LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028882.D
Acq On : 24 Feb 2021 16:55
Operator : CG/JU
Sample : M1470-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-591

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.357	397	403	412	rBB	130877	187569	15.22%	3.744%
2	6.987	675	680	690	rBB	76486	131066	10.64%	2.616%
3	7.804	813	819	825	rBB	55448	83348	6.76%	1.663%
4	8.981	1011	1019	1026	rVB	167772	264940	21.50%	5.288%
5	9.957	1178	1185	1190	rBV	9033	14462	1.17%	0.289%
6	10.604	1289	1295	1304	rBB	77009	124918	10.14%	2.493%
7	13.080	1709	1716	1722	rBV	446166	629205	51.06%	12.558%
8	13.927	1855	1860	1865	rVB	13093	16531	1.34%	0.330%
9	14.463	1941	1951	1958	rVV	121383	170784	13.86%	3.409%
10	14.892	2019	2024	2029	rBV	25714	33193	2.69%	0.662%
11	15.715	2156	2164	2168	rBV3	9170	13350	1.08%	0.266%
12	15.962	2200	2206	2213	rBV	437786	607396	49.29%	12.123%
13	16.074	2220	2225	2232	rBV	36463	49584	4.02%	0.990%
14	16.610	2312	2316	2322	rBV2	10503	13443	1.09%	0.268%
15	17.209	2411	2418	2423	rBV	149979	209844	17.03%	4.188%
16	18.104	2563	2570	2579	rBV	183845	250250	20.31%	4.995%
17	19.256	2762	2766	2771	rVB3	12653	18090	1.47%	0.361%
18	19.374	2781	2786	2796	rBV	76493	100164	8.13%	1.999%
19	19.645	2825	2832	2836	rBV2	24488	34597	2.81%	0.690%
20	19.827	2857	2863	2867	rBV	972576	1232345	100.00%	24.595%
21	21.068	3070	3074	3085	rVB	184052	221354	17.96%	4.418%
22	21.274	3105	3109	3114	rBV	31552	35199	2.86%	0.703%
23	21.368	3120	3125	3130	rBV	228896	289271	23.47%	5.773%
24	22.191	3262	3265	3269	rVB3	17520	22017	1.79%	0.439%
25	23.580	3495	3501	3512	rVB2	140946	257545	20.90%	5.140%

Sum of corrected areas: 5010465

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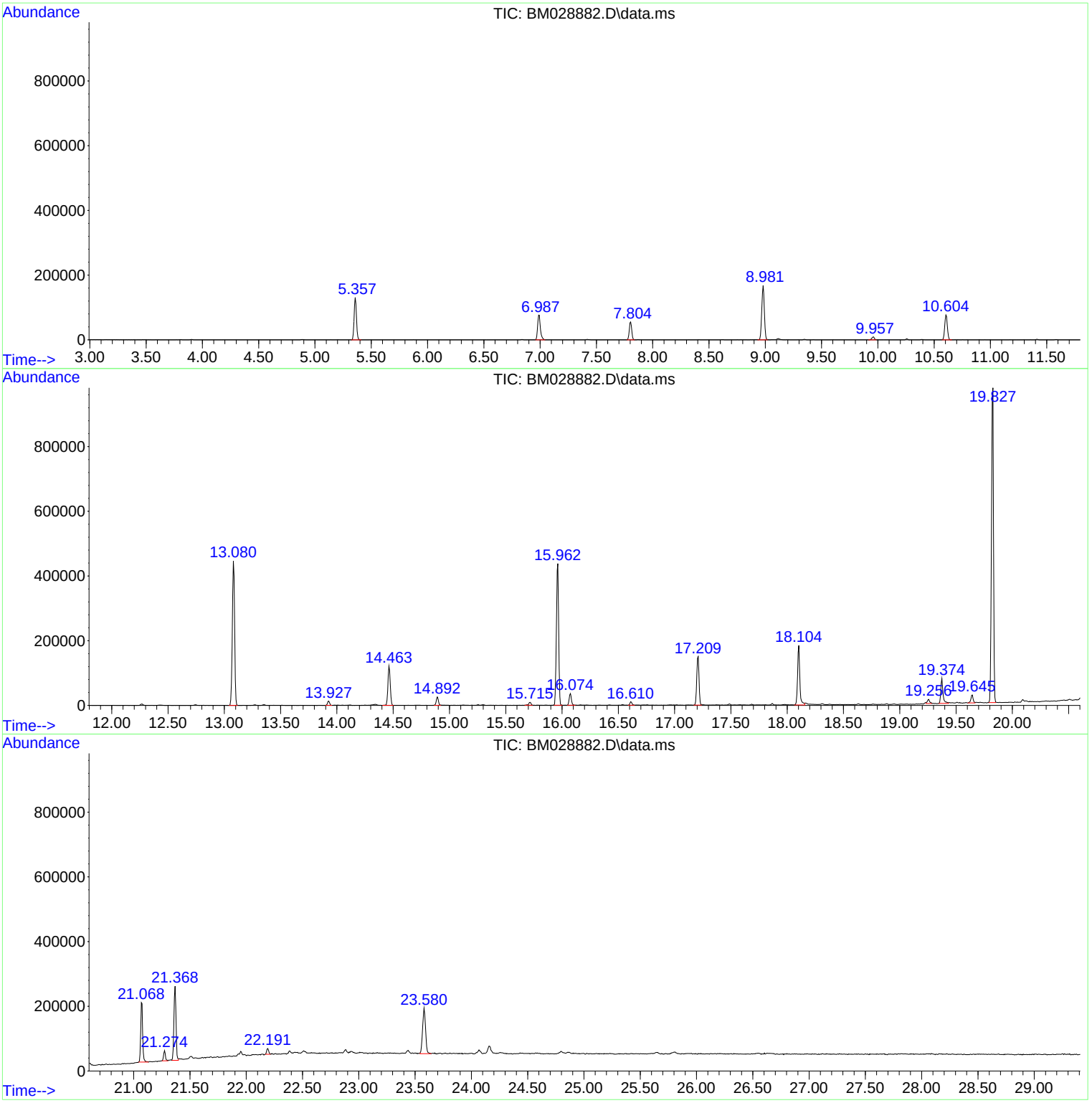
BNA_M
ClientSampleId :
CBH-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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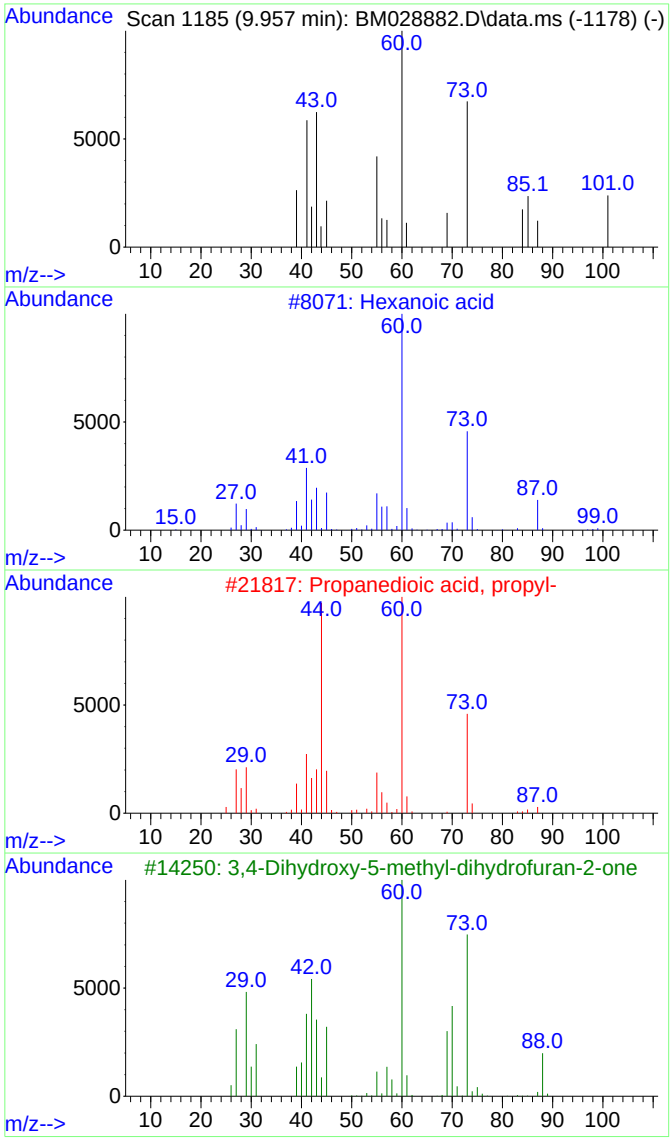
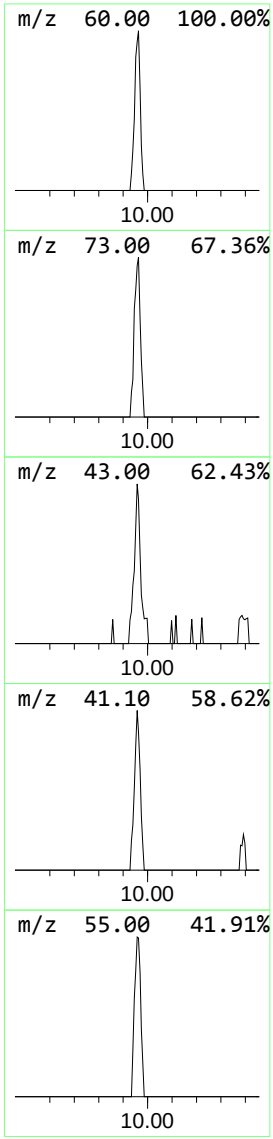
****

Peak Number 1 Hexanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.957	2.32 ng	14462	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	53
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
3	3,4-Dihydroxy-5-methyl-dihydrofu...	132	C5H8O4	1000193-83-1	50
4	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	40
5	Pentanoic acid	102	C5H10O2	000109-52-4	10





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Operator : CG/JU
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Instrument : BNA_M
ClientSampleId : CBH-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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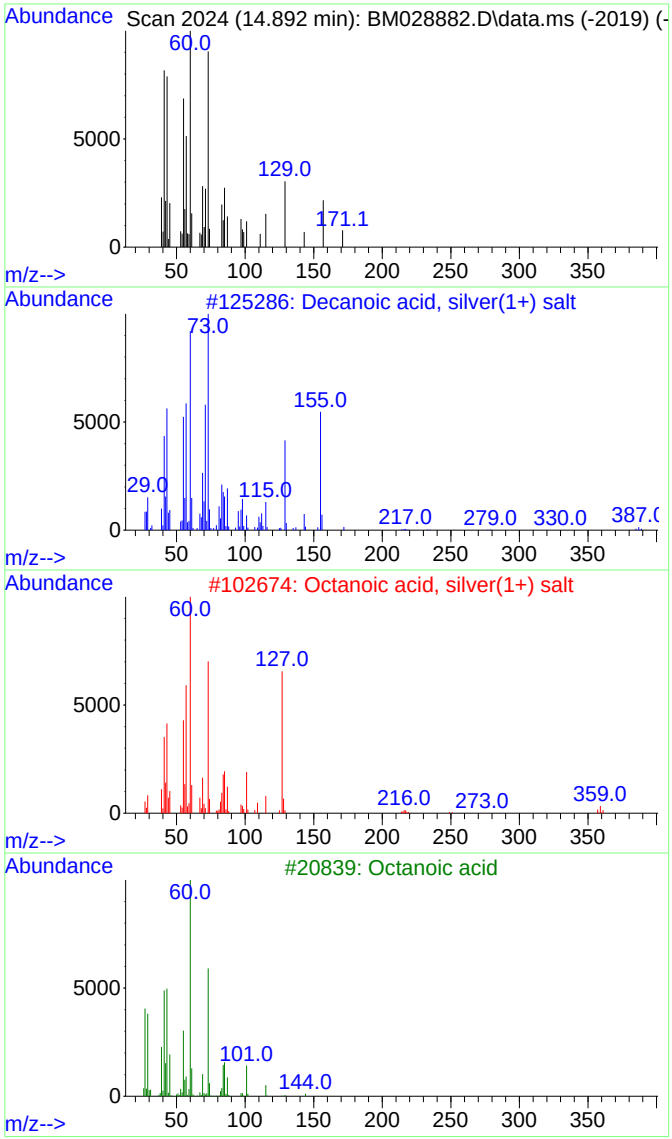
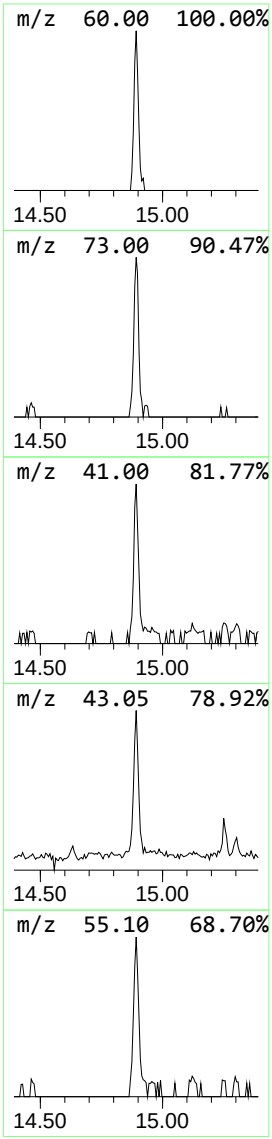
****
Peak Number 2 Decanoic acid, silver(1+) salt Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	3.89 ng	33193	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
3	Octanoic acid	144	C8H16O2	000124-07-2	47
4	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	38
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	35





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Instrument : BNA_M
ClientSampleId : CBH-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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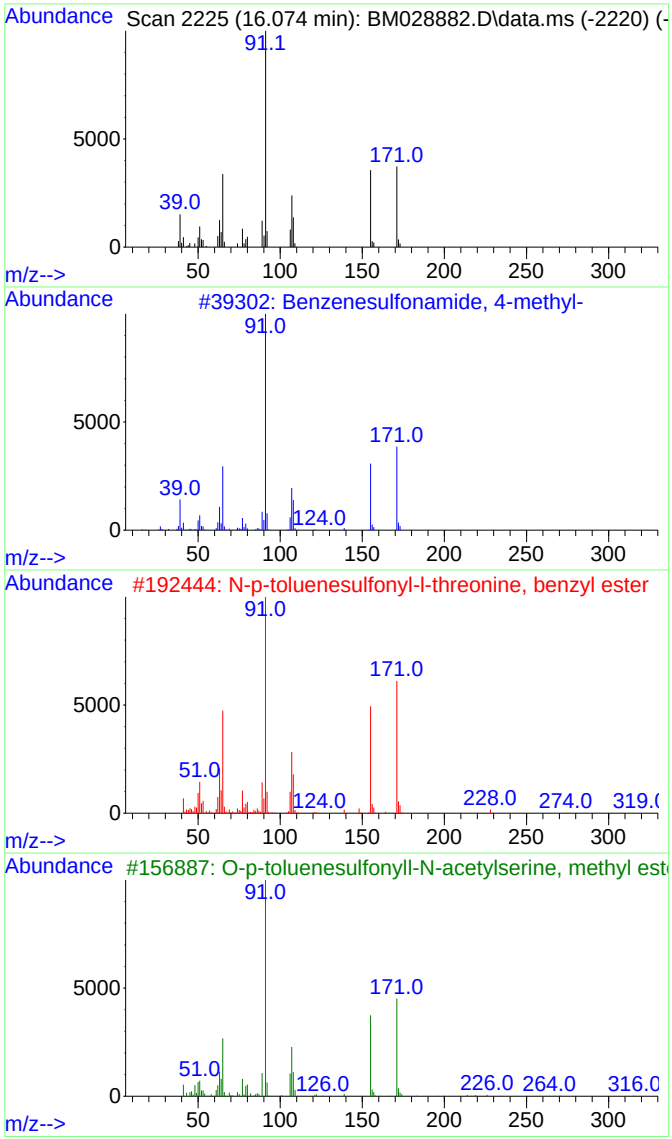
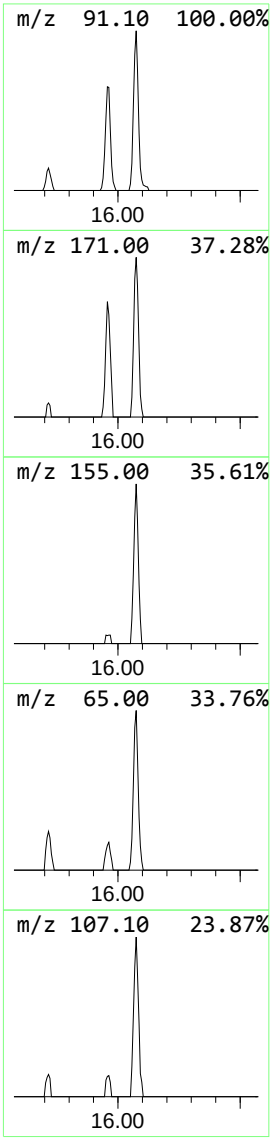
****

Peak Number 3 Benzenesulfonamide, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.074	4.73 ng	49584	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	91
3	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	91
4	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	83
5	Tolbutamide	270	C12H18N2O3S	000064-77-7	53





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Instrument : BNA_M
ClientSampleId : CBH-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

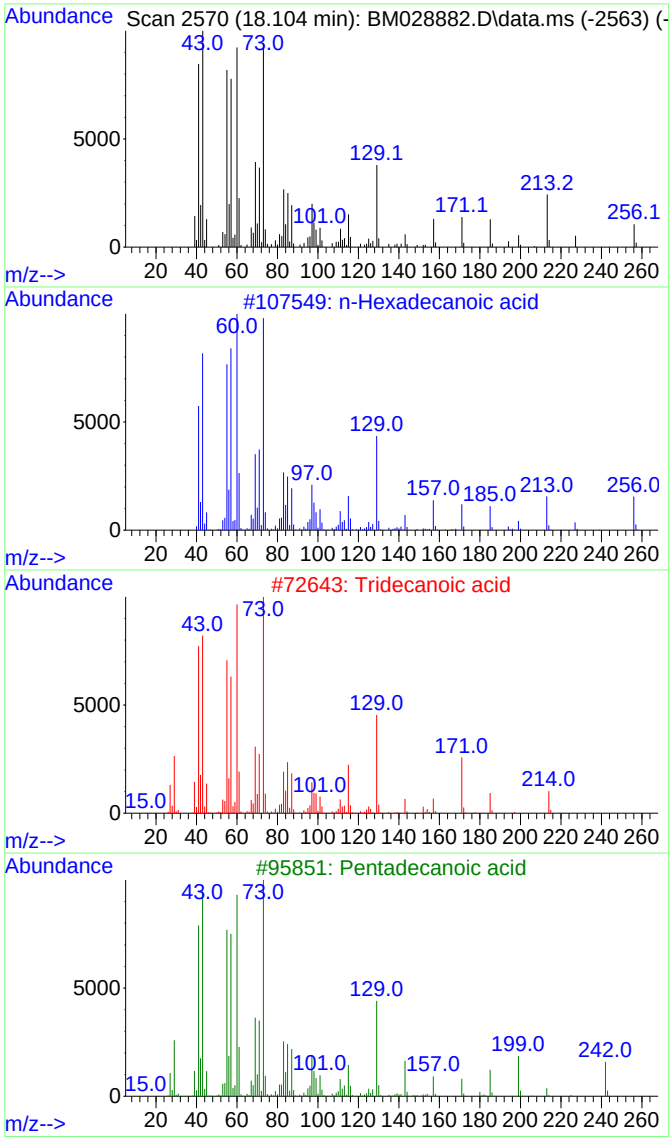
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

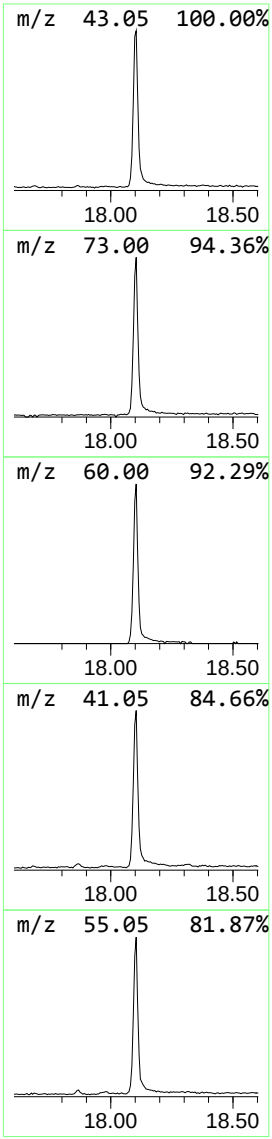
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	23.85 ng	250250	Phenanthrene-d10	17.209

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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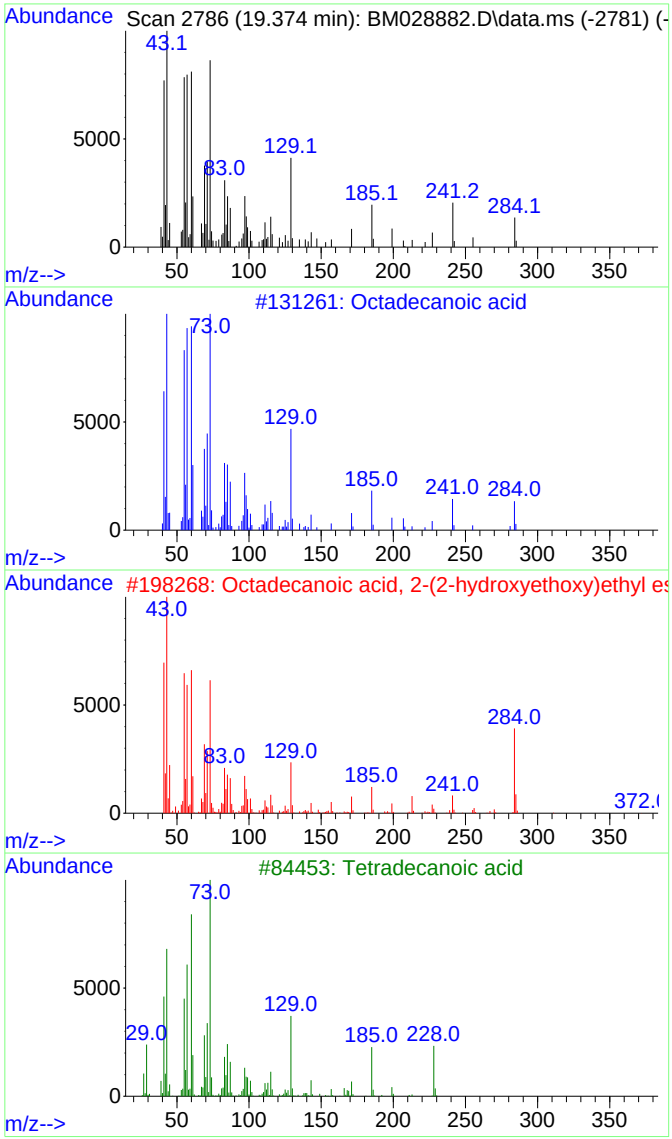
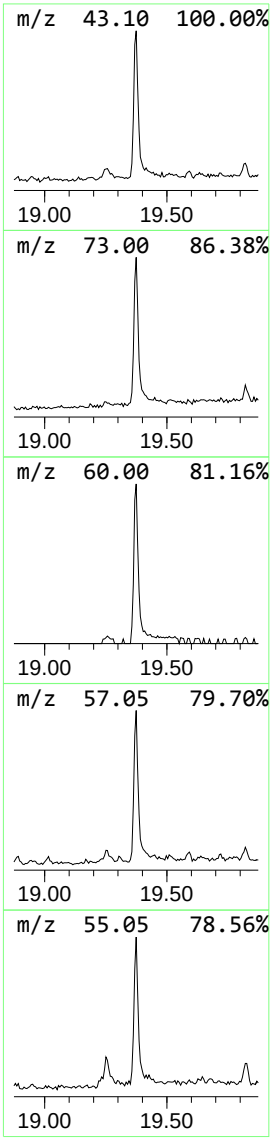
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	6.93 ng	100164	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	45





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Instrument : BNA_M
ClientSampleId : CBH-591

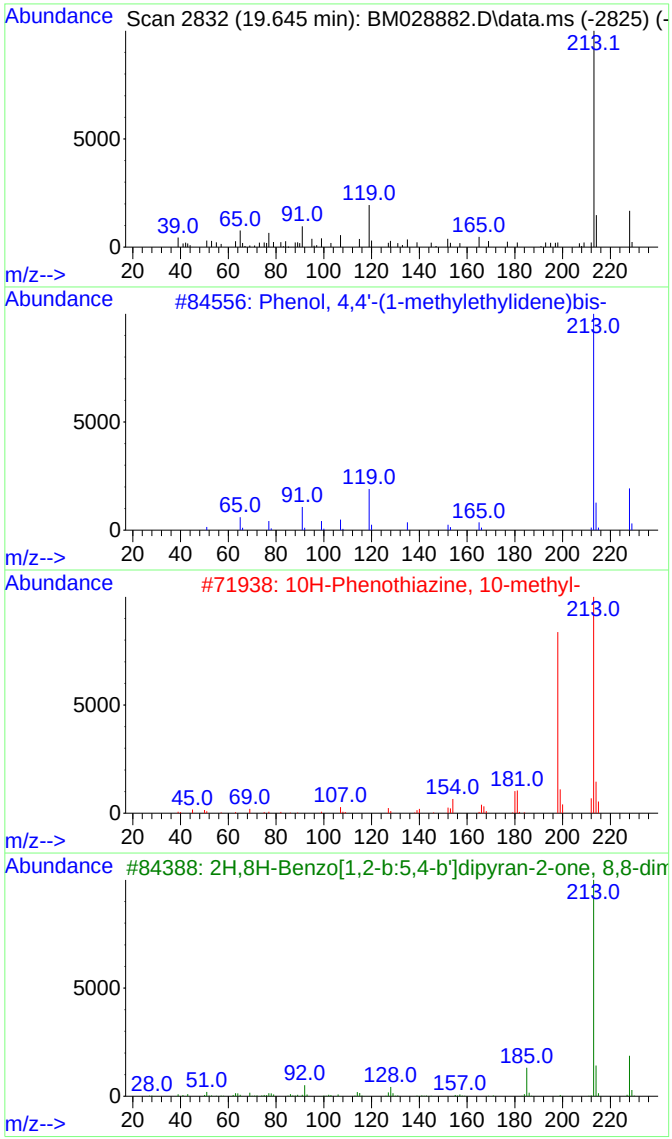
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

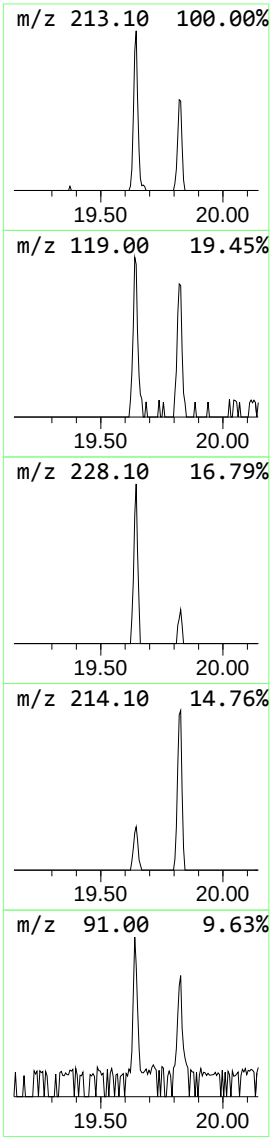
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.645	2.39 ng	34597	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	95
2	10H-Phenothiazine, 10-methyl-	213	C13H11NS	001207-72-3	50
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	50
4	2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	42
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	40





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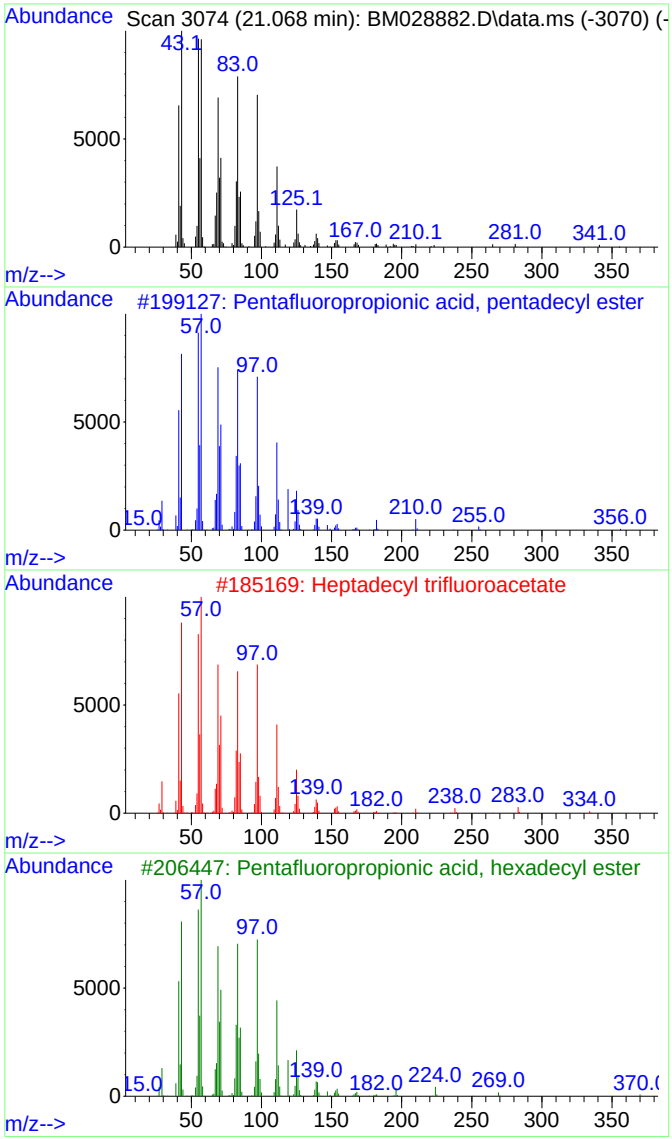
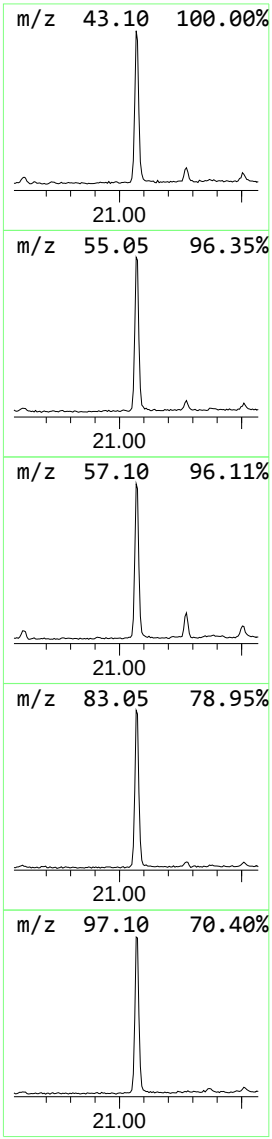
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.068	15.30 ng	221354	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexanoic acid	9.957	2.3	ng	14462	2	10.604	124918	20.0
Decanoic acid, ...	14.892	3.9	ng	33193	3	14.463	170784	20.0
Benzenesulfonam...	16.074	4.7	ng	49584	4	17.209	209844	20.0
n-Hexadecanoic ...	18.104	23.9	ng	250250	4	17.209	209844	20.0
Octadecanoic acid	19.374	6.9	ng	100164	5	21.368	289271	20.0
Phenol, 4,4'-(1...	19.645	2.4	ng	34597	5	21.368	289271	20.0
Pentafluoroprop...	21.068	15.3	ng	221354	5	21.368	289271	20.0