LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090221\
Data File : BM032034.D
Acq On : 03 Sep 2021 00:56
Operator : CG/JU
Sample : M3610-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : YORK-ST-MH-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_M\Methods\8270-BM090221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.699	270	274	286	rVB	65243	99306	2.30%	0.622%
2	5.134	343	348	359	rVB	343831	486834	11.29%	3.048%
3	6.693	607	613	624	rBV	186622	311448	7.22%	1.950%
4	7.493	740	749	758	rBV	261141	408490	9.47%	2.558%
5	8.645	938	945	963	rBV	731507	1211626	28.09%	7.587%
6	10.251	1210	1218	1228	rBV	313728	527377	12.23%	3.302%
7	12.745	1634	1642	1656	rBV	1929724	2802433	64.96%	17.547%
8	14.133	1871	1878	1885	rBV	502583	731906	16.97%	4.583%
9	15.410	2089	2095	2101	rBV	51955	85199	1.97%	0.533%
10	15.639	2126	2134	2142	rBV	867220	1306398	30.28%	8.180%
11	15.892	2170	2177	2183	rBV3	88328	148751	3.45%	0.931%
12	16.716	2312	2317	2329	rVB	55684	99141	2.30%	0.621%
13	16.892	2341	2347	2352	rBV	615618	872752	20.23%	5.465%
14	17.810	2499	2503	2512	rVB3	106011	156370	3.62%	0.979%
15	19.098	2718	2722	2729	rBV3	73666	96451	2.24%	0.604%
16	19.539	2791	2797	2804	rBV	3824734	4313884	100.00%	27.011%
17	20.833	3013	3017	3023	rBV3	83825	130927	3.04%	0.820%
18	21.092	3056	3061	3069	rBV	783938	1057266	24.51%	6.620%
19	23.227	3418	3424	3436	rVB2	608759	1124210	26.06%	7.039%

Sum of corrected areas: 15970769

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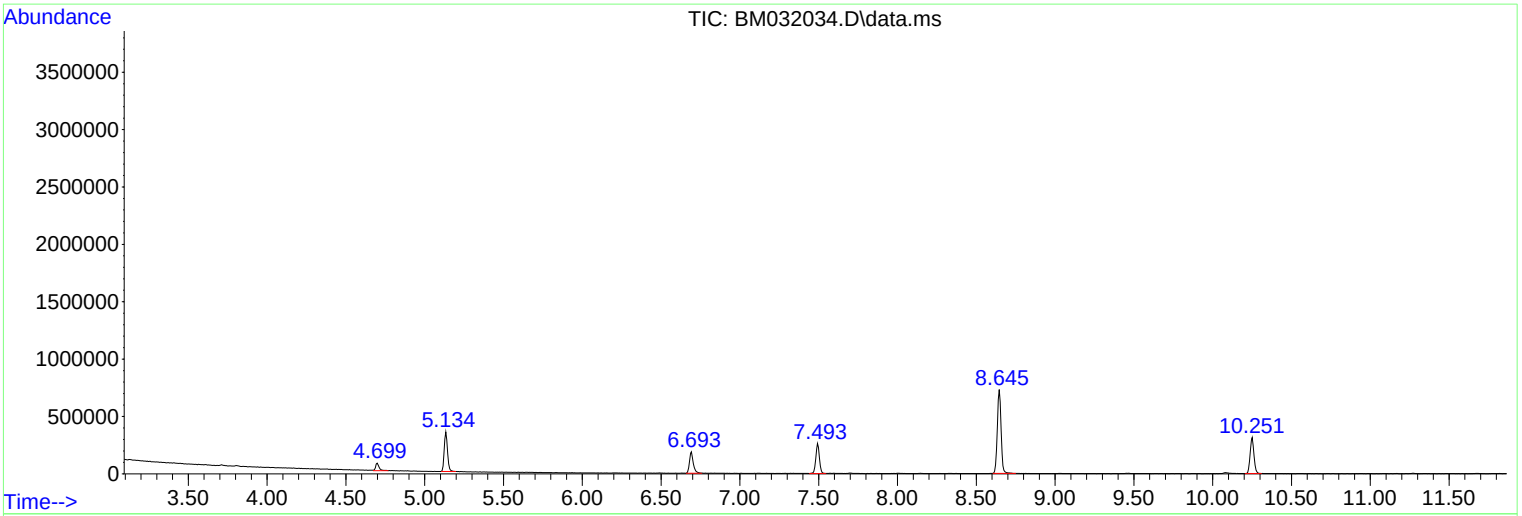
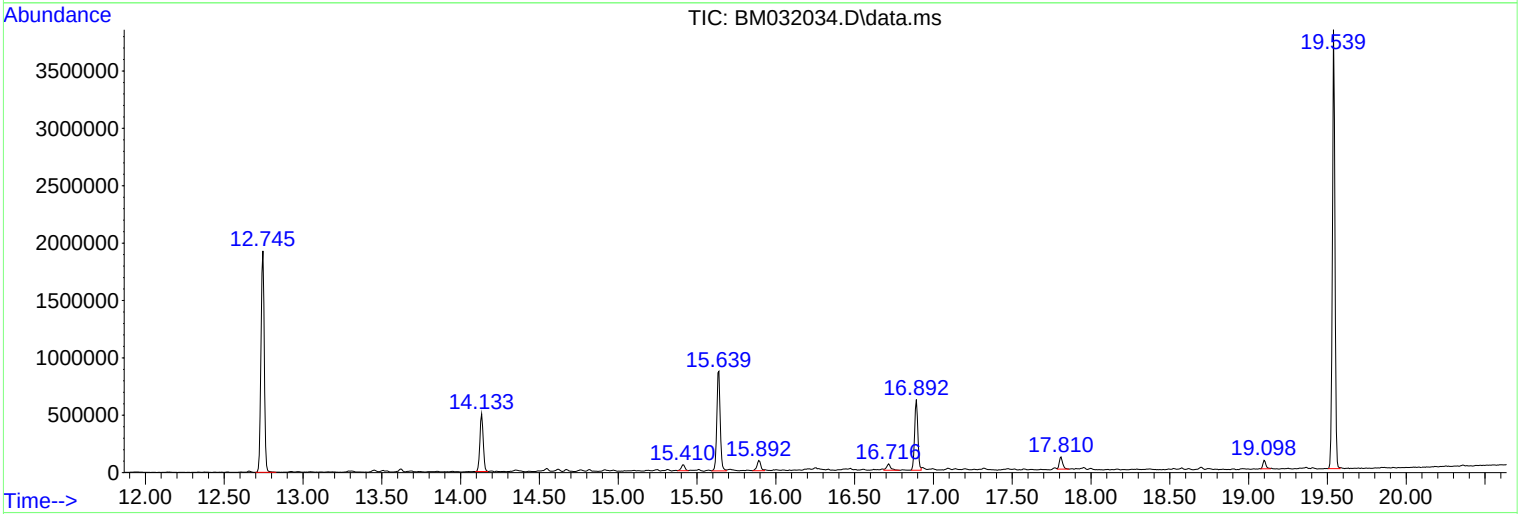
Misc :
ALS Vial : 17 Sample Multiplier: 1

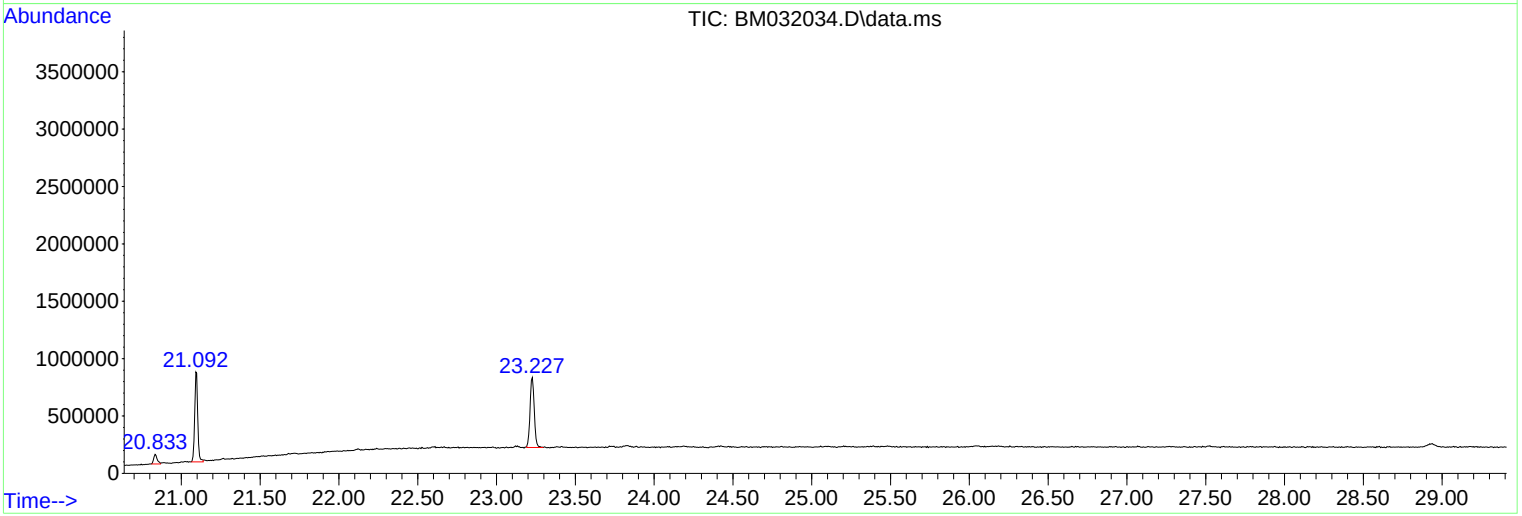
Instrument :
BNA_M
ClientSampleId :
YORK-ST-MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM090221.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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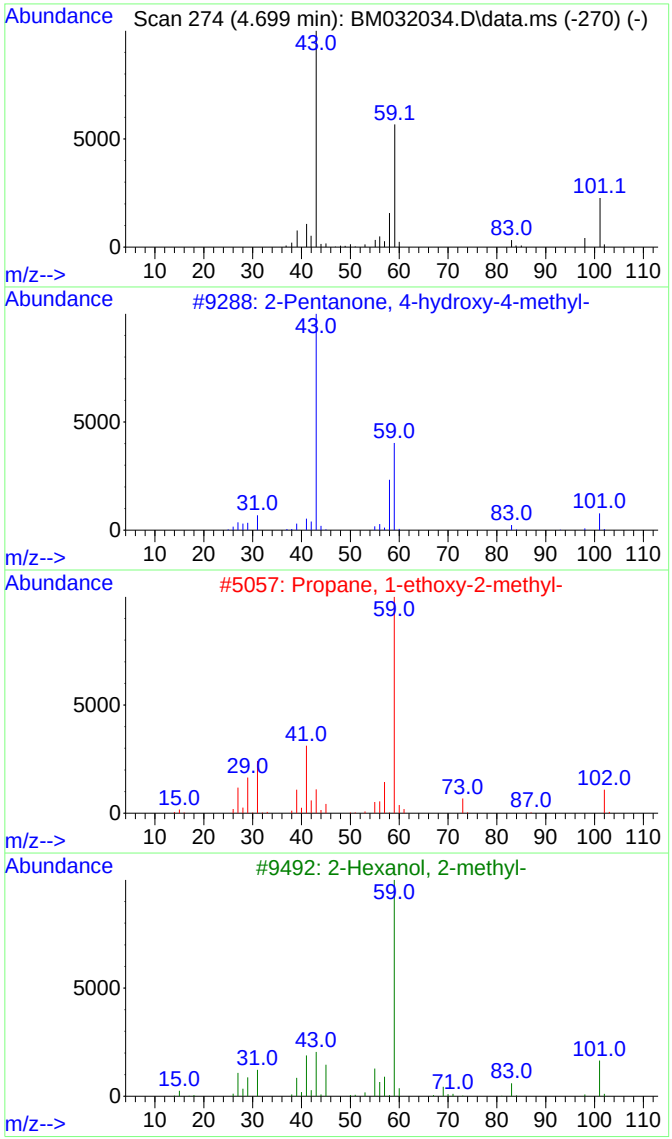
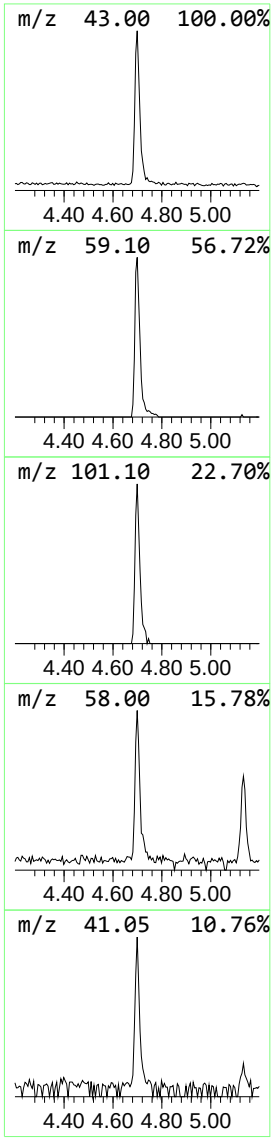
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.699	4.86 ng	99306	1,4-Dichlorobenzene-d4	7.493

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	17
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16





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Misc :
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Instrument :
BNA_M
ClientSampleId :
YORK-ST-MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM090221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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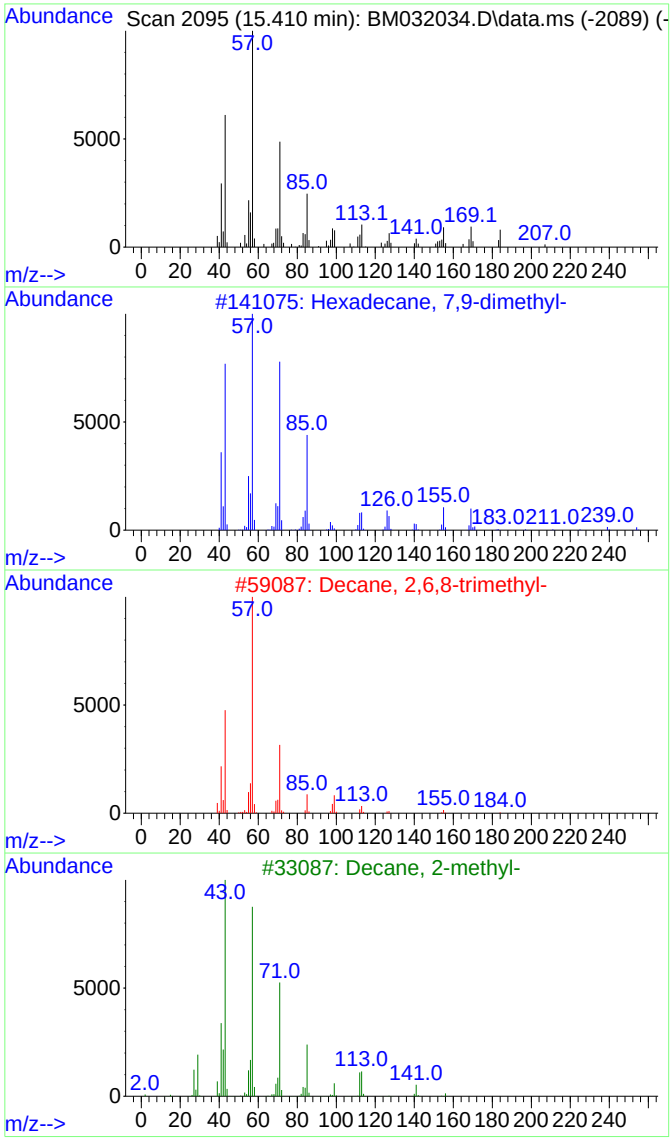
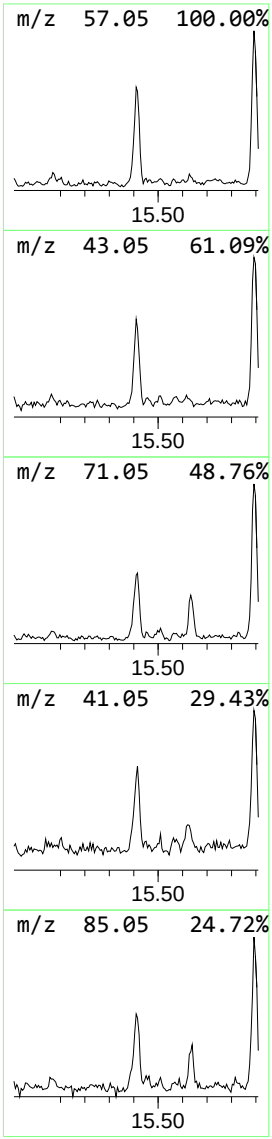
****

Peak Number 2 Hexadecane, 7,9-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	2.33 ng	85199	Acenaphthene-d10	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	64
2	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	60
3	Decane, 2-methyl-	156	C11H24	006975-98-0	58
4	5-Ethyldecane	170	C12H26	017302-36-2	58
5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	58





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Acq On : 03 Sep 2021 00:56
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Sample : M3610-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
YORK-ST-MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM090221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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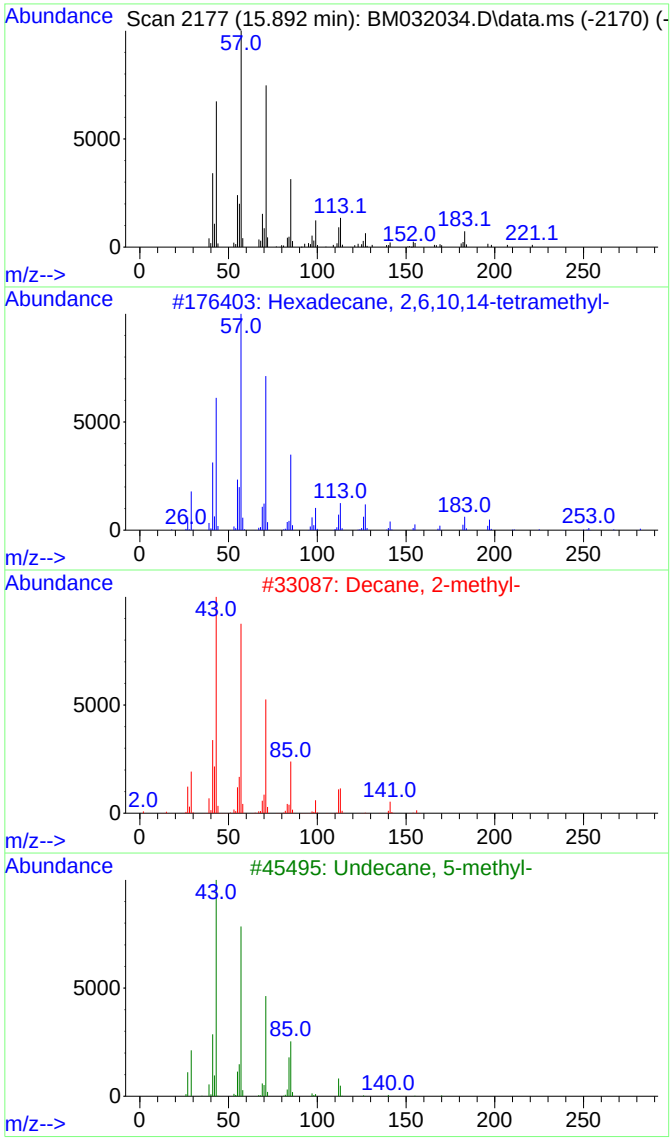
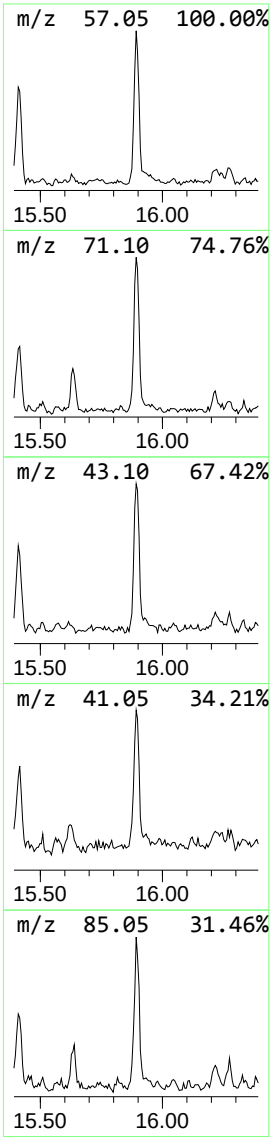
****
Peak Number 3 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	3.41 ng	148751	Phenanthrene-d10	16.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Decane, 2-methyl-	156	C11H24	006975-98-0	90
3	Undecane, 5-methyl-	170	C12H26	001632-70-8	87
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
5	2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	86





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Sample : M3610-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
YORK-ST-MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM090221.M
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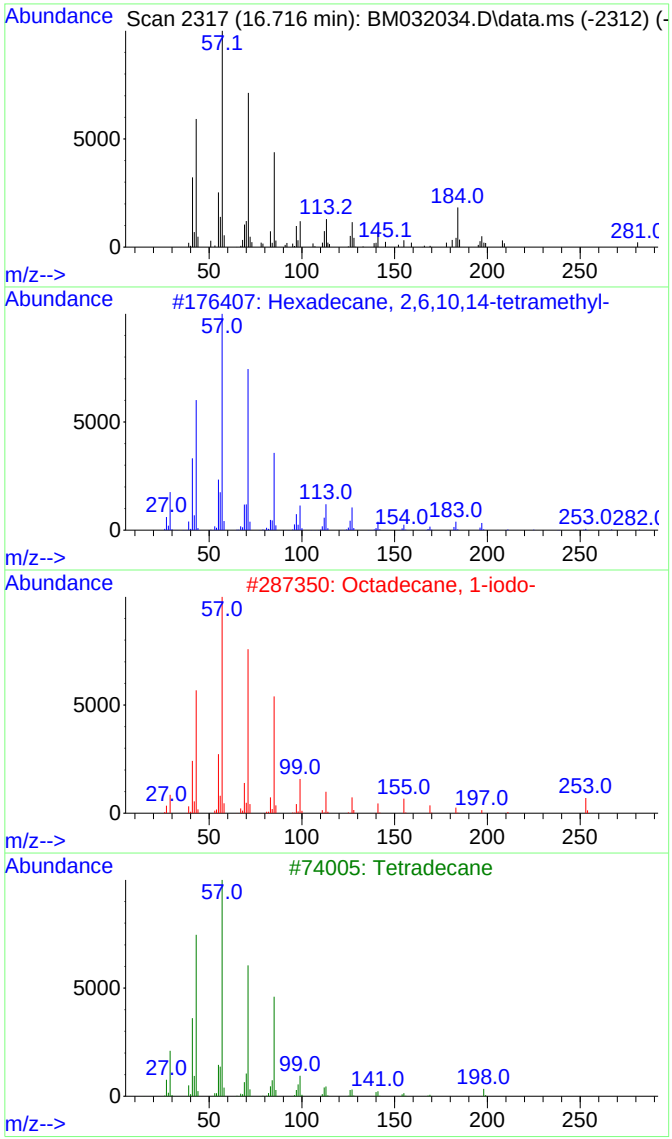
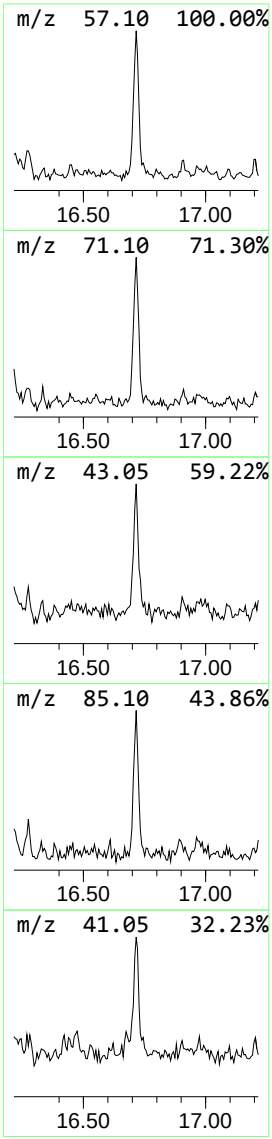
Peak Number 4 Octadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.715	2.27 ng	99141	Phenanthrene-d10	16.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
3	Tetradecane	198	C14H30	000629-59-4	76
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
5	Hexadecane	226	C16H34	000544-76-3	72





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Sample : M3610-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM090221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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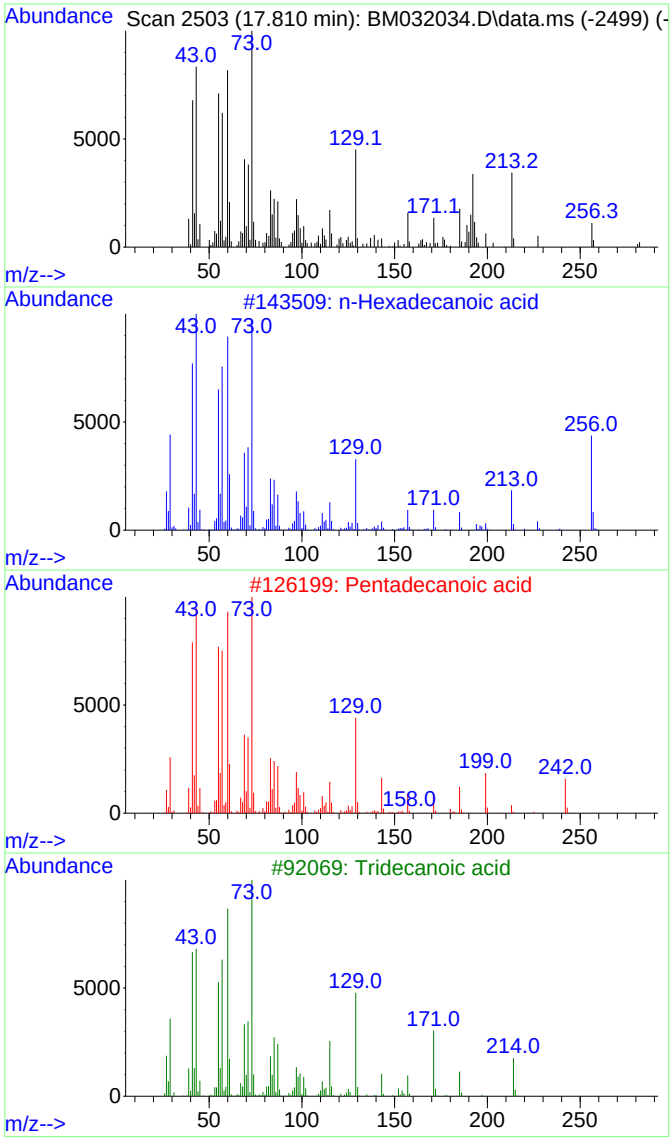
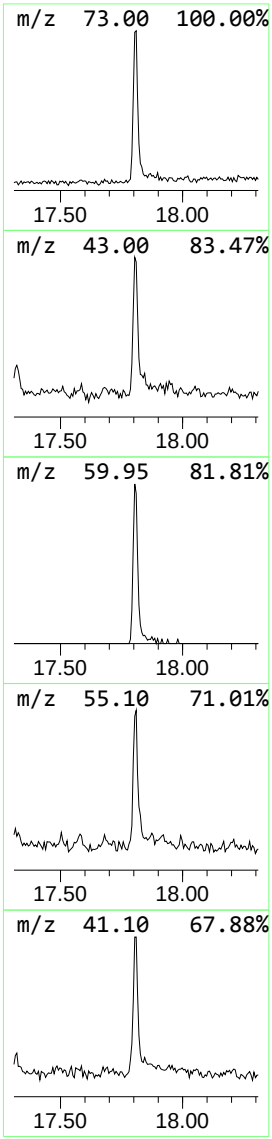
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.810	3.58 ng	156370	Phenanthrene-d10	16.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	N-(3,4-Difluorophenyl)-2,2-dimet...	213	C11H13F2NO	1000486-60-2	25





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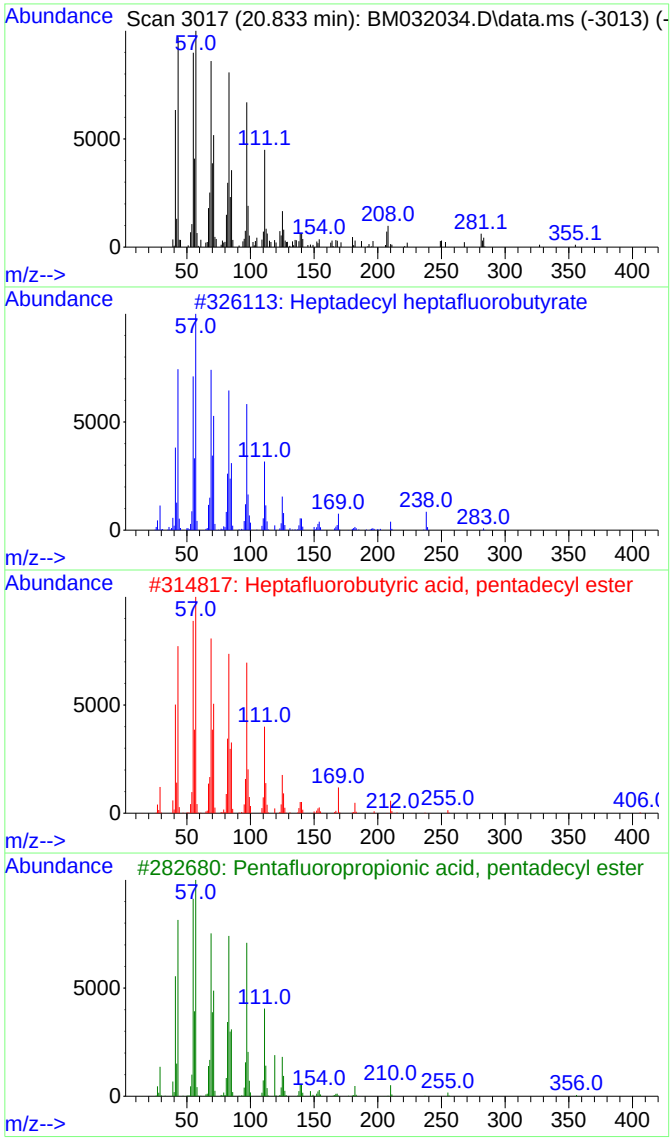
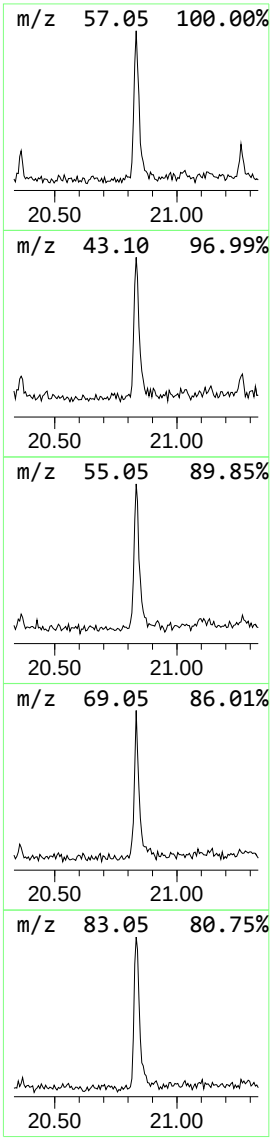
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.833	2.48 ng	130927	Chrysene-d12	21.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	1-Tetracosene	336	C24H48	010192-32-2	91





Tentatively Identified Compound (LSC) summary

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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-...	4.699	4.9	ng	99306	1	7.493	408490	20.0
Hexadecane, 7,9...	15.410	2.3	ng	85199	3	14.133	731906	20.0
Hexadecane, 2,6...	15.892	3.4	ng	148751	4	16.892	872752	20.0
Octadecane, 1-i...	16.715	2.3	ng	99141	4	16.892	872752	20.0
n-Hexadecanoic ...	17.810	3.6	ng	156370	4	16.892	872752	20.0
Heptadecyl hept...	20.833	2.5	ng	130927	5	21.092	1057270	20.0