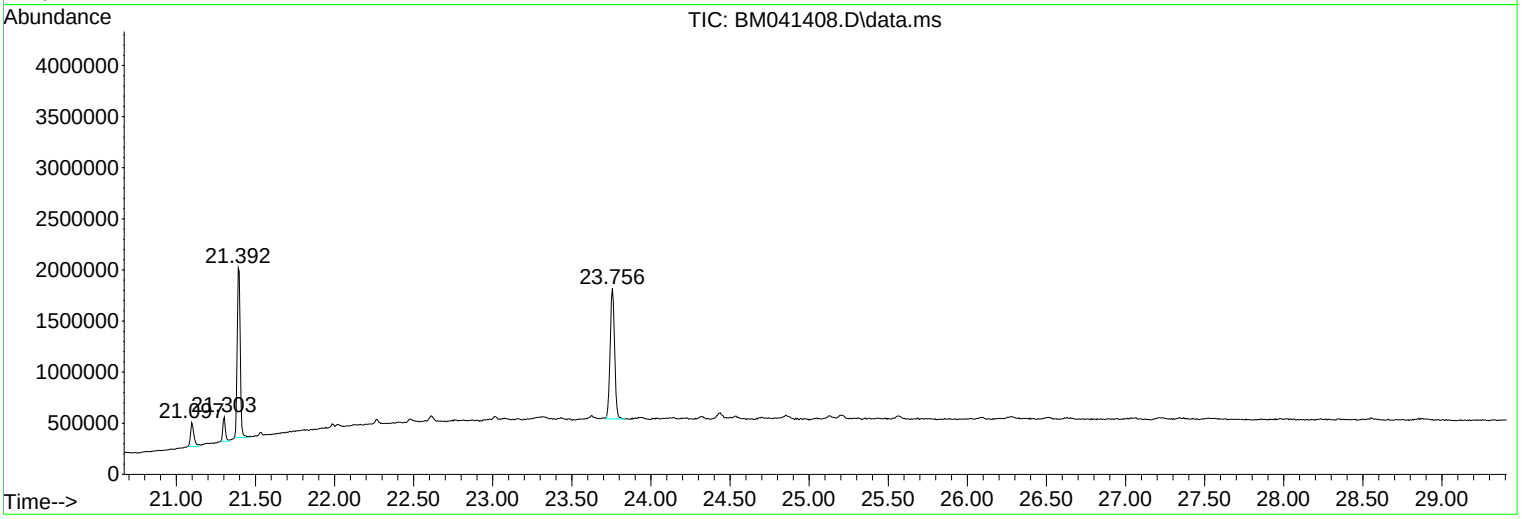
ClientSampleId :
PNNL-APM2-0811-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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

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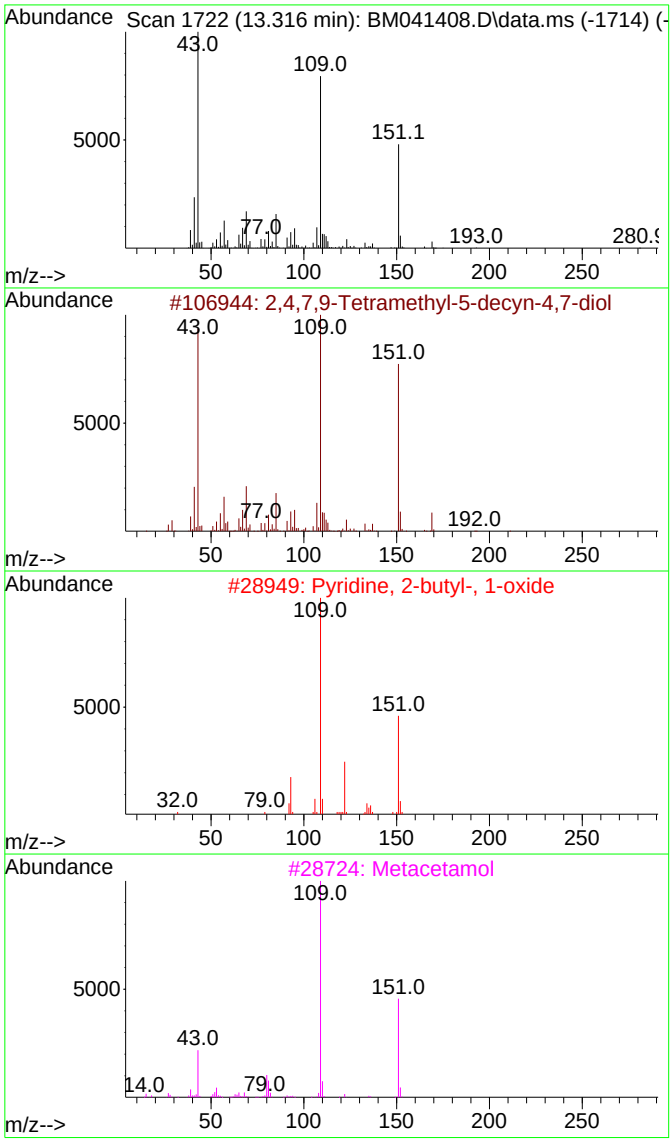
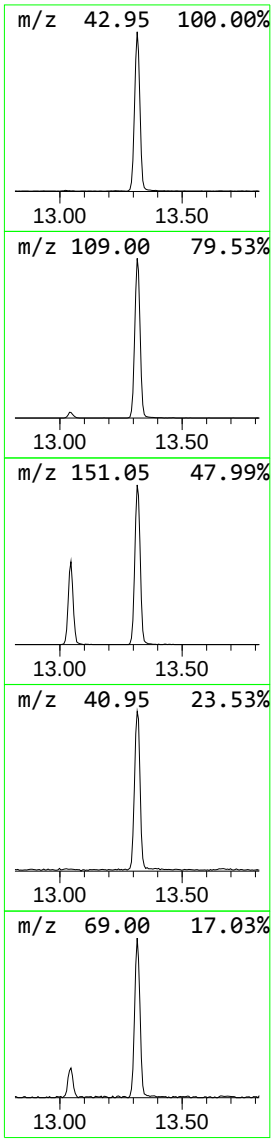
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.316	16.57 ng	1287760	Acenaphthene-d10	14.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	59
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	45





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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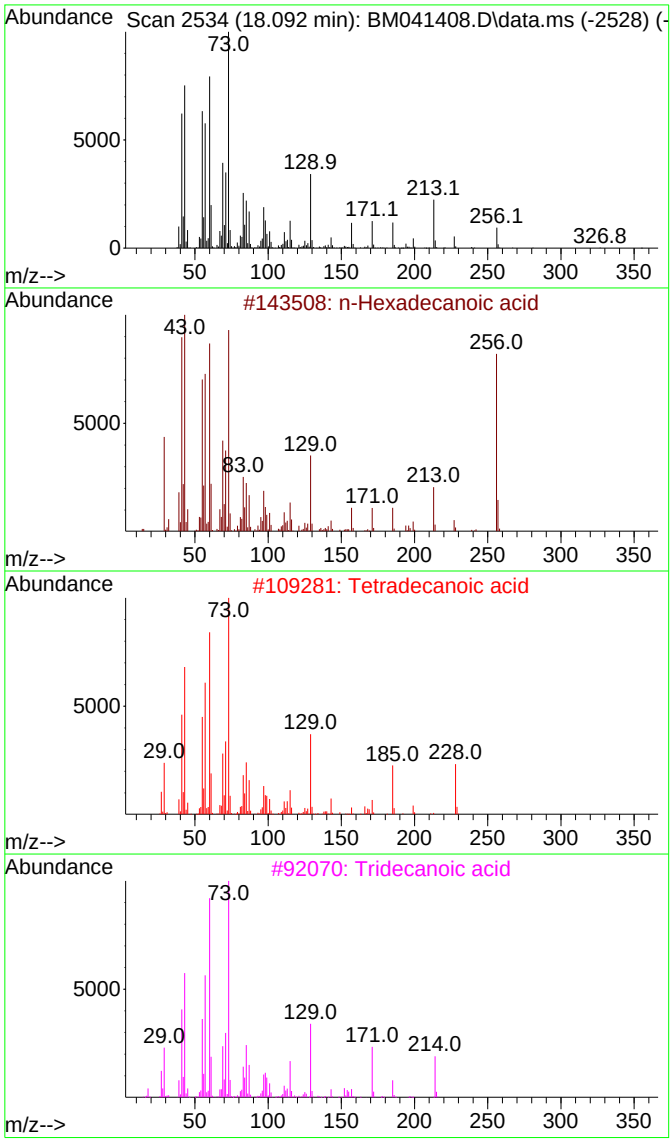
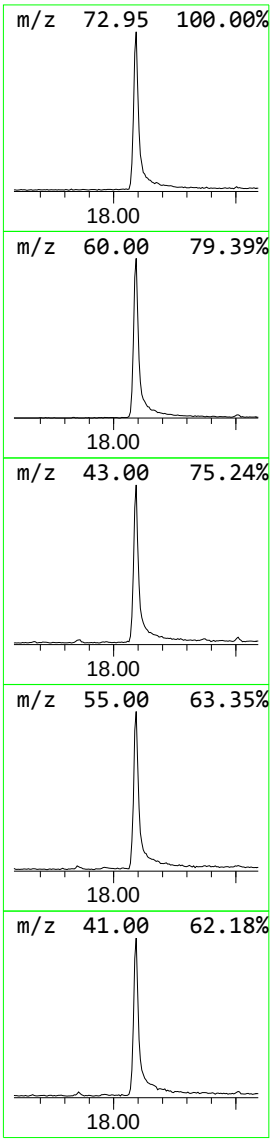
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	17.03 ng	1560260	Phenanthrene-d10	17.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Data File : BM041408.D
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Operator : MA/JU
Sample : 03985-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PNNL-APM2-0811-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
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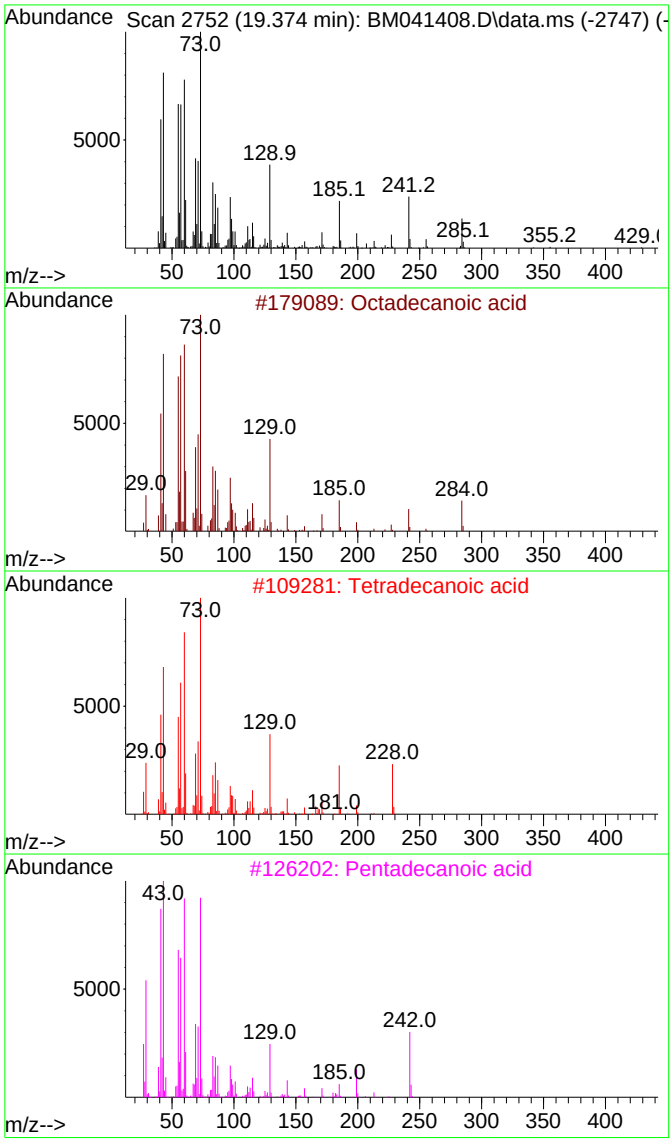
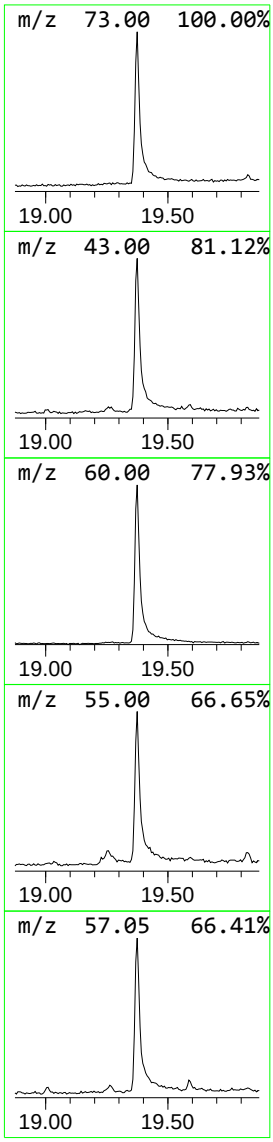
Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	8.51 ng	940085	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PNNL-APM2-0811-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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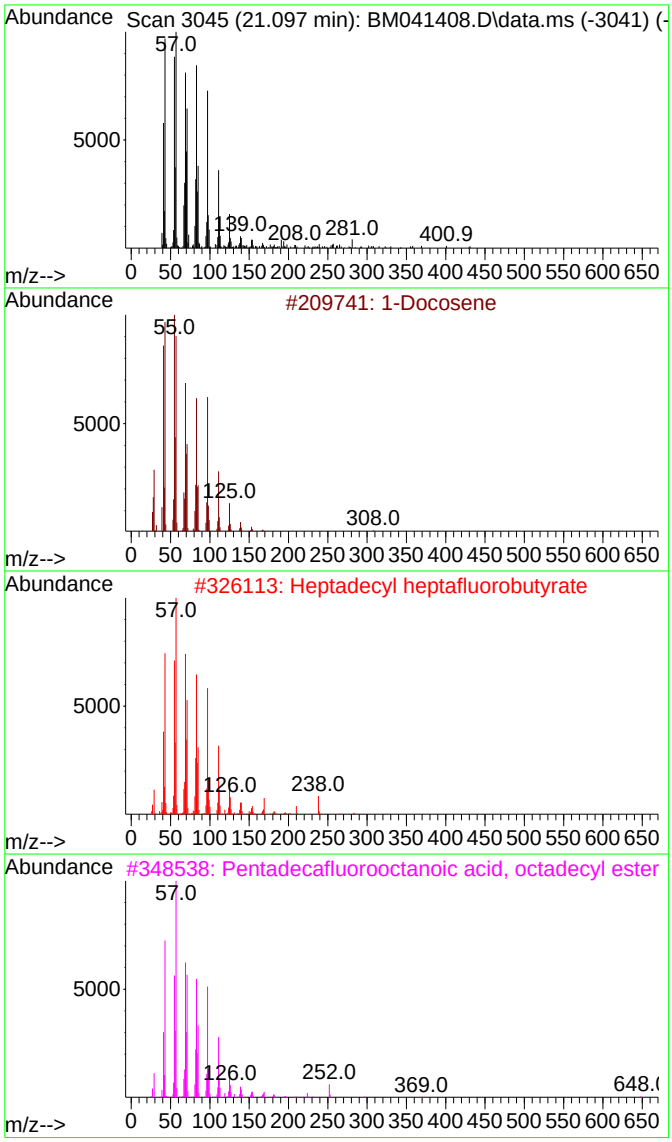
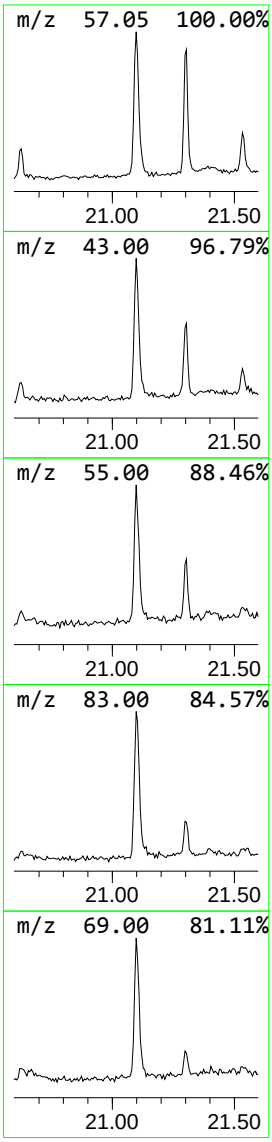
Peak Number 4 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	3.14 ng	347021	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Heptacos-1-ene	378	C27H54	015306-27-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081523\
Data File : BM041408.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.316	16.6	ng	1287760	3	14.427	1553990	20.0
n-Hexadecanoic ...	18.092	17.0	ng	1560260	4	17.186	1832080	20.0
Octadecanoic acid	19.374	8.5	ng	940085	5	21.392	2208390	20.0
1-Docosene	21.098	3.1	ng	347021	5	21.392	2208390	20.0