LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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: BM028880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.363	397	404	413	rBV	165855	237925	27.82%	4.989%
2	6.993	674	681	691	rVB	97075	152842	17.87%	3.205%
3	7.804	813	819	826	rVB	73385	108248	12.66%	2.270%
4	8.981	1012	1019	1028	rBV	196707	316658	37.02%	6.640%
5	10.386	1251	1258	1265	rBV	11749	17682	2.07%	0.371%
6	10.604	1288	1295	1302	rBV	89593	148201	17.33%	3.107%
7	12.280	1574	1580	1596	rBV	13665	36813	4.30%	0.772%
8	13.080	1710	1716	1722	rVB	451710	665076	77.76%	13.945%
9	13.927	1854	1860	1865	rVB	18233	23206	2.71%	0.487%
10	14.357	1928	1933	1941	rVB3	6248	12017	1.40%	0.252%
11	14.463	1945	1951	1957	rVB	121672	177696	20.78%	3.726%
12	15.292	2085	2092	2099	rVB3	3761	8697	1.02%	0.182%
13	15.751	2161	2170	2179	rVB2	8693	23798	2.78%	0.499%
14	15.963	2200	2206	2211	rBV	383595	525746	61.47%	11.024%
15	16.715	2330	2334	2343	rBV	11426	20178	2.36%	0.423%
16	17.210	2412	2418	2423	rBV	134485	183546	21.46%	3.849%
17	18.098	2564	2569	2578	rBV	133142	187613	21.93%	3.934%
18	19.374	2777	2786	2795	rBV	74596	118418	13.84%	2.483%
19	19.645	2828	2832	2837	rBV	17545	20430	2.39%	0.428%
20	19.821	2857	2862	2867	rBV	693725	855316	100.00%	17.934%
21	20.133	2911	2915	2922	rVB3	11471	18103	2.12%	0.380%
22	20.568	2974	2989	3005	rVB3	38371	182615	21.35%	3.829%
23	21.068	3070	3074	3083	rVB	113362	133557	15.61%	2.800%
24	21.368	3120	3125	3129	rBV	149055	183447	21.45%	3.846%
25	21.597	3156	3164	3177	rVB4	81048	240382	28.10%	5.040%
26	23.580	3496	3501	3508	rVB2	96208	171011	19.99%	3.586%

Sum of corrected areas: 4769221

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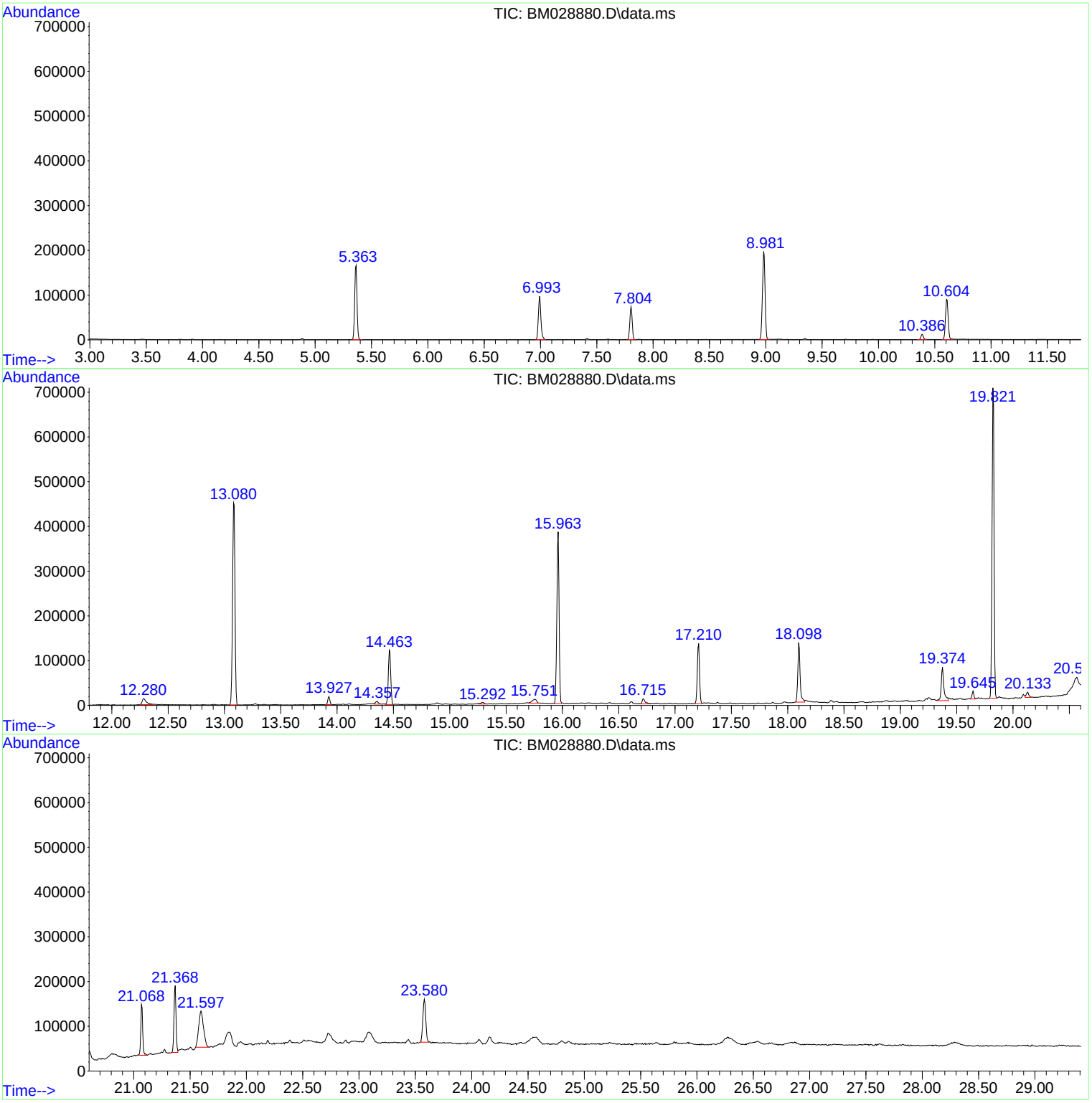
Instrument :
BNA_M
ClientSampleId :
CBH-594

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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Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
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Instrument : BNA_M
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TIC Integration Parameters: LSCINT.P

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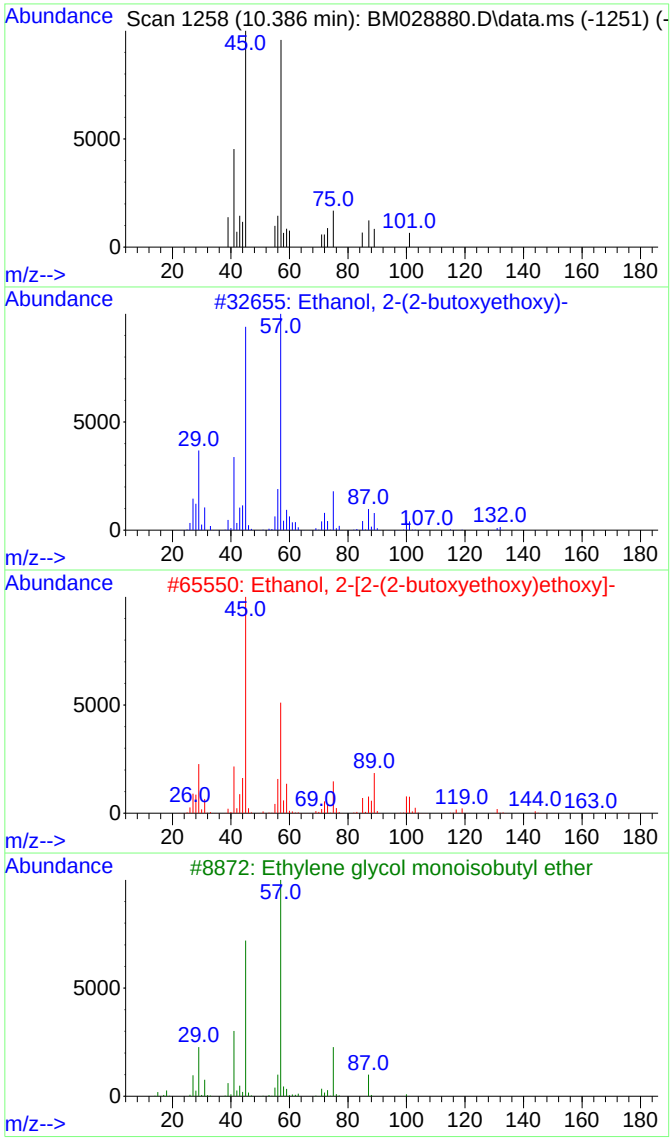
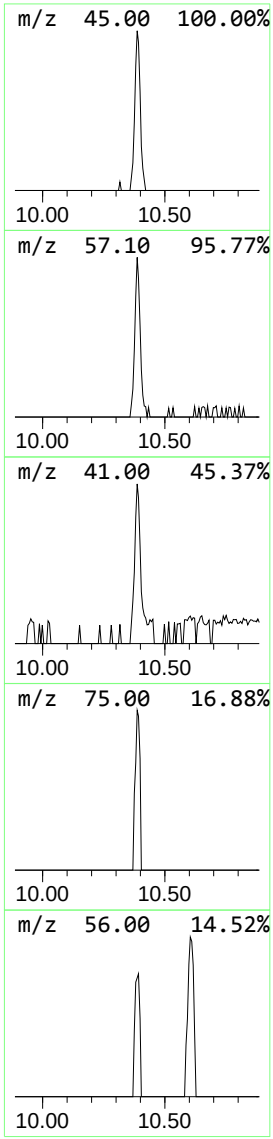
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.386	2.39 ng	17682	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	42
5	Oxirane, (ethoxymethyl)-	102	C5H10O2	004016-11-9	39





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Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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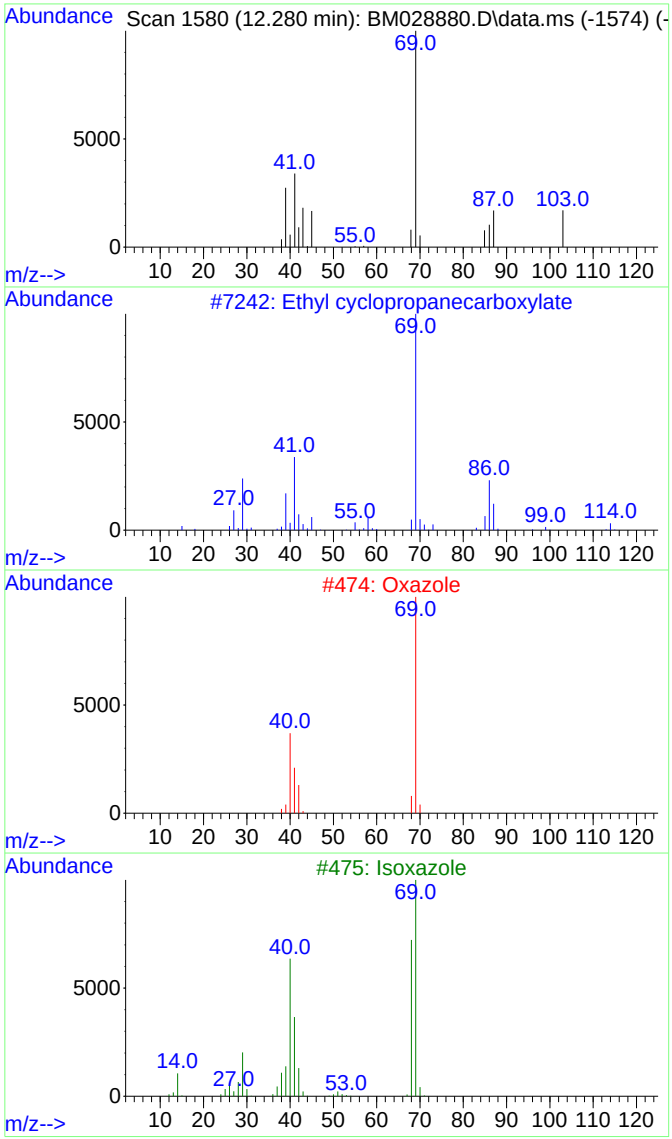
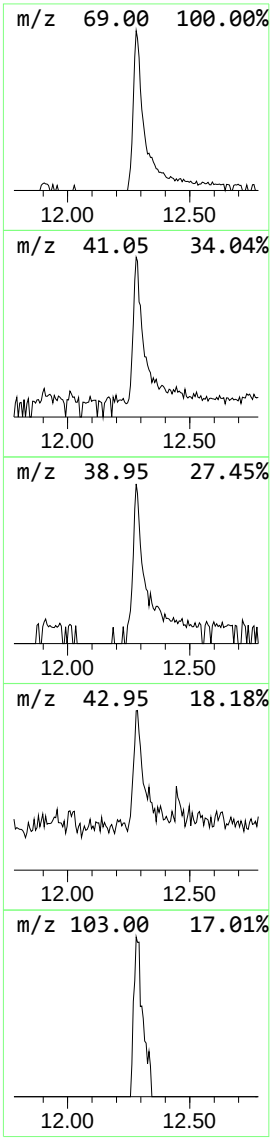
Peak Number 2 unknown12.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.280	4.97 ng	36813	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
2	Oxazole	69	C3H3NO	000288-42-6	9
3	Isoxazole	69	C3H3NO	000288-14-2	9
4	Cyclopropanecarboxylic acid,isob...	142	C8H14O2	064969-79-5	9
5	meso-5,6-Decanediol	174	C10H22O2	003266-25-9	9





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Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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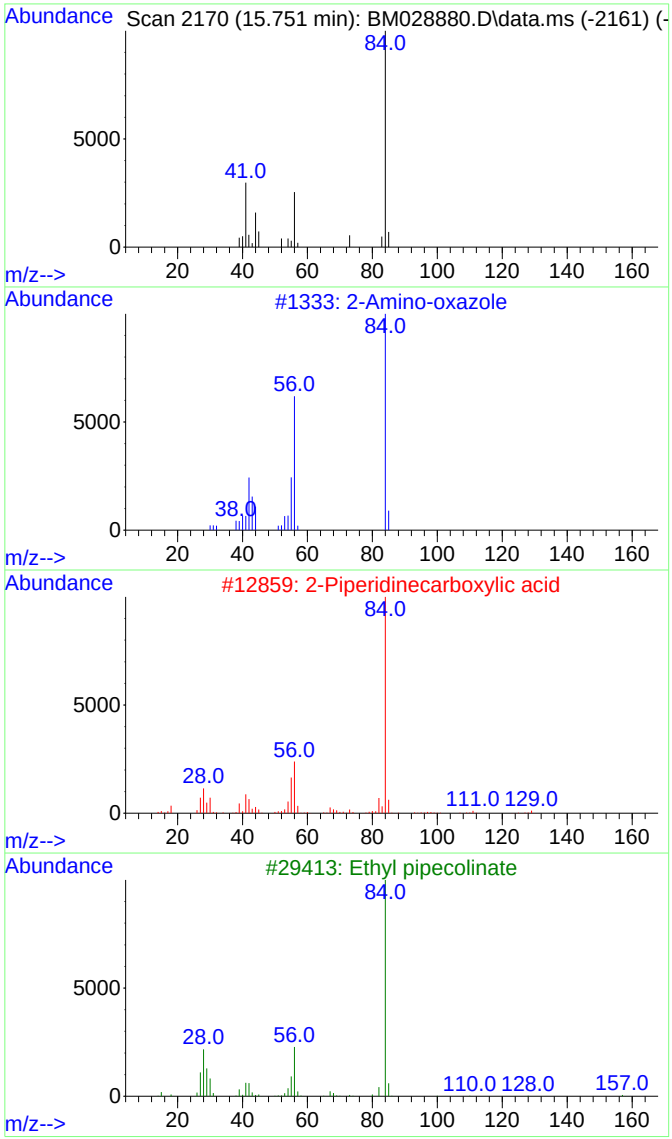
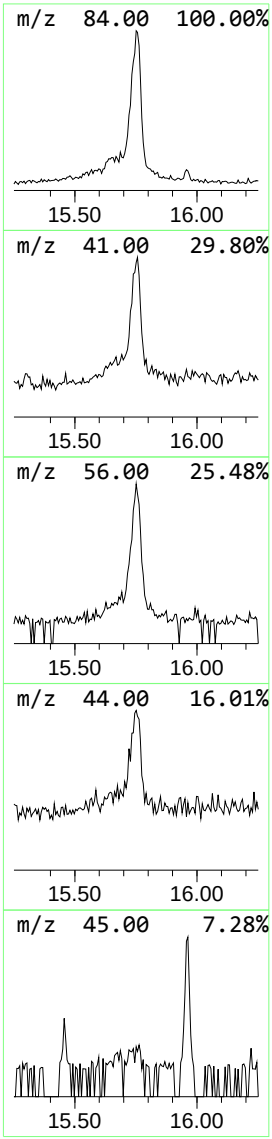
Peak Number 3 2-Amino-oxazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.68 ng	23798	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-oxazole	84	C3H4N2O	004570-45-0	50
2	2-Piperidinecarboxylic acid	129	C6H11NO2	000535-75-1	40
3	Ethyl pipecolinate	157	C8H15NO2	015862-72-3	39
4	Propane, 2-isocyanato-2-methyl-	99	C5H9NO	001609-86-5	38
5	1,5-Pentanediamine	102	C5H14N2	000462-94-2	10





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Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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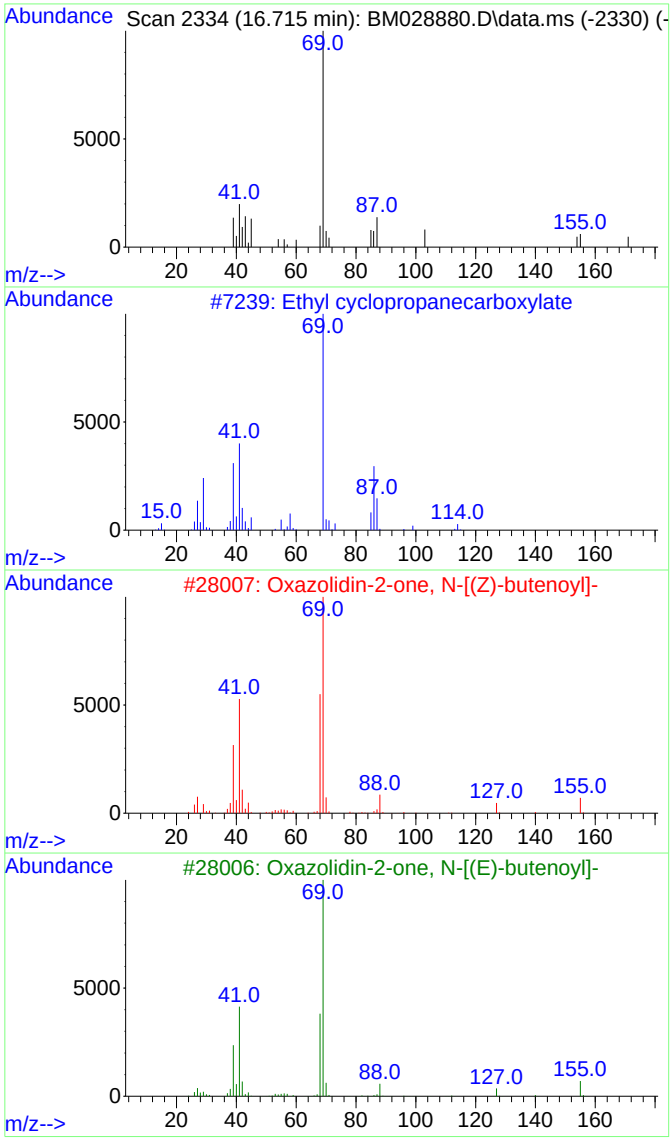
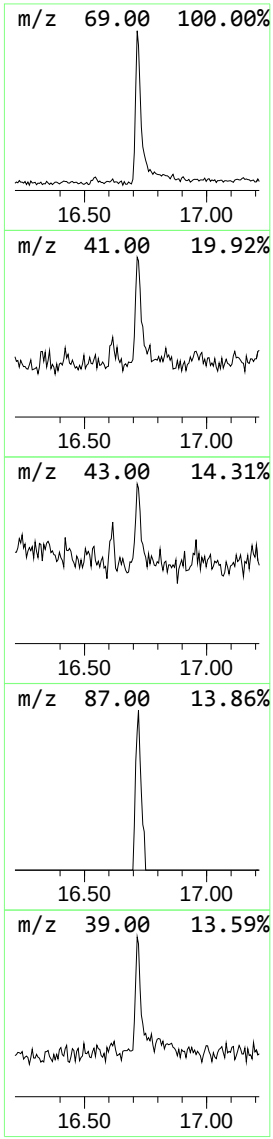
Peak Number 4 unknown16.71 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.715	2.20 ng	20178	Phenanthrene-d10	17.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	42
2	Oxazolidin-2-one, N-[(Z)-butenoyl]-	155	C7H9NO3	1000156-45-4	9
3	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1000156-45-5	9
4	Oxazole	69	C3H3NO	000288-42-6	9
5	2-Decene, 2-methyl-	154	C11H22	023381-92-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
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Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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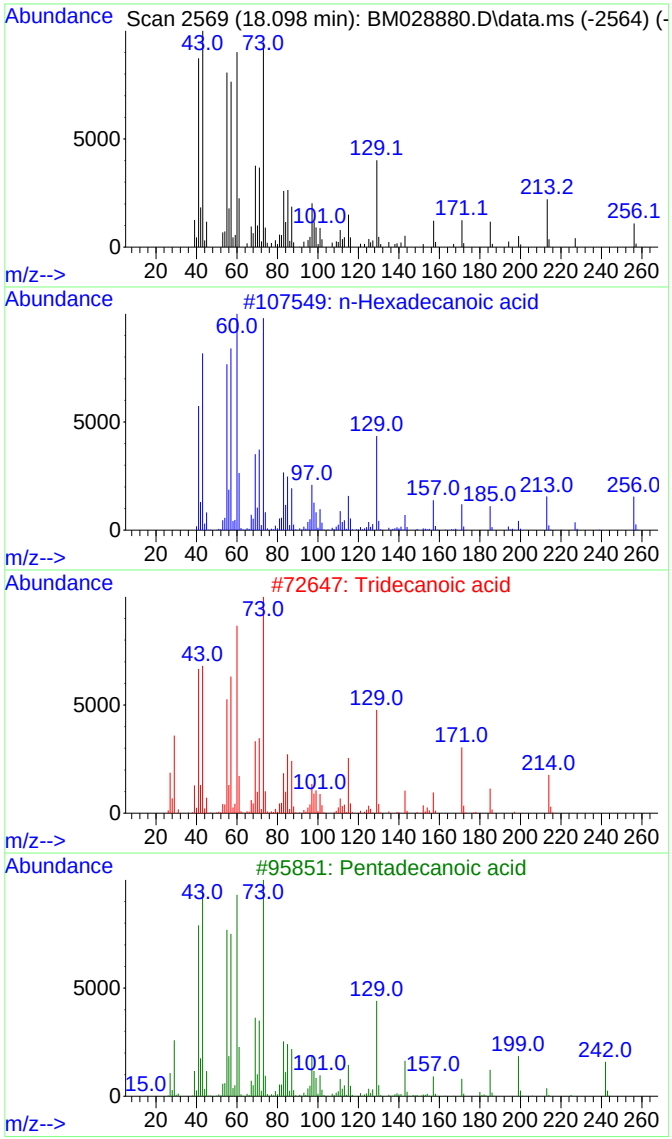
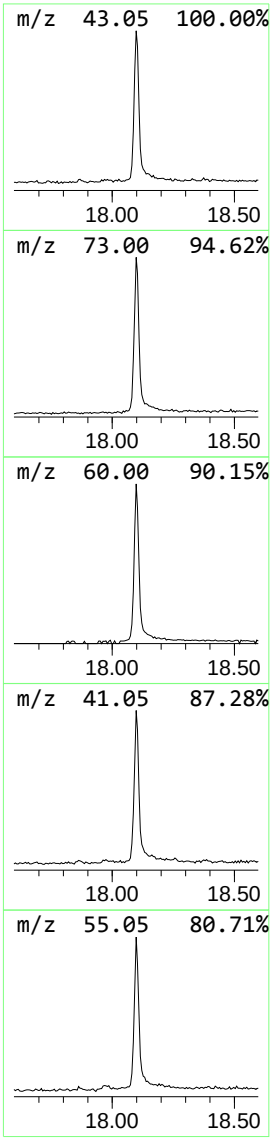
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	20.44 ng	187613	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	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





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Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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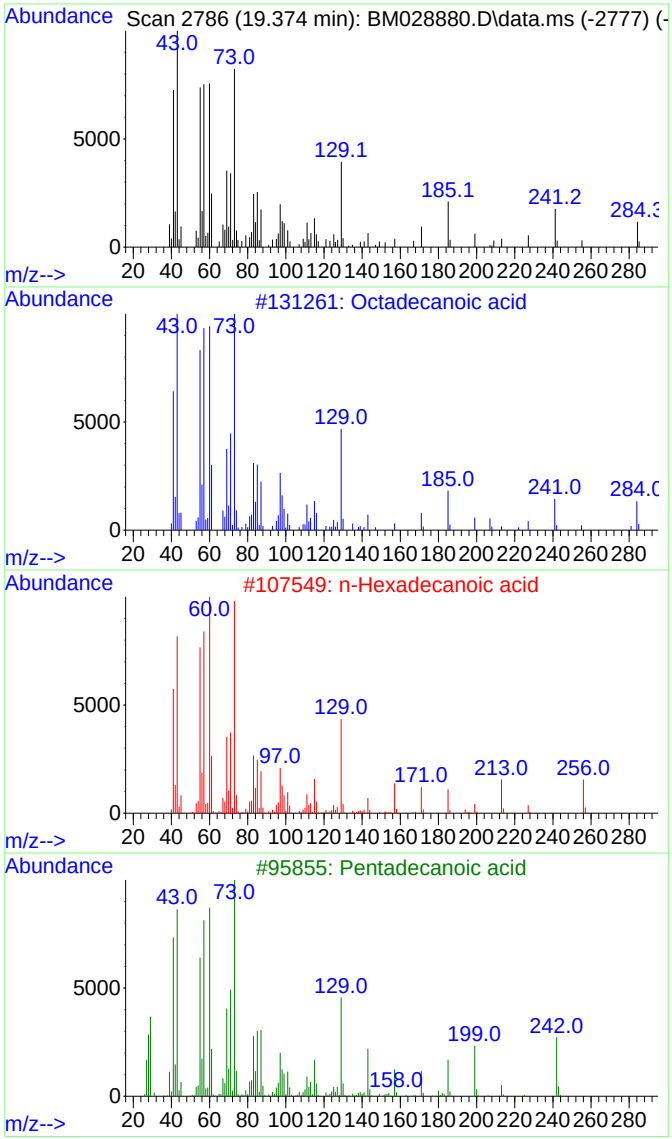
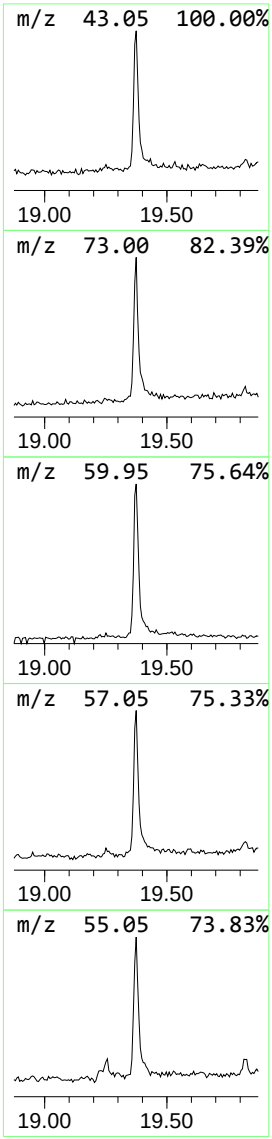
Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	12.91 ng	118418	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74





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Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CBH-594

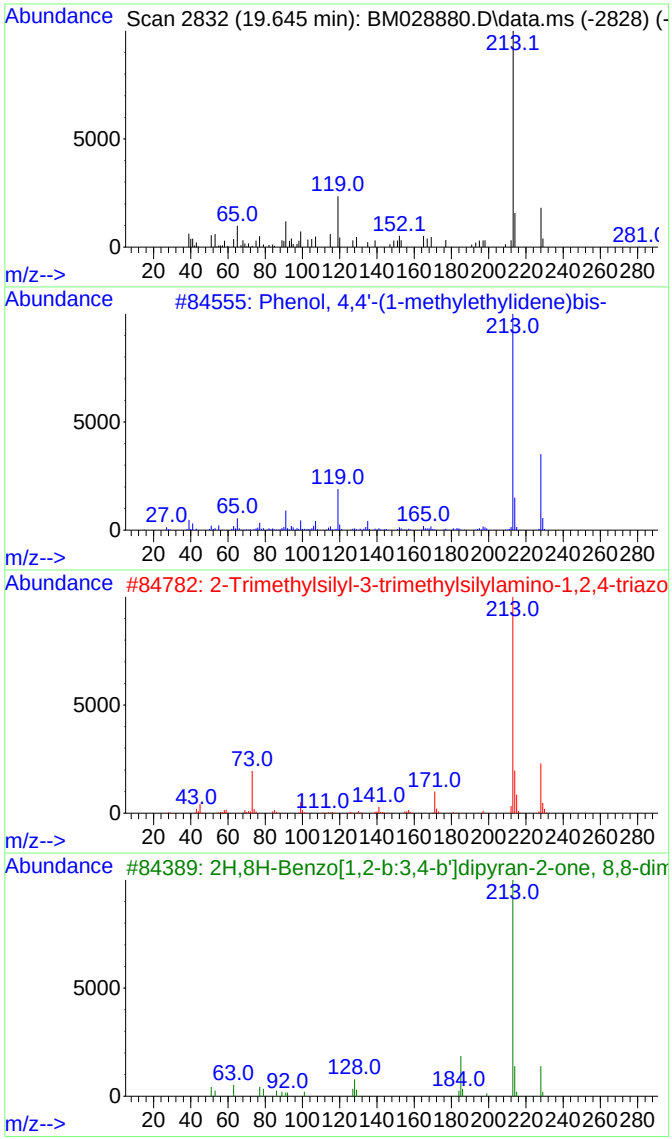
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

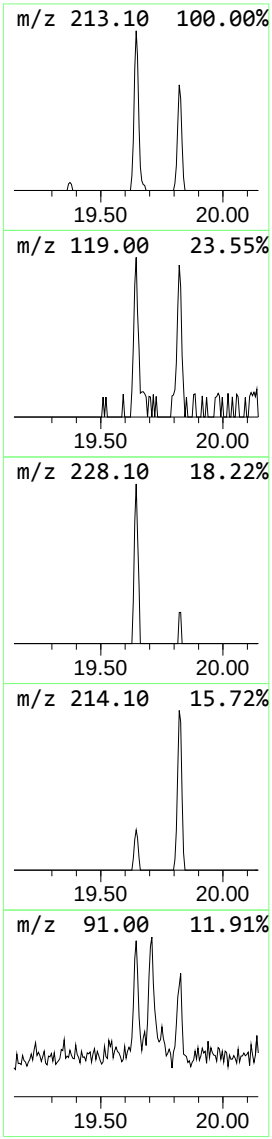
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.645	2.23 ng	20430	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	64
3	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	58
4	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52





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Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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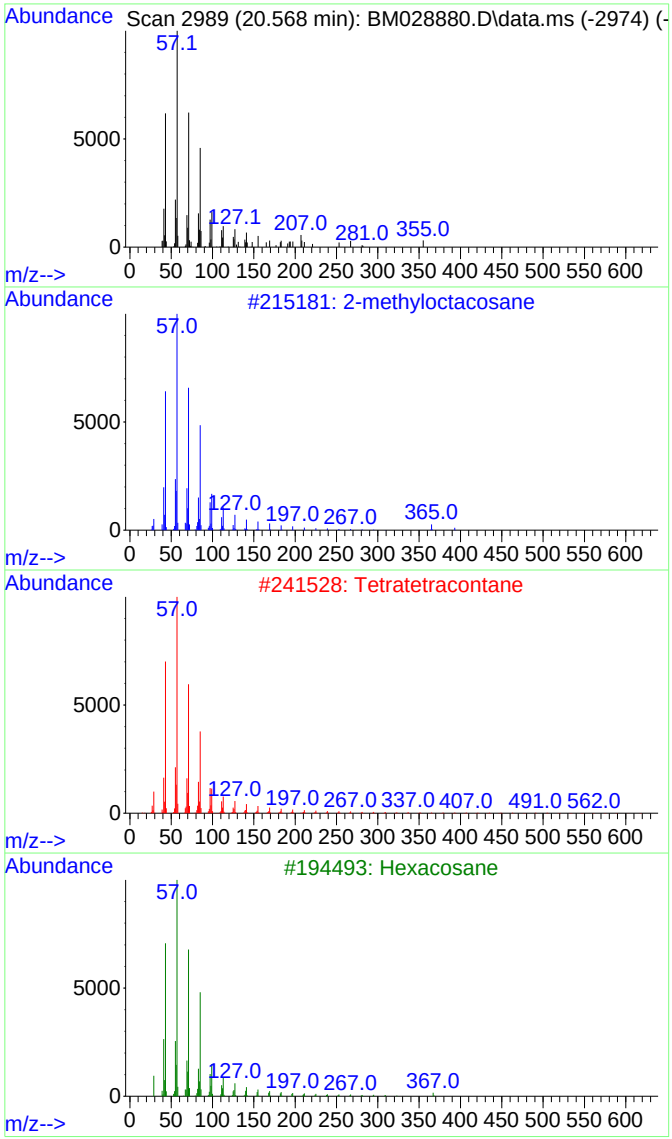
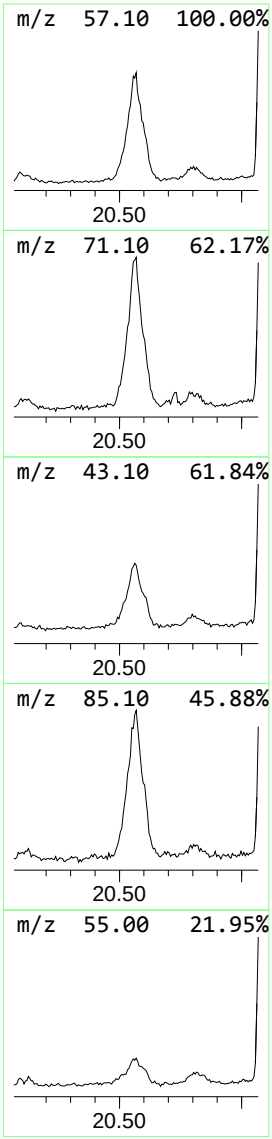
Peak Number 8 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.568	19.91 ng	182615	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Octacosane	394	C28H58	000630-02-4	90





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Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CBH-594

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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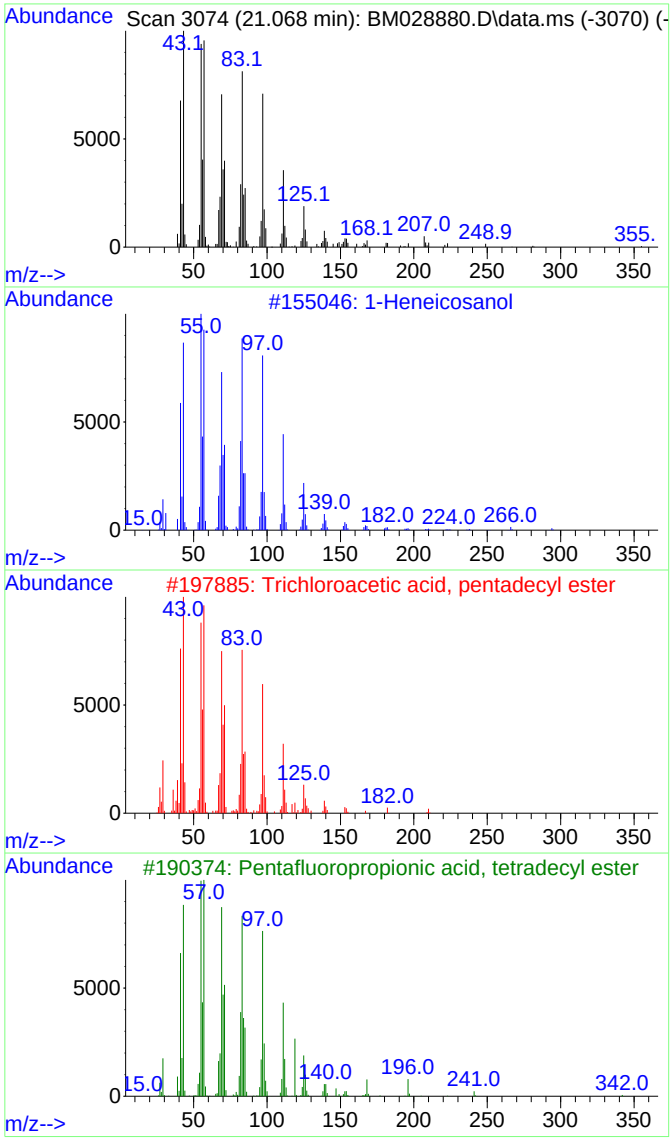
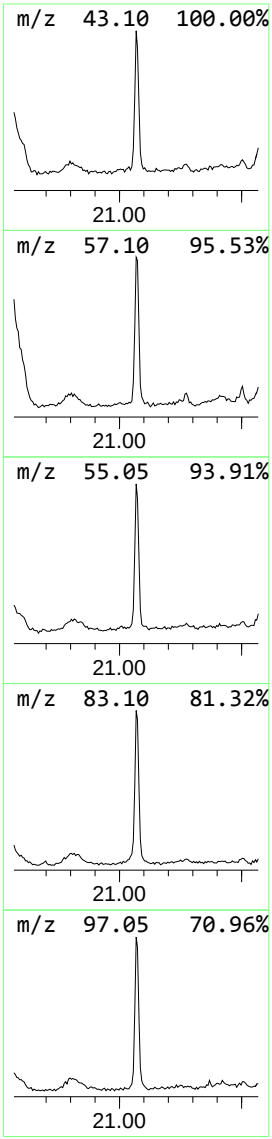
Peak Number 9 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.068	14.56 ng	133557	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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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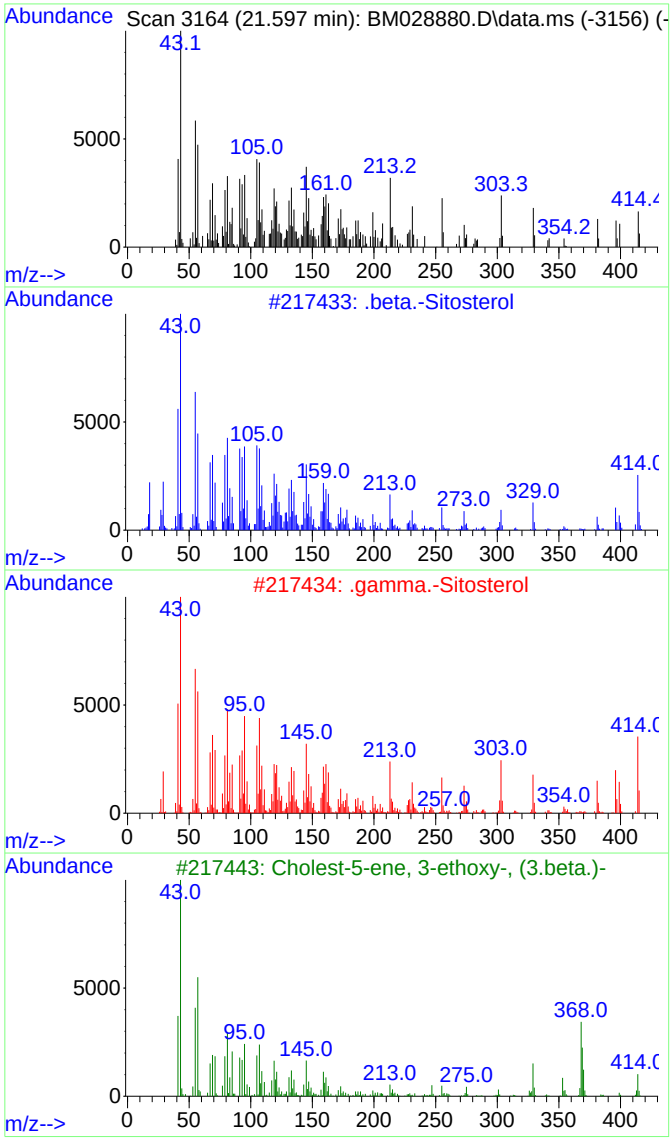
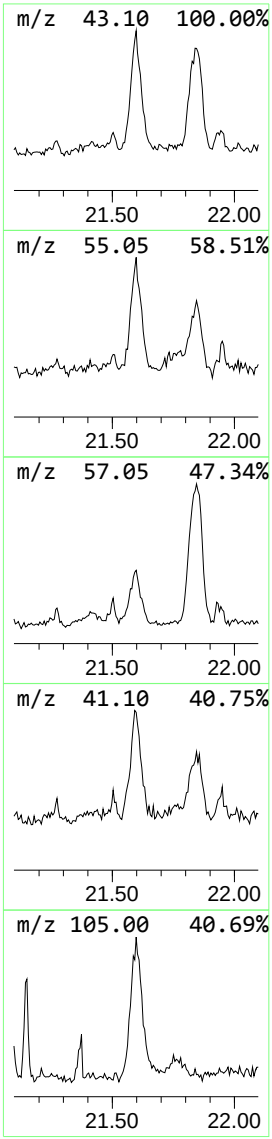
Peak Number 10 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.598	26.21 ng	240382	Chrysene-d12	21.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	98
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	46
4	Pregn-5-en-20-one, 16,17-epoxy-3...	330	C21H30O3	000974-23-2	27
5	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022421\
Data File : BM028880.D
Acq On : 24 Feb 2021 15:41
Operator : CG/JU
Sample : M1470-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CBH-594

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.386	2.4	ng	17682	2	10.604	148201	20.0
unknown12.28	12.280	5.0	ng	36813	2	10.604	148201	20.0
2-Amino-oxazole	15.751	2.7	ng	23798	3	14.463	177696	20.0
unknown16.71	16.715	2.2	ng	20178	4	17.209	183546	20.0
n-Hexadecanoic ...	18.098	20.4	ng	187613	4	17.209	183546	20.0
Octadecanoic acid	19.374	12.9	ng	118418	5	21.368	183447	20.0
Phenol, 4,4'-(1...	19.645	2.2	ng	20430	5	21.368	183447	20.0
2-methyloctacosane	20.568	19.9	ng	182615	5	21.368	183447	20.0
1-Heneicosanol	21.068	14.6	ng	133557	5	21.368	183447	20.0
.beta.-Sitosterol	21.598	26.2	ng	240382	5	21.368	183447	20.0