LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029261.D
Acq On : 30 Mar 2021 01:23
Operator : CG/JU
Sample : M1786-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-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-BM032621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	17	22	27	rBV	685292	813618	11.27%	1.951%
2	3.058	27	29	38	rVB2	56762	73255	1.01%	0.176%
3	5.364	415	421	433	rBV	2419923	3457374	47.90%	8.292%
4	6.940	681	689	703	rBV	2353569	3767219	52.19%	9.035%
5	7.758	821	828	836	rBV	471521	750952	10.40%	1.801%
6	8.910	1014	1024	1033	rBV	1476679	2427616	33.63%	5.822%
7	10.540	1292	1301	1310	rBV	614529	1039292	14.40%	2.493%
8	12.187	1573	1581	1592	rBV	40385	95983	1.33%	0.230%
9	13.004	1713	1720	1727	rBV	3357994	5054570	70.03%	12.122%
10	13.839	1858	1862	1872	rVB	79053	122620	1.70%	0.294%
11	14.387	1948	1955	1966	rVB	865988	1328352	18.40%	3.186%
12	14.975	2048	2055	2060	rBV	106798	155735	2.16%	0.373%
13	15.869	2201	2207	2216	rBV	2264988	3363606	46.60%	8.067%
14	17.122	2414	2420	2430	rVB	1071563	1507203	20.88%	3.615%
15	18.022	2568	2573	2590	rBV	659344	1072701	14.86%	2.573%
16	19.186	2762	2771	2786	rBV	1460900	4097326	56.77%	9.826%
17	19.304	2787	2791	2805	rVB	415503	783189	10.85%	1.878%
18	19.745	2860	2866	2871	rBV	5988423	7218010	100.00%	17.311%
19	20.510	2993	2996	3000	rBV	232574	245879	3.41%	0.590%
20	21.004	3077	3080	3089	rVB	777427	903680	12.52%	2.167%
21	21.286	3124	3128	3134	rBV	1306835	1678770	23.26%	4.026%
22	23.527	3504	3509	3516	rVB	931680	1739791	24.10%	4.172%

Sum of corrected areas: 41696741

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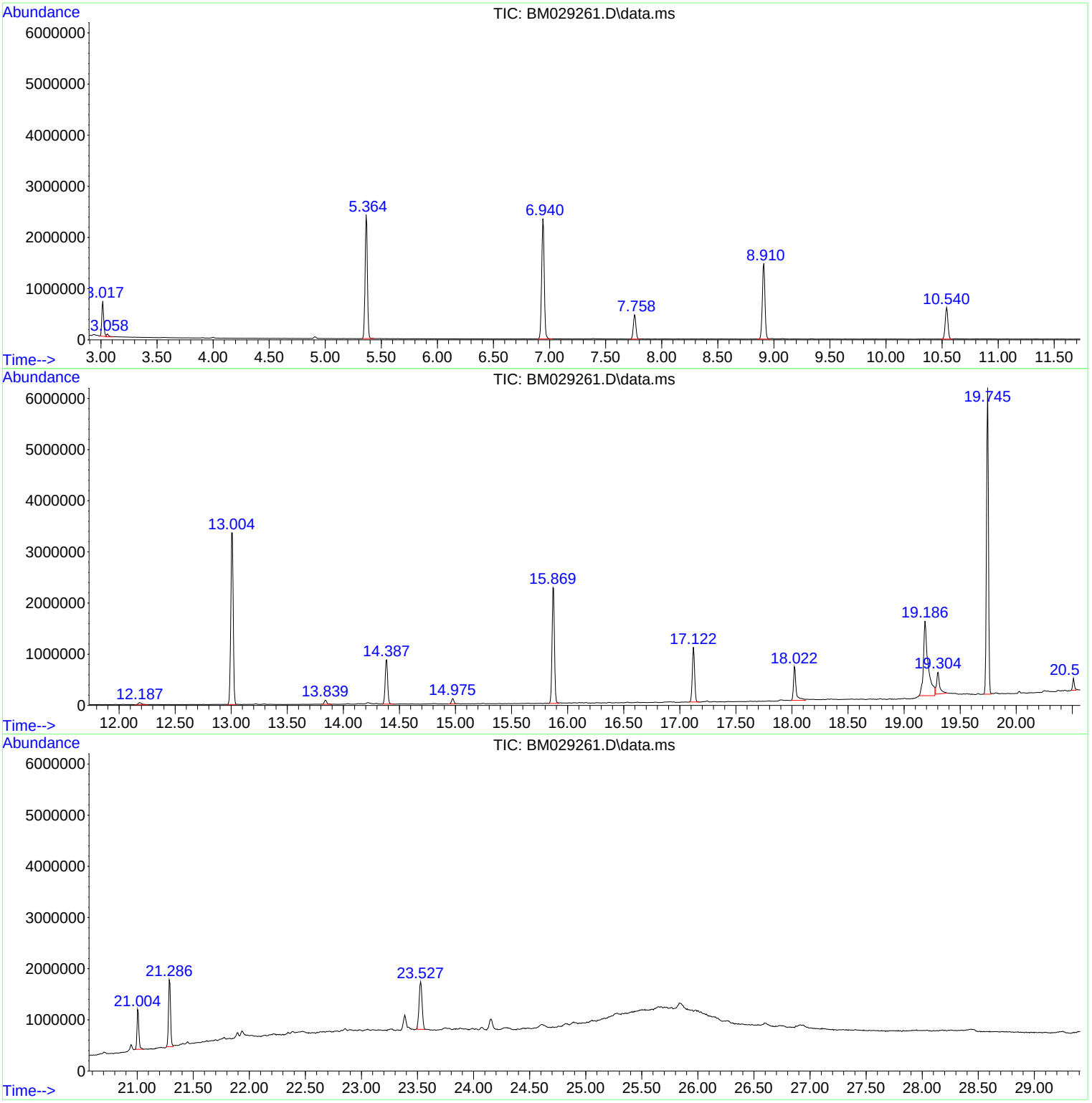
Instrument :
BNA_M
ClientSampleId :
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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 : BM029261.D
Acq On : 30 Mar 2021 01:23
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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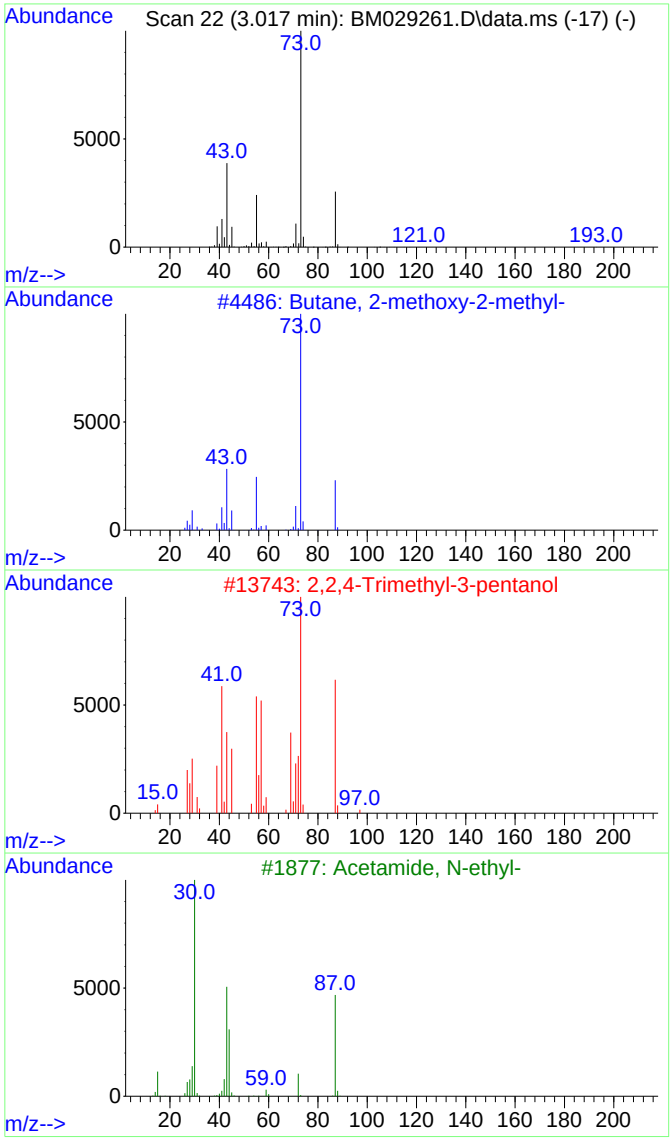
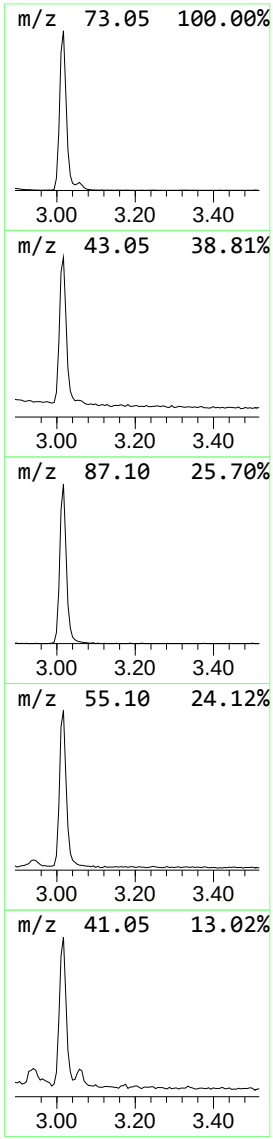
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.017	21.67 ng	813618	1,4-Dichlorobenzene-d4	7.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : CG/JU
Sample : M1786-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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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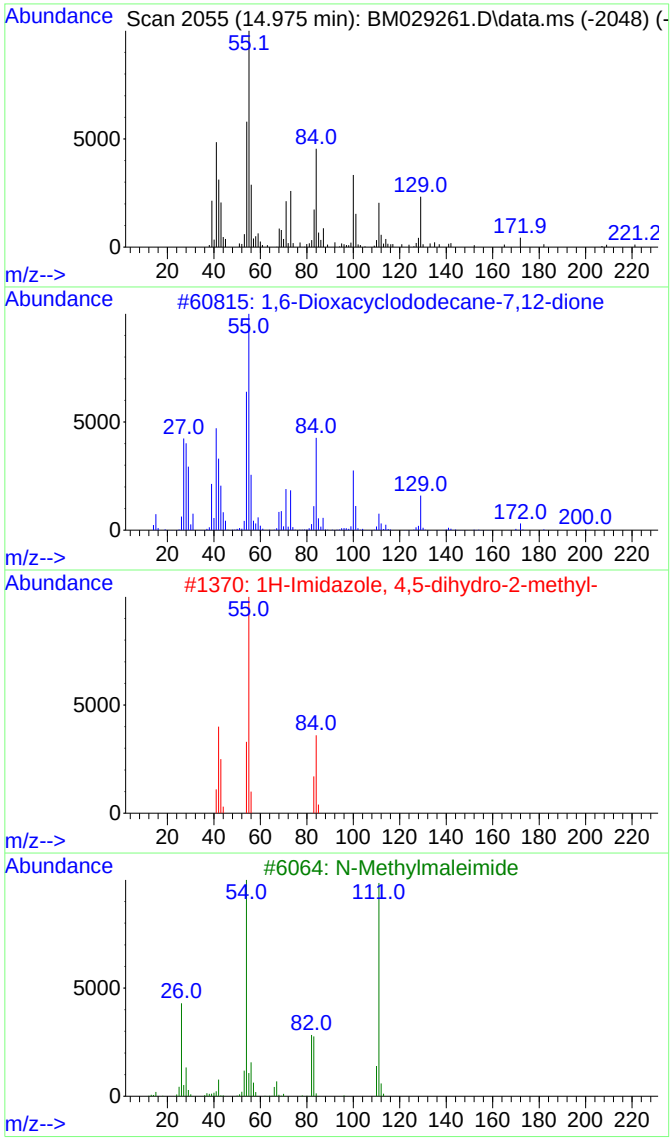
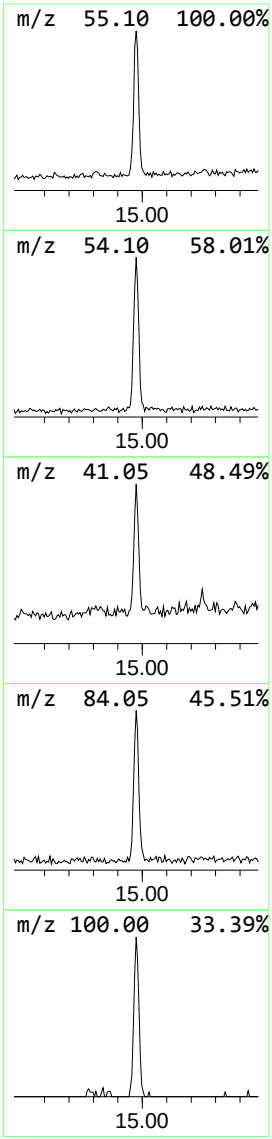
Peak Number 2 1,6-Dioxacyclododecane-7,12... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.975	2.34 ng	155735	Acenaphthene-d10	14.387

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Dioxacyclododecane-7,12-dione	200	C10H16O4	000777-95-7	72
2	1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	14
3	N-Methylmaleimide	111	C5H5NO2	000930-88-1	14
4	Cyclopentanone	84	C5H8O	000120-92-3	11
5	3-Ethyl-6-trifluoroacetoxyoctane	254	C12H21F3O2	1000215-97-3	10





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Operator : CG/JU
Sample : M1786-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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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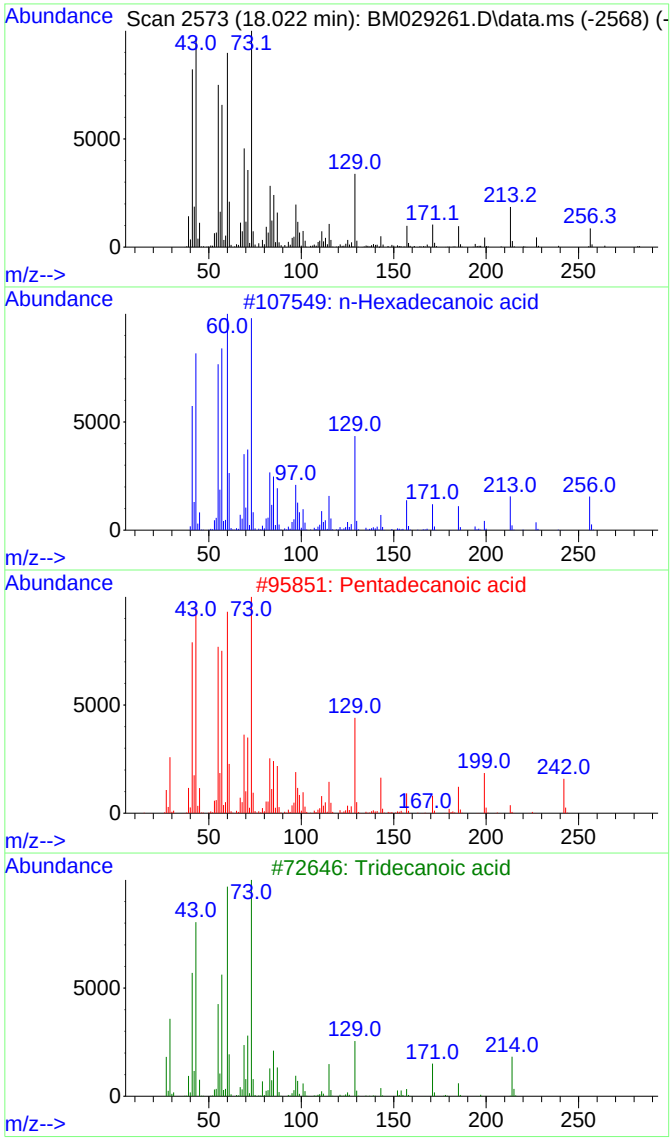
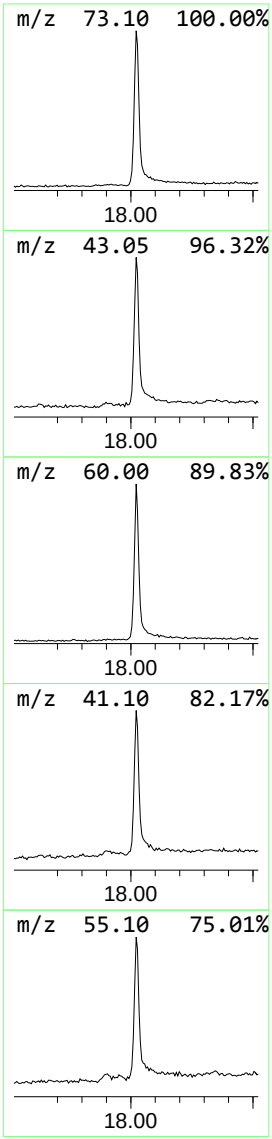
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	14.23 ng	1072700	Phenanthrene-d10	17.122

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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Acq On : 30 Mar 2021 01:23
Operator : CG/JU
Sample : M1786-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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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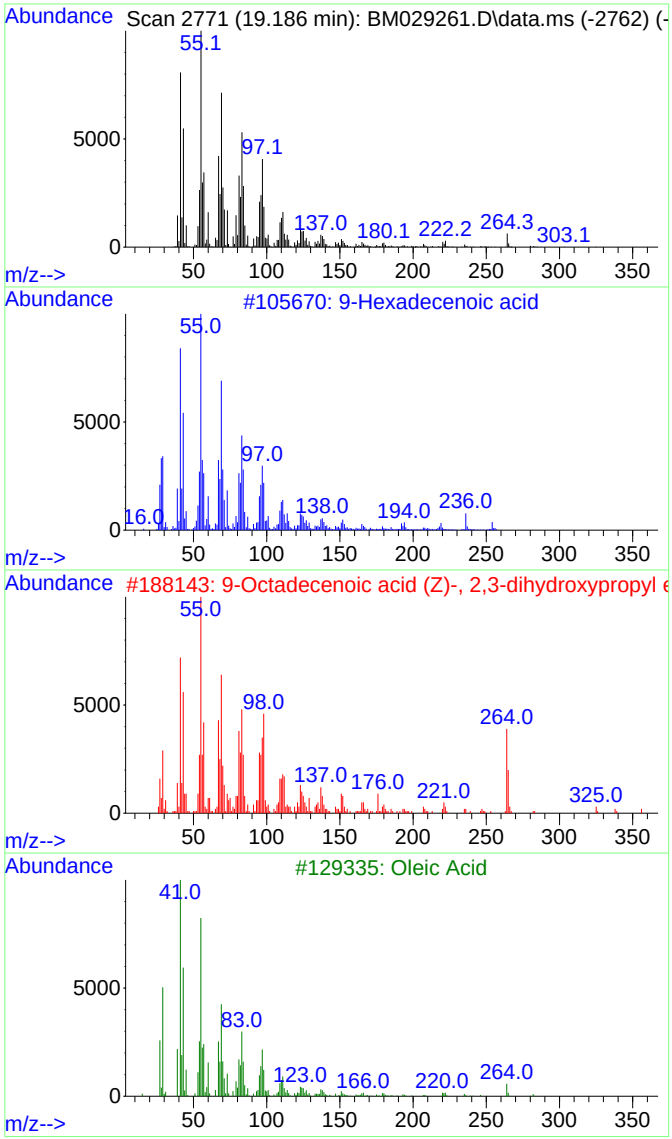
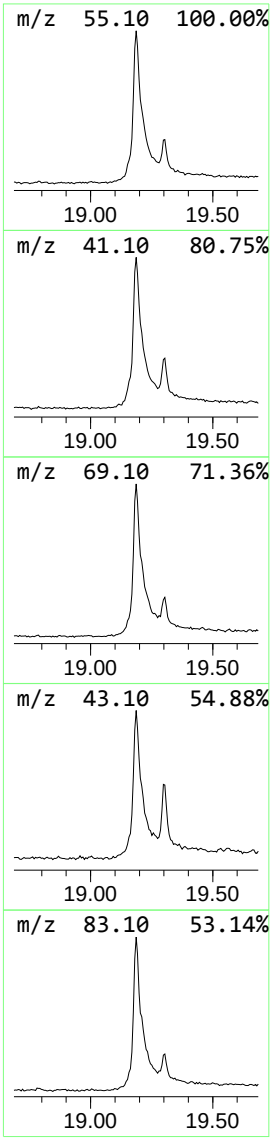
Peak Number 4 9-Hexadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	54.37 ng	4097330	Phenanthrene-d10	17.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	91
2	9-Octadecenoic acid (Z)-, 2,3-di...	356	C21H40O4	000111-03-5	87
3	Oleic Acid	282	C18H34O2	000112-80-1	81
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	76
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	68





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Data File : BM029261.D
Acq On : 30 Mar 2021 01:23
Operator : CG/JU
Sample : M1786-01
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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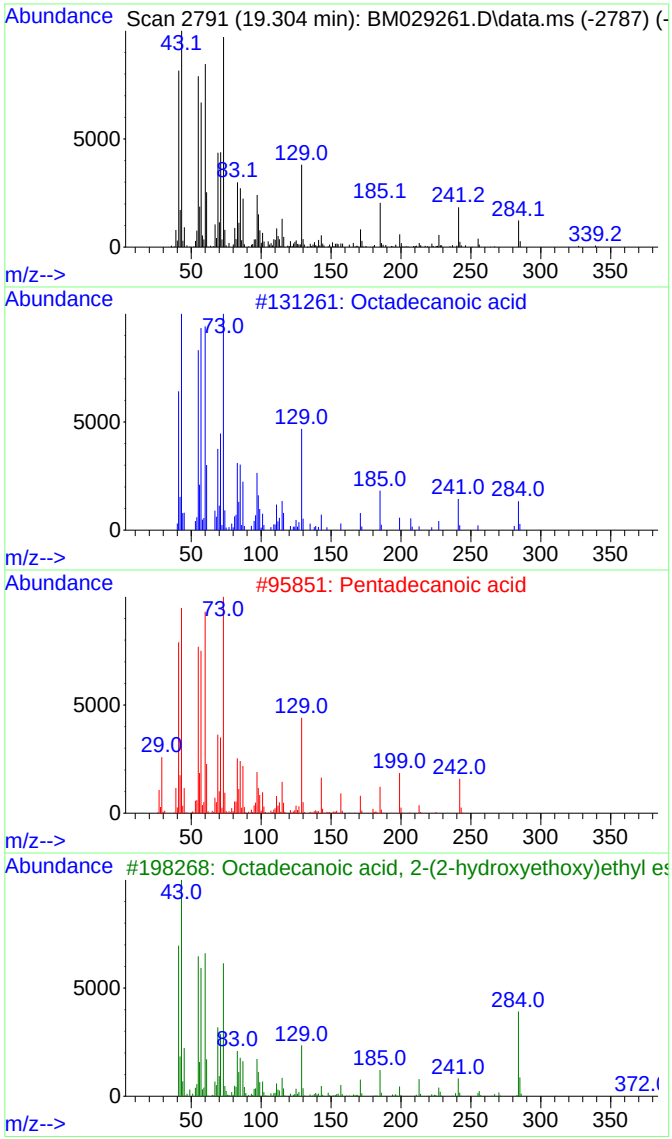
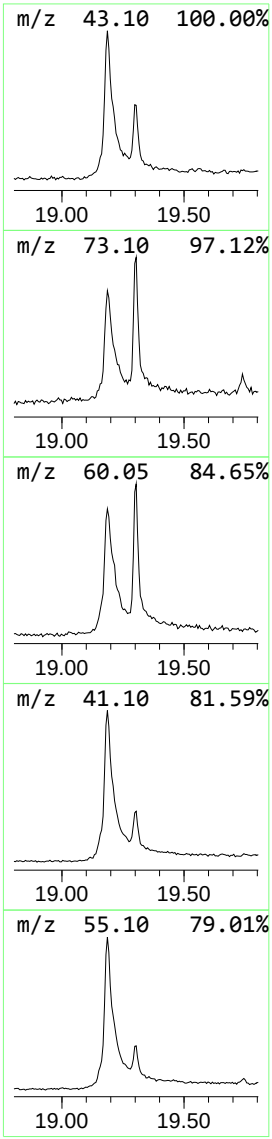
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.304	9.33 ng	783189	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Instrument : BNA_M
ClientSampleId : SP-1

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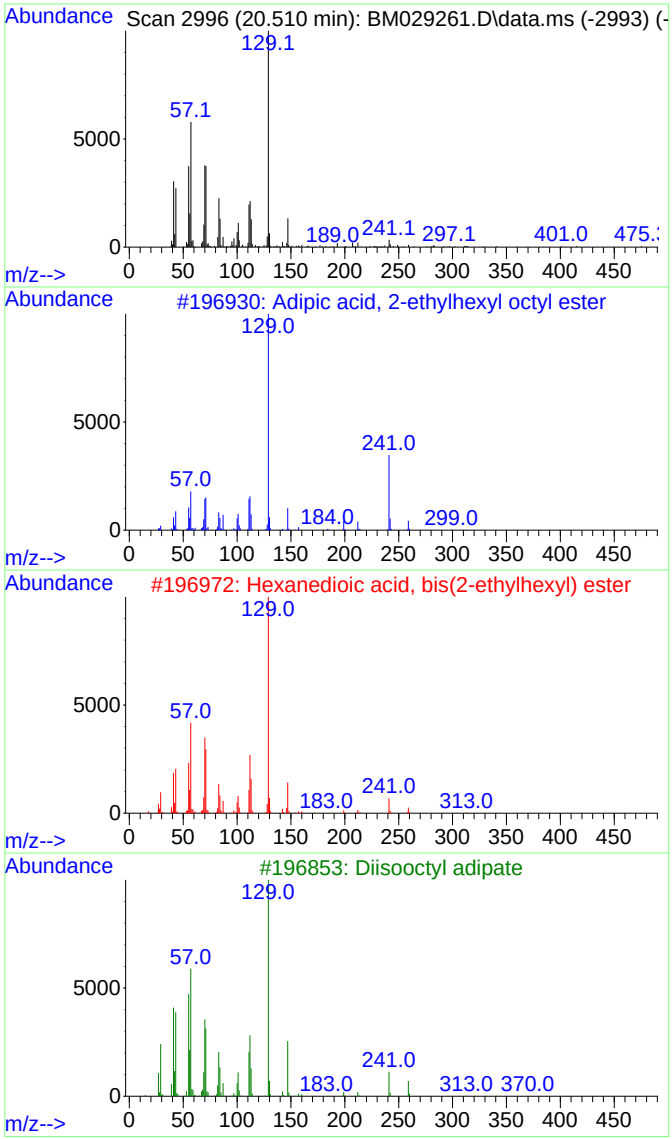
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

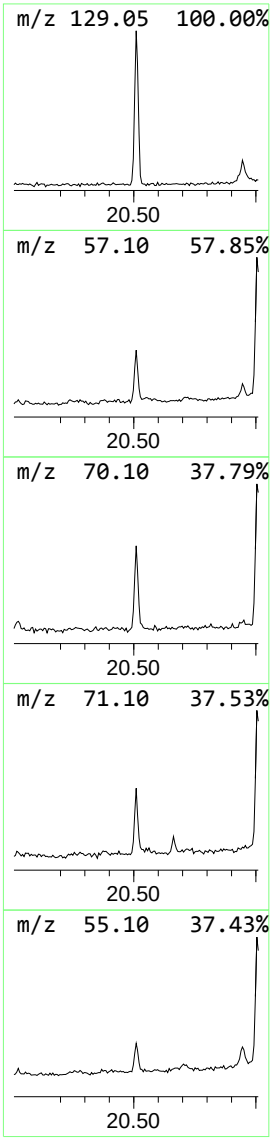
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Adipic acid, 2-ethylhexyl o... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.510	2.93 ng	245879	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	83
3	Diisooctyl adipate	370	C22H42O4	001330-86-5	72
4	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
5	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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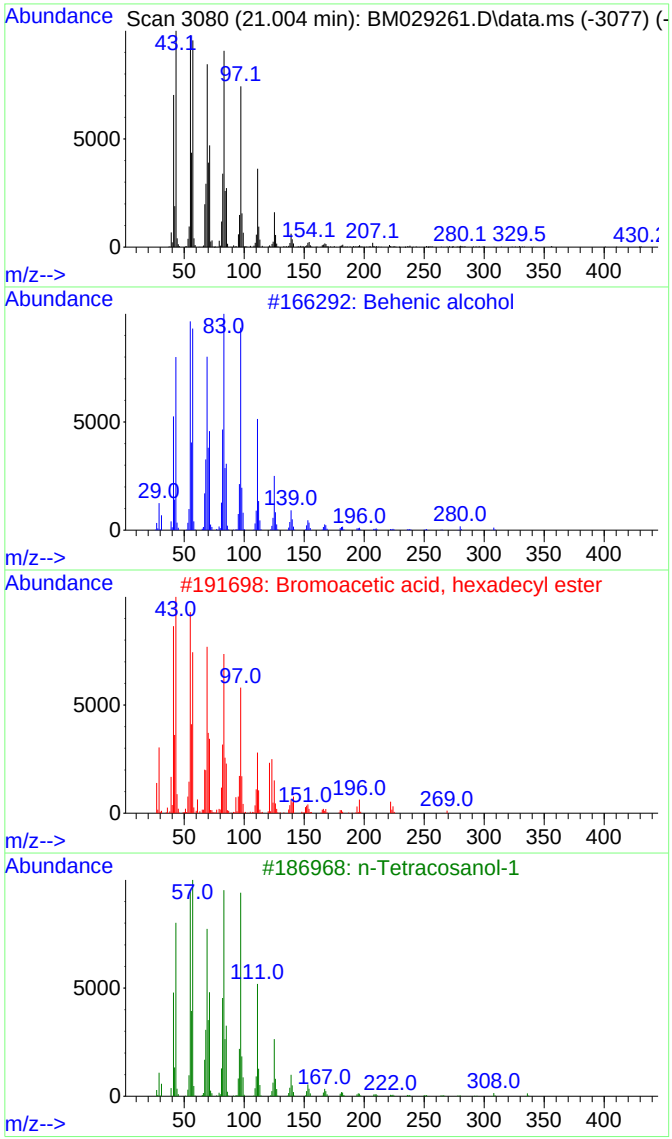
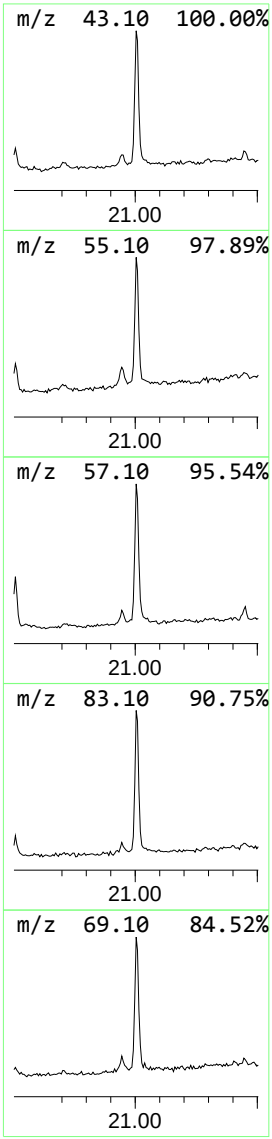
Peak Number 7 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.004	10.77 ng	903680	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Docosene	308	C22H44	001599-67-3	93
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93





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
Butane, 2-metho...	3.017	21.7	ng	813618	1	7.758	750952	20.0
1,6-Dioxacyclod...	14.975	2.3	ng	155735	3	14.387	1328350	20.0
n-Hexadecanoic ...	18.022	14.2	ng	1072700	4	17.122	1507200	20.0
9-Hexadecenoic ...	19.186	54.4	ng	4097330	4	17.122	1507200	20.0
Octadecanoic acid	19.304	9.3	ng	783189	5	21.286	1678770	20.0
Adipic acid, 2-...	20.510	2.9	ng	245879	5	21.286	1678770	20.0
Behenic alcohol	21.004	10.8	ng	903680	5	21.286	1678770	20.0