LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029003.D
Acq On : 05 Mar 2021 19:30
Operator : CG/JU
Sample : M1565-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-4

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: BM029003.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.240	378	383	396	rVB	162884	226957	87.78%	11.422%
2	6.863	653	659	672	rVB	149775	233684	90.38%	11.761%
3	7.675	792	797	804	rVB	35058	50831	19.66%	2.558%
4	8.852	990	997	1007	rBV	91485	145077	56.11%	7.301%
5	10.469	1266	1272	1280	rVB	42507	65873	25.48%	3.315%
6	12.957	1689	1695	1703	rVB	166938	224146	86.69%	11.281%
7	13.234	1737	1742	1747	rVB	3620	4757	1.84%	0.239%
8	13.810	1835	1840	1846	rBV	6401	8001	3.09%	0.403%
9	14.345	1925	1931	1937	rBV	53920	74859	28.95%	3.768%
10	15.839	2180	2185	2192	rVB	138408	184310	71.28%	9.276%
11	17.092	2393	2398	2404	rBV	62425	81956	31.70%	4.125%
12	17.986	2545	2550	2555	rBV	23069	29305	11.33%	1.475%
13	18.374	2609	2616	2620	rBV	32268	42619	16.48%	2.145%
14	18.457	2625	2630	2637	rBV3	32866	42819	16.56%	2.155%
15	18.733	2672	2677	2681	rBV	6978	9439	3.65%	0.475%
16	19.269	2764	2768	2776	rBV	12080	15383	5.95%	0.774%
17	19.668	2833	2836	2839	rBV2	2590	2746	1.06%	0.138%
18	19.716	2839	2844	2849	rVV	217483	258556	100.00%	13.013%
19	20.698	3008	3011	3015	rVB5	2441	2718	1.05%	0.137%
20	20.980	3055	3059	3068	rBV	35639	46430	17.96%	2.337%
21	21.268	3103	3108	3112	rBV	92058	109055	42.18%	5.489%
22	21.680	3175	3178	3181	rBV2	4134	4882	1.89%	0.246%
23	23.427	3470	3475	3484	rVB2	68715	122548	47.40%	6.168%

Sum of corrected areas: 1986951

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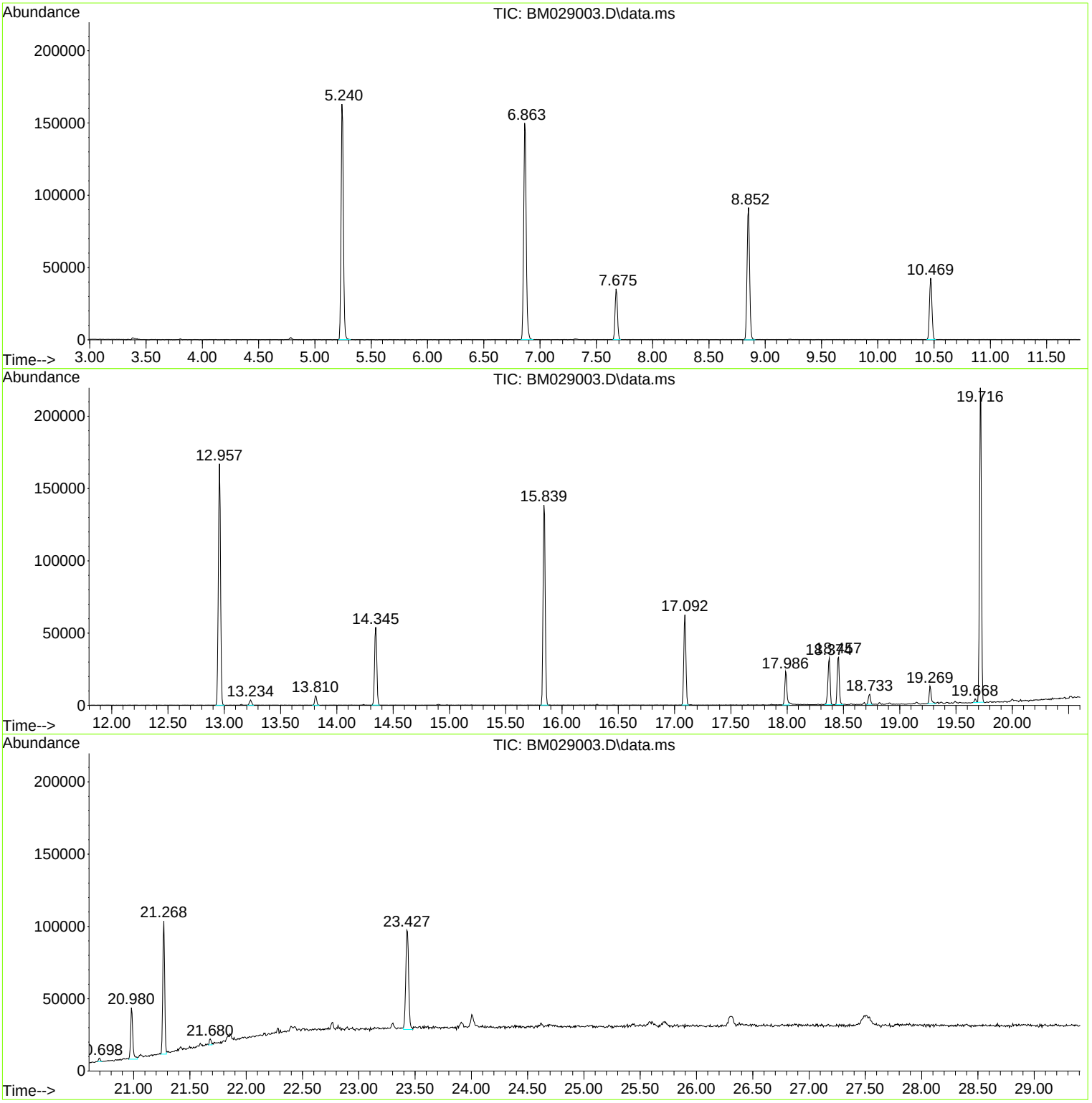
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM029003.D
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TIC Library : C:\DATABASE\NIST11.L
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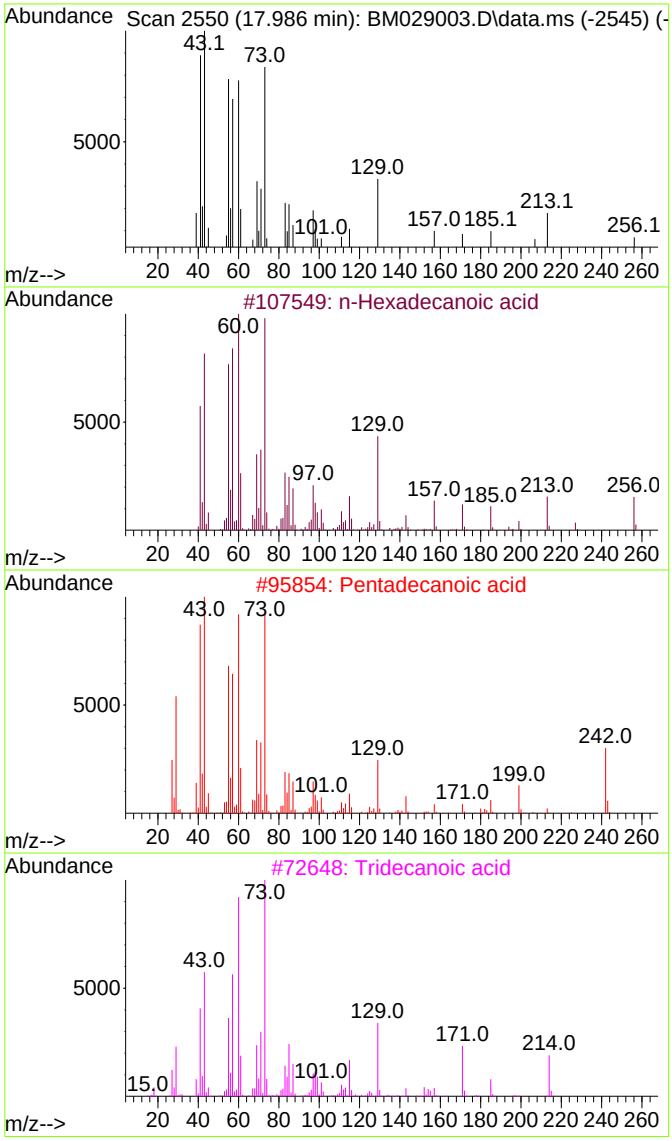
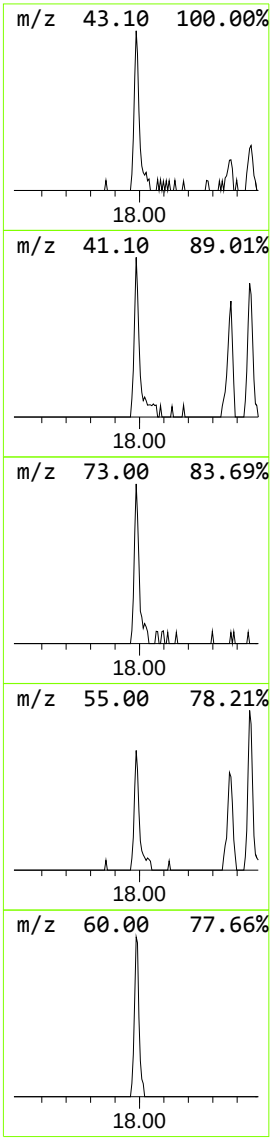
Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	7.15 ng	29305	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Trehalose	342	C12H22O11	000099-20-7	50





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-4

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

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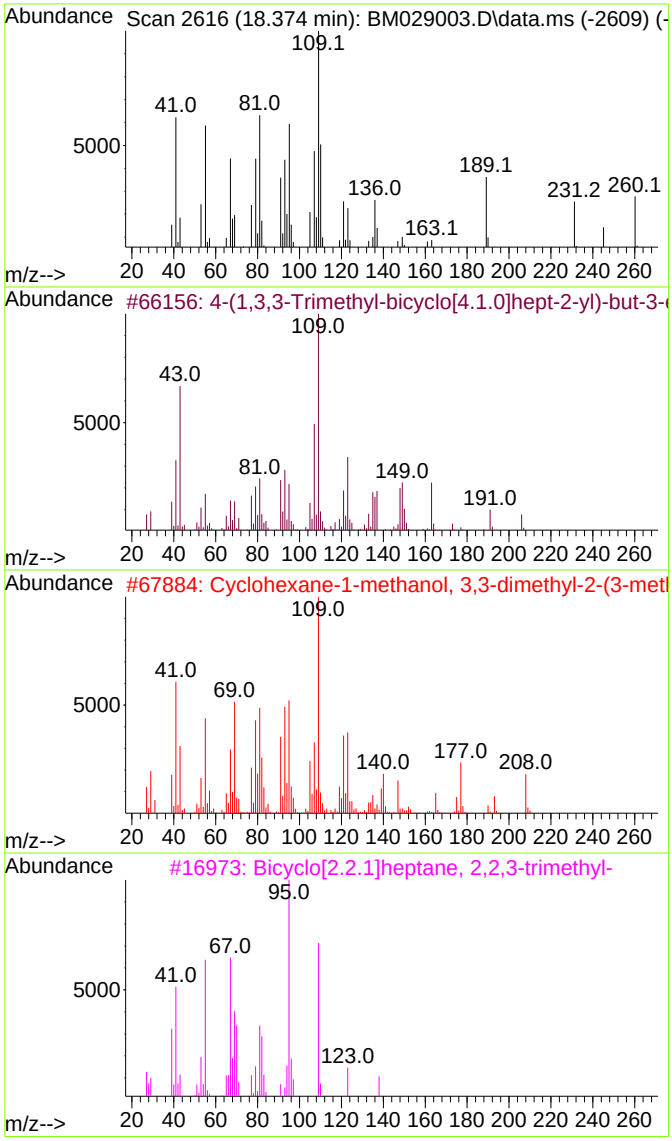
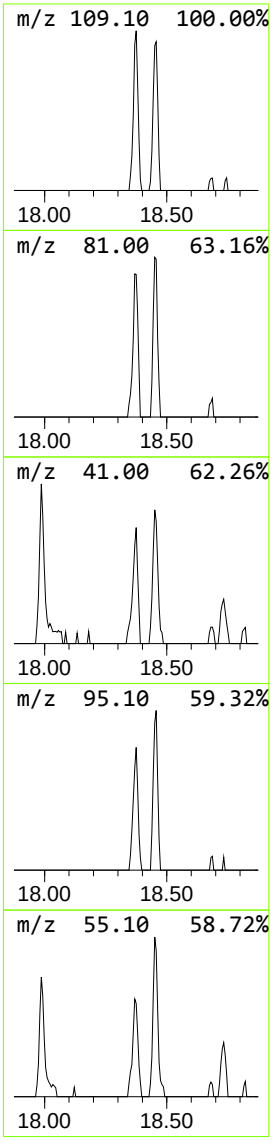
Peak Number 2 unknown18.374 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	10.40 ng	42619	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	43
2	Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	38
3	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	35
4	1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	35
5	Ethyl Camphorsulfonates	260	C12H20O4S	1000373-95-5	35





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Data File : BM029003.D
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Operator : CG/JU
Sample : M1565-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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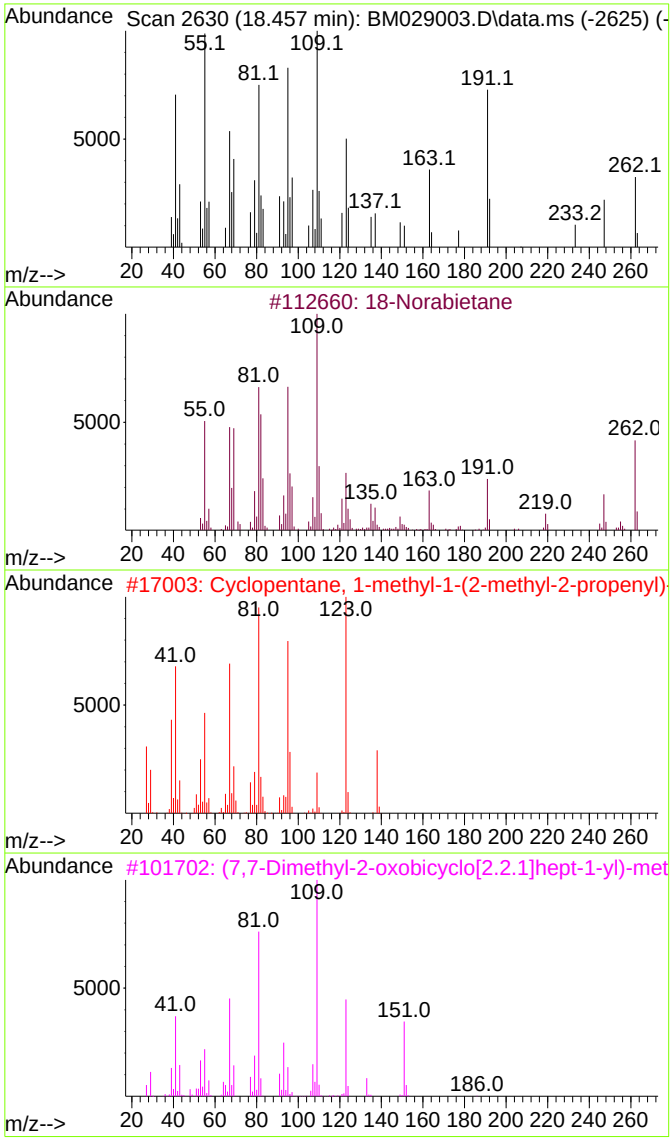
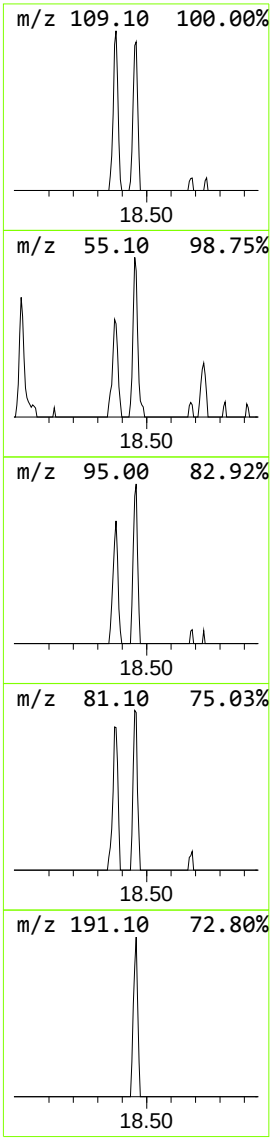
Peak Number 3 unknown18.457 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.457	10.45 ng	42819	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Norabietane	262	C19H34	1000293-16-6	41
2	Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	38
3	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	38
4	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	27
5	2-Cyclopenten-1-one, 3,5,5-trime...	124	C8H12O	024156-95-4	27





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Instrument : BNA_M
ClientSampleId : TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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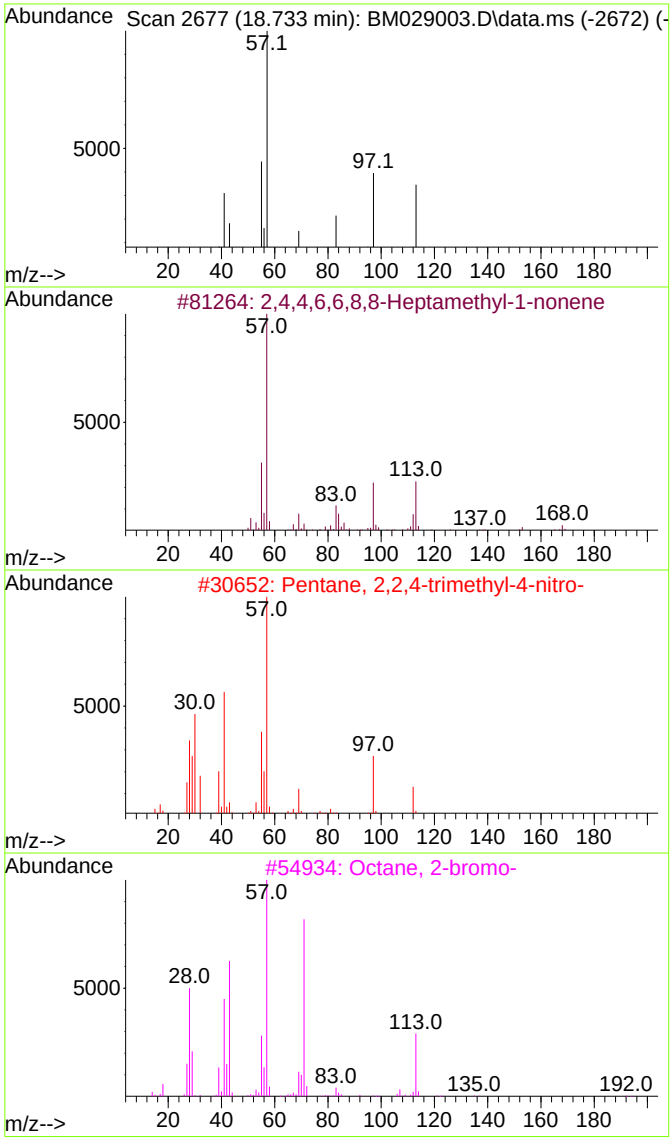
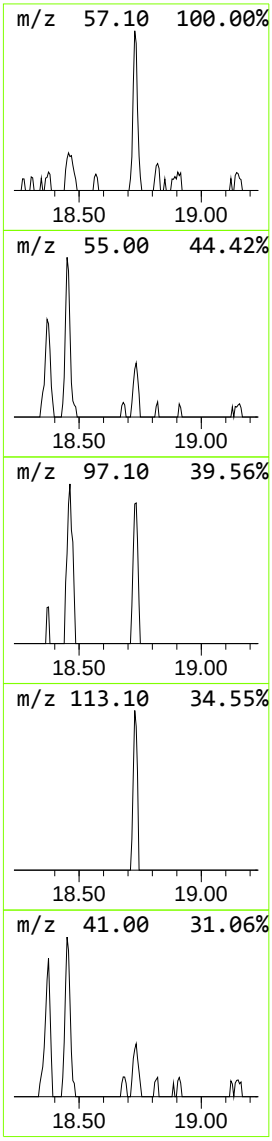
Peak Number 4 unknown18.733 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.733	2.30 ng	9439	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	9
2	Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	9
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	9
4	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	9
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	9





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Instrument : BNA_M
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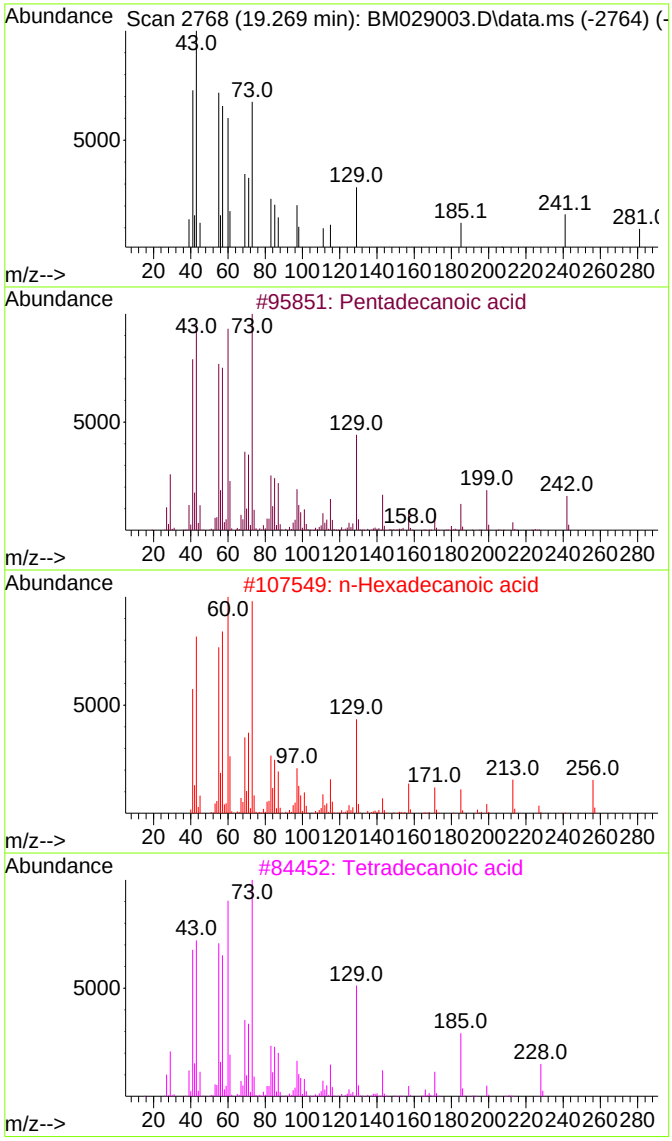
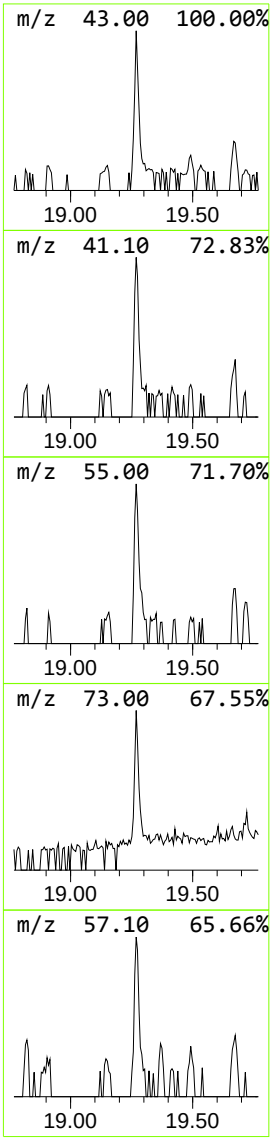
Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.269	2.82 ng	15383	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Maltose	342	C12H22O11	000069-79-4	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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ClientSampleId :
TP-4

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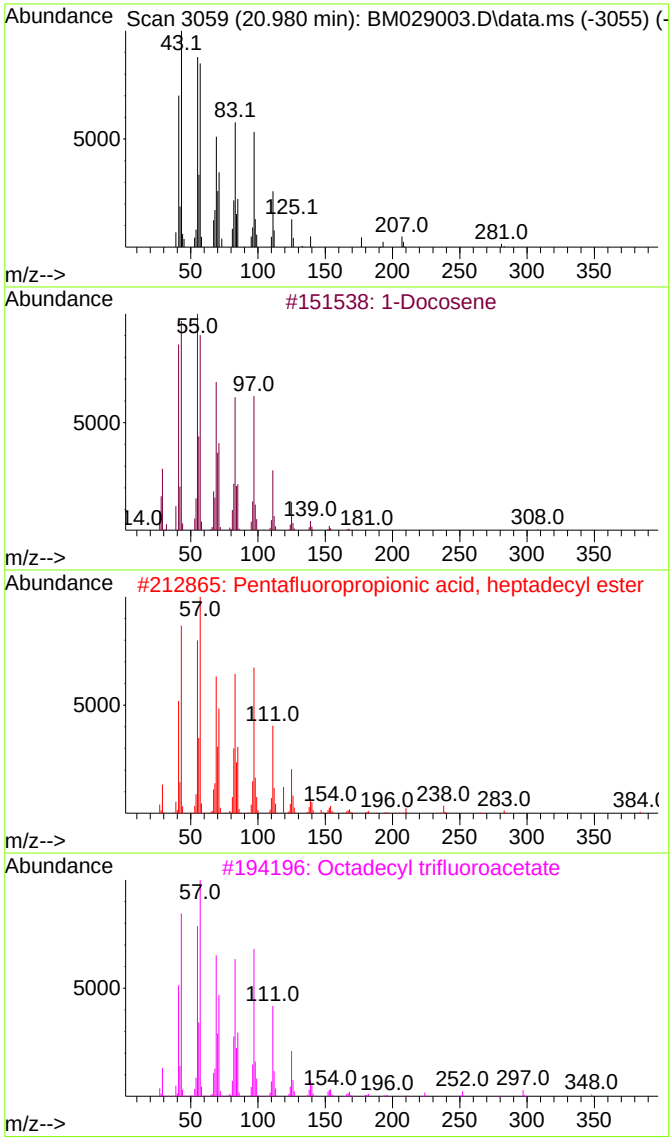
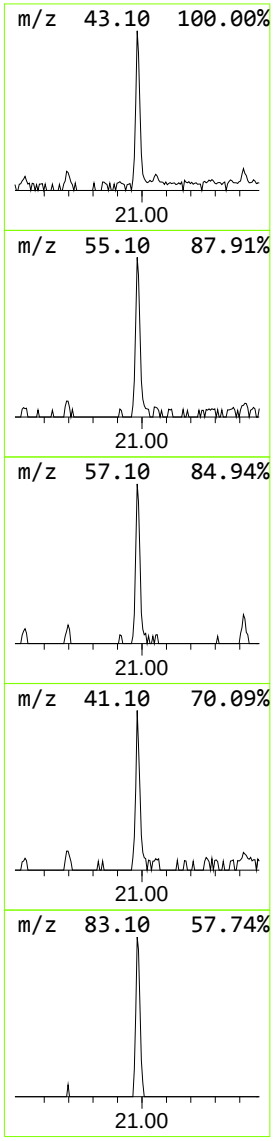
Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	8.51 ng	46430	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	17.986	7.2	ng	29305	4	17.092	81956	20.0
unknown18.374	18.374	10.4	ng	42619	4	17.092	81956	20.0
unknown18.457	18.457	10.4	ng	42819	4	17.092	81956	20.0
unknown18.733	18.733	2.3	ng	9439	4	17.092	81956	20.0
Pentadecanoic acid	19.269	2.8	ng	15383	5	21.268	109055	20.0
1-Docosene	20.980	8.5	ng	46430	5	21.268	109055	20.0