LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047253.D
Acq On : 19 Aug 2024 15:28
Operator : RC/JU
Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	356	362	371	rBV	607628	975310	8.24%	2.009%
2	6.581	621	628	636	rBV	430302	682809	5.77%	1.407%
3	7.363	755	761	769	rBV	334117	513438	4.34%	1.058%
4	8.510	949	956	964	rBV	909553	1440186	12.16%	2.967%
5	10.122	1223	1230	1239	rBV	436220	715253	6.04%	1.474%
6	10.881	1352	1359	1369	rBV2	58844	122768	1.04%	0.253%
7	12.633	1649	1657	1664	rBV	2394661	3535201	29.86%	7.283%
8	13.916	1869	1875	1887	rVB3	69159	183377	1.55%	0.378%
9	14.027	1888	1894	1901	rVB	705585	1046420	8.84%	2.156%
10	14.263	1928	1934	1935	rBV	871594	1067281	9.01%	2.199%
11	14.280	1935	1937	1949	rVB	1047967	1278940	10.80%	2.635%
12	14.880	2033	2039	2047	rBV	104366	170094	1.44%	0.350%
13	15.298	2104	2110	2120	rVB	56966	133288	1.13%	0.275%
14	15.533	2144	2150	2161	rBV	3499577	4941318	41.73%	10.180%
15	16.792	2358	2364	2370	rVB	967826	1388614	11.73%	2.861%
16	16.868	2373	2377	2382	rBV	175642	217136	1.83%	0.447%
17	17.727	2517	2523	2531	rBV	2062476	3302260	27.89%	6.803%
18	18.686	2683	2686	2690	rVB	126621	135946	1.15%	0.280%
19	18.827	2706	2710	2715	rBV	167066	239565	2.02%	0.494%
20	18.909	2720	2724	2731	rVV2	172788	379380	3.20%	0.782%
21	19.039	2738	2746	2769	rBV	6966853	11840860	100.00%	24.394%
22	19.456	2812	2817	2822	rBV	7371923	8872184	74.93%	18.278%
23	20.121	2928	2930	2934	rBV3	100432	125573	1.06%	0.259%
24	20.768	3037	3040	3045	rBV2	282633	368963	3.12%	0.760%
25	21.033	3080	3085	3090	rVB	1574718	2108079	17.80%	4.343%
26	23.733	3538	3544	3557	rVB	1200323	2755669	23.27%	5.677%

Sum of corrected areas: 48539912

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Instrument :
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ClientSampleId :
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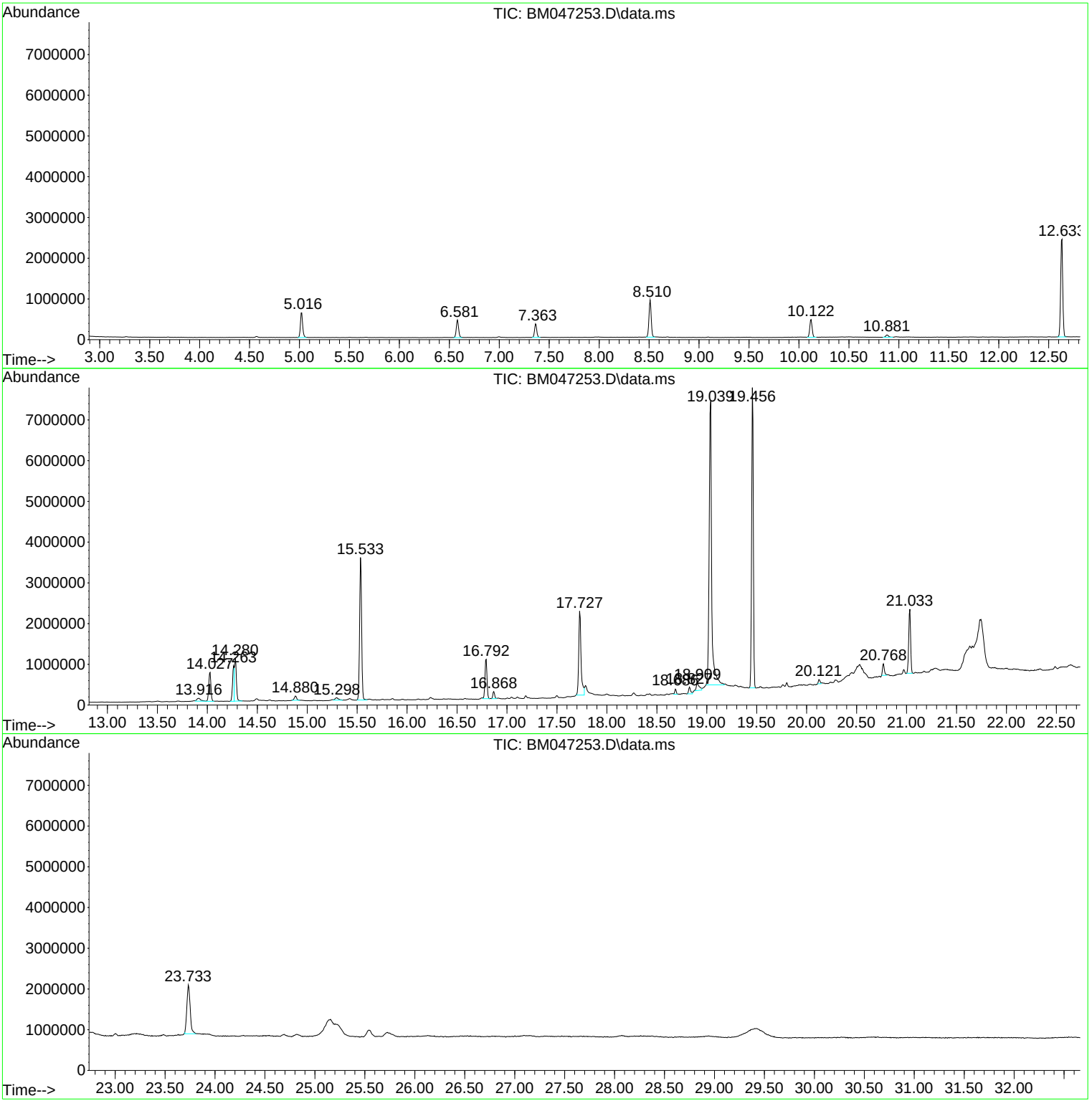
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
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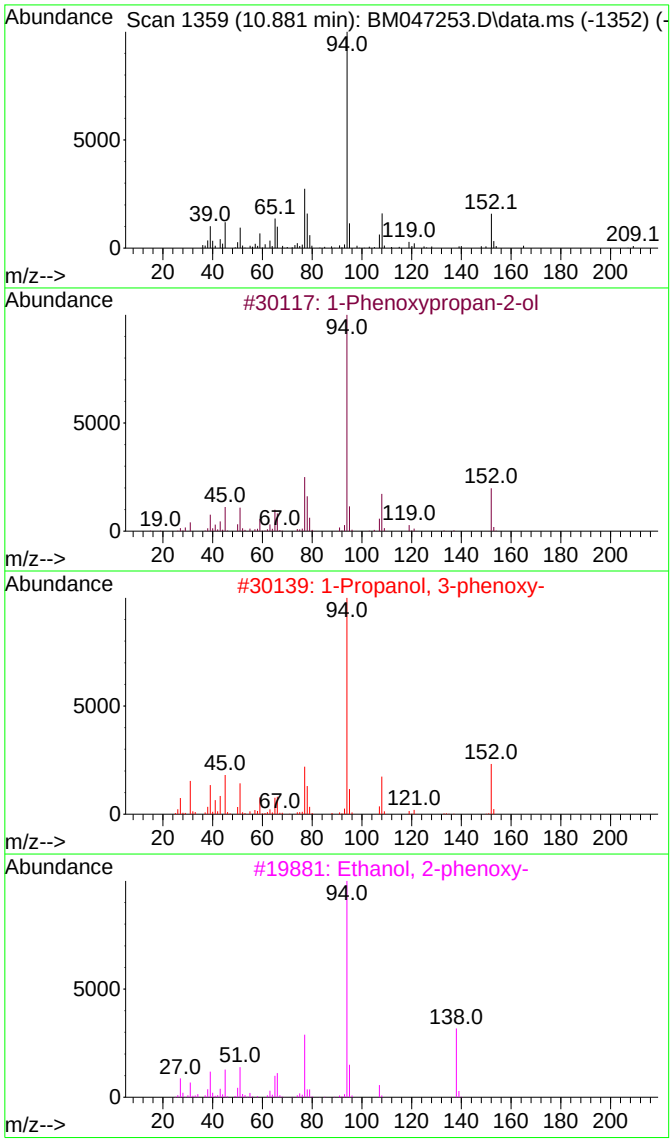
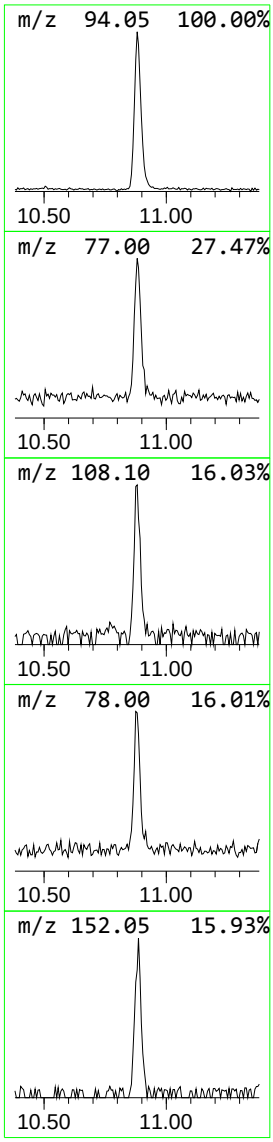
Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	3.43 ng	122768	Naphthalene-d8	10.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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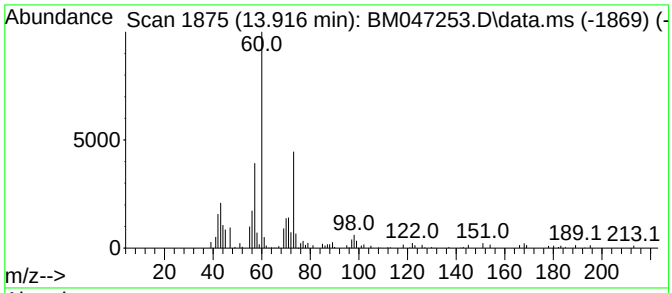
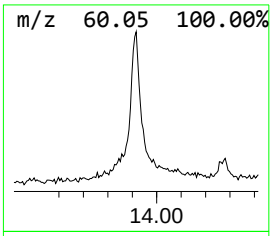
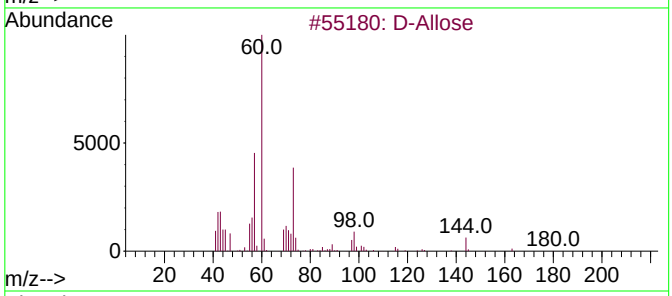
Peak Number 2 D-Allose Concentration Rank 6

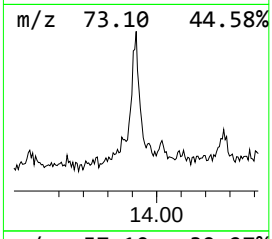
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	3.50 ng	183377	Acenaphthene-d10	14.027

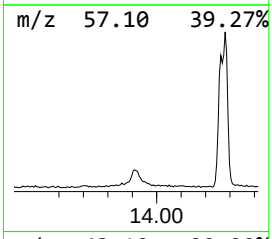
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	90
2	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	74
3	Heptanoic acid	130	C7H14O2	000111-14-8	59
4	3,4-Altrosan	162	C6H10O5	1000129-76-4	58
5	Hexanoic acid	116	C6H12O2	000142-62-1	47

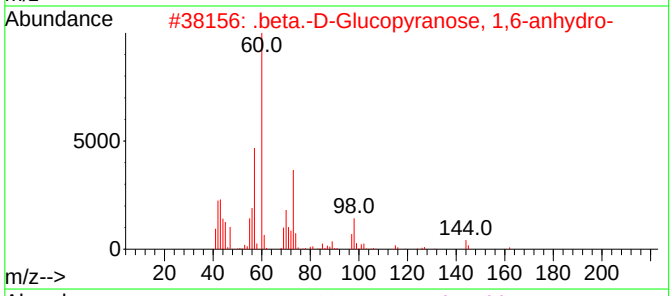


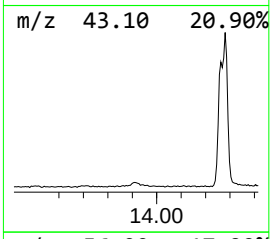


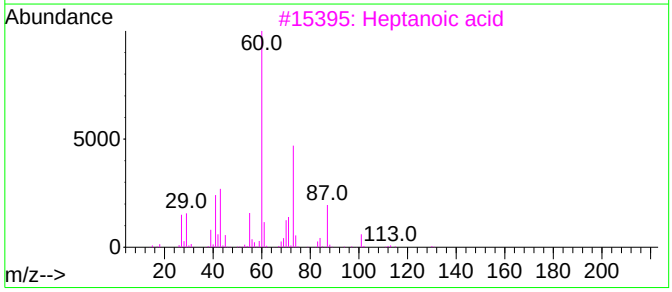


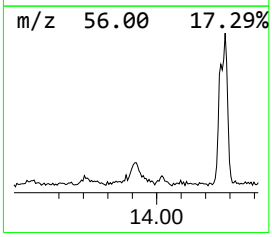












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Data File : BM047253.D
Acq On : 19 Aug 2024 15:28
Operator : RC/JU
Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

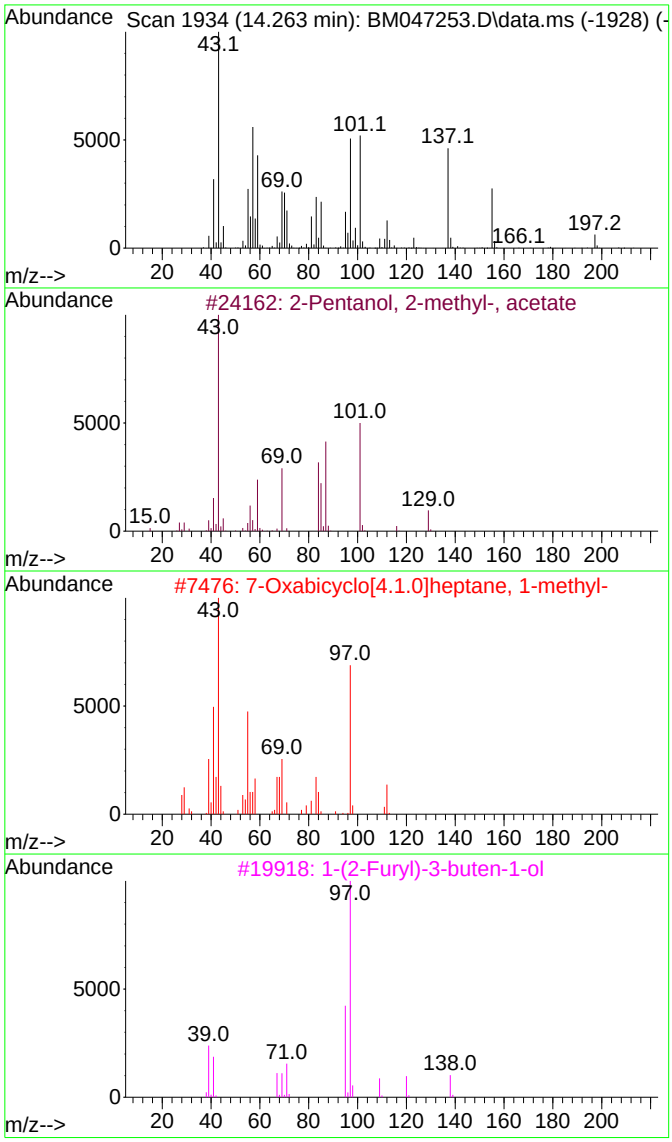
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

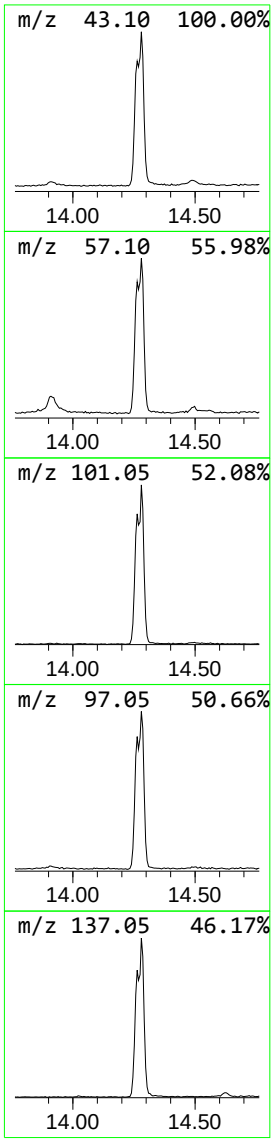
****

Peak Number 3 unknown14.263 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	20.40 ng	1067280	Acenaphthene-d10	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
2	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10
3	1-(2-Furyl)-3-buten-1-ol	138	C8H10O2	1000311-94-9	10
4	2-Pyrazoline, 1,4,5-trimethyl-	112	C6H12N2	007423-11-2	10
5	Succinic acid, hexyl 2-methylcyc...	298	C17H30O4	1000329-82-0	10





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Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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TIC Library : C:\Database\NIST20.L
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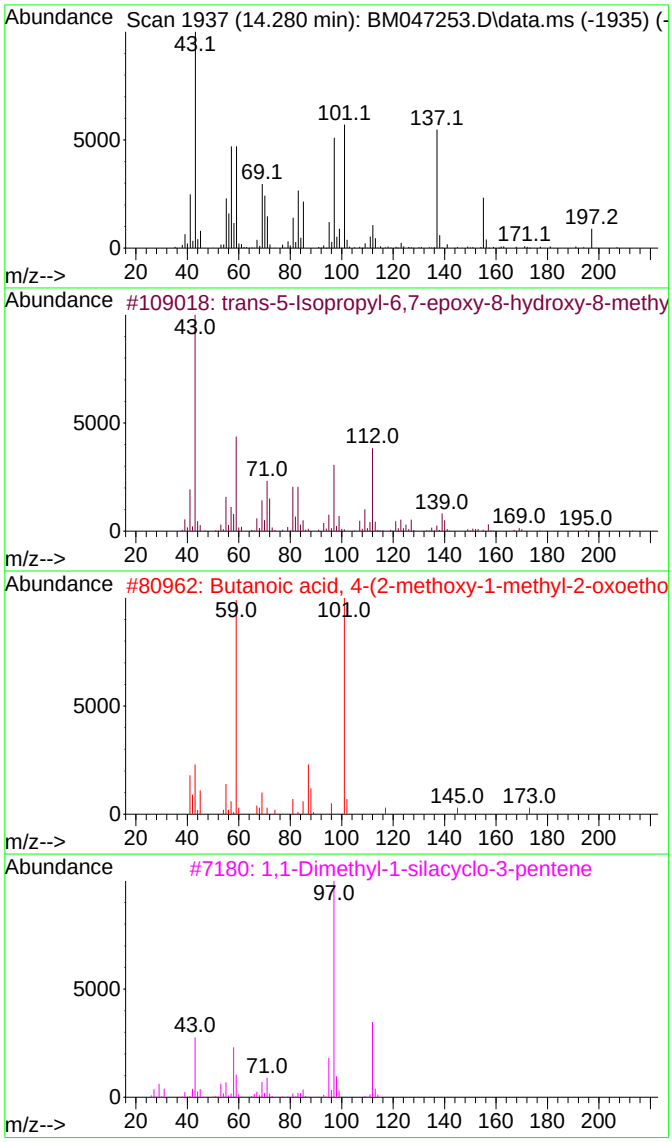
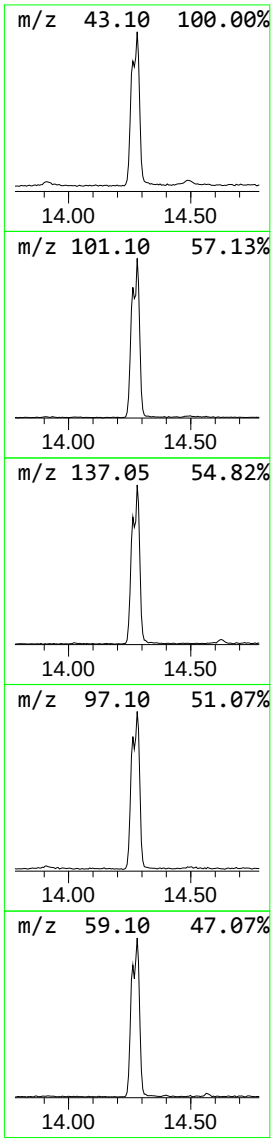
Peak Number 4 unknown14.280 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	24.44 ng	1278940	Acenaphthene-d10	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	22
2	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	14
3	1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	14
4	Succinic acid, cyclohexylmethyl ...	282	C16H26O4	1010391-26-3	12
5	Acetoxyacetic acid, 3-tetradecyl...	314	C18H34O4	1000308-80-8	10





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Instrument :
BNA_M
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918-J-WS-081324-FD

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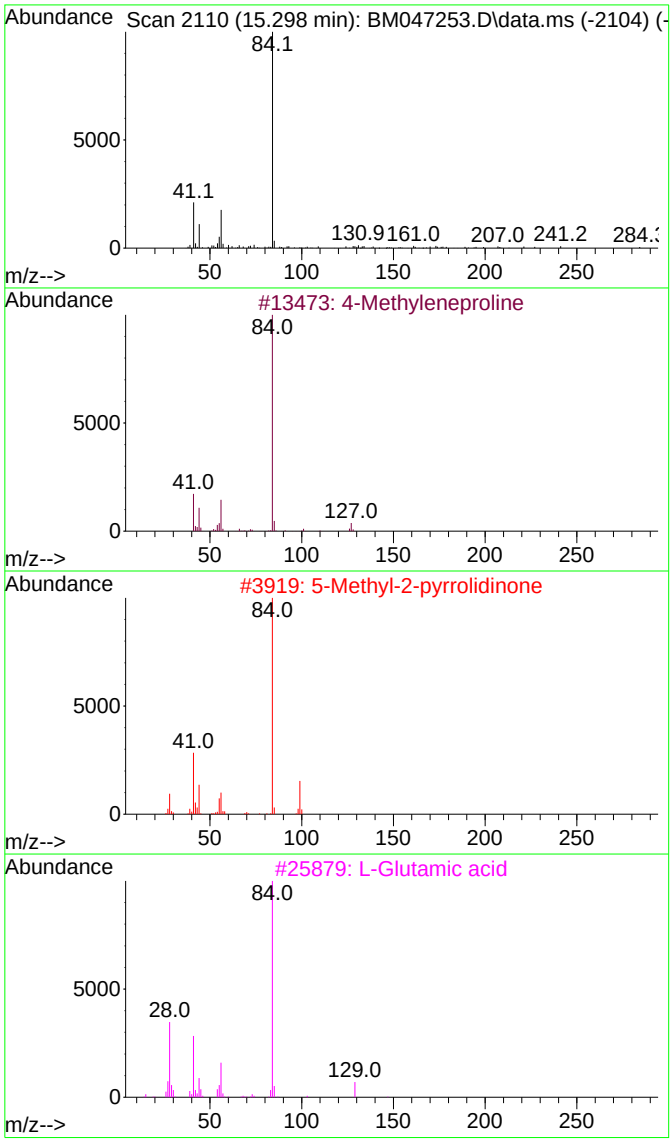
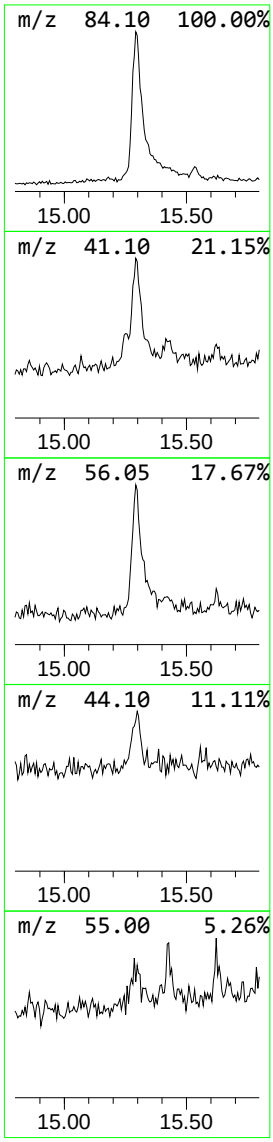
Peak Number 5 4-Methyleneproline Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.55 ng	133288	Acenaphthene-d10	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyleneproline	127	C6H9NO2	1000131-14-7	56
2	5-Methyl-2-pyrrolidinone	99	C5H9NO	000108-27-0	56
3	L-Glutamic acid	147	C5H9NO4	000056-86-0	56
4	DL-Proline, 5-oxo-	129	C5H7NO3	000149-87-1	45
5	.gamma.-L-glutamyl-L-glutamic acid	276	C10H16N2O7	001116-22-9	39





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ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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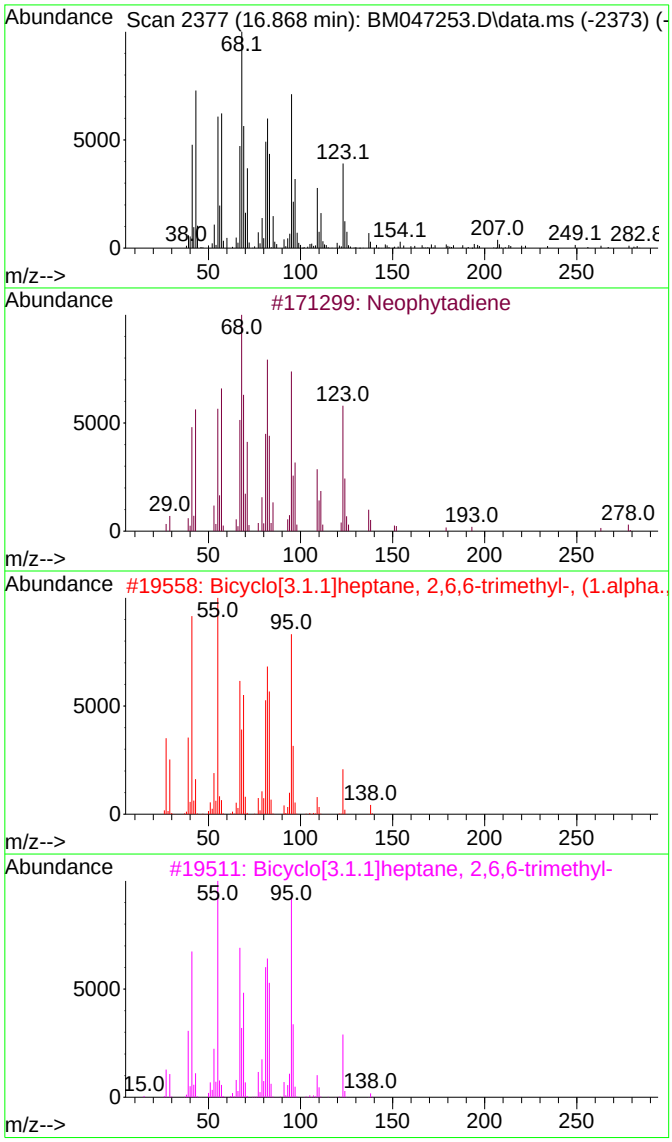
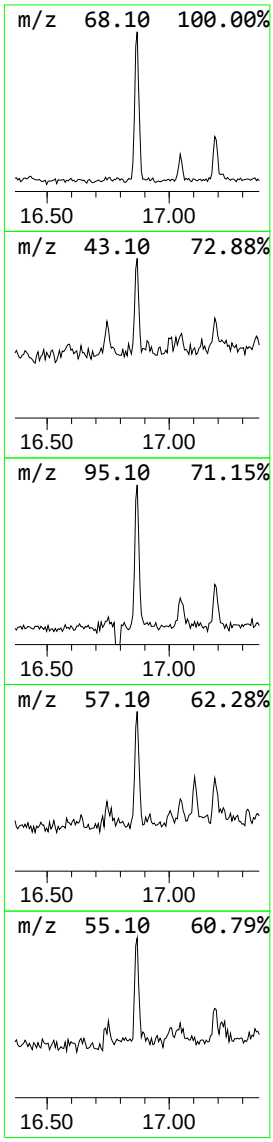
Peak Number 6 Neophytadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.868	3.13 ng	217136	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neophytadiene	278	C20H38	000504-96-1	64
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	60
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	46
4	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	43
5	11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	43





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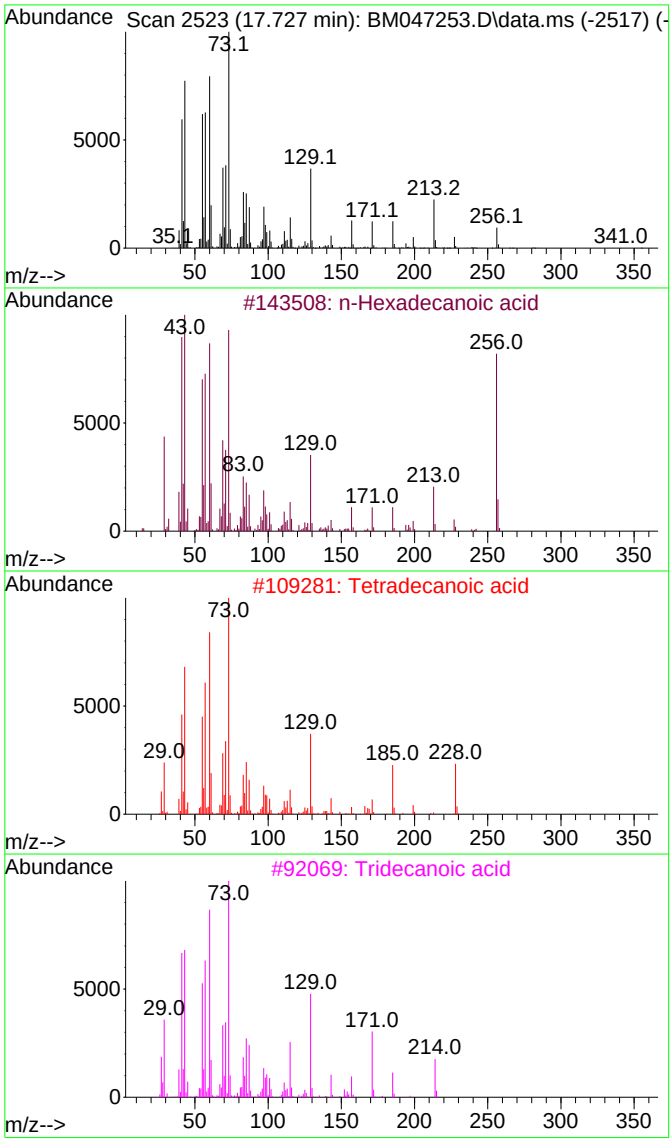
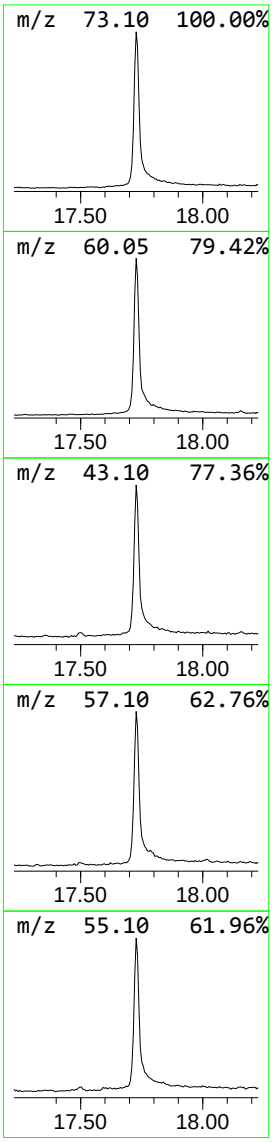
Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	47.56 ng	3302260	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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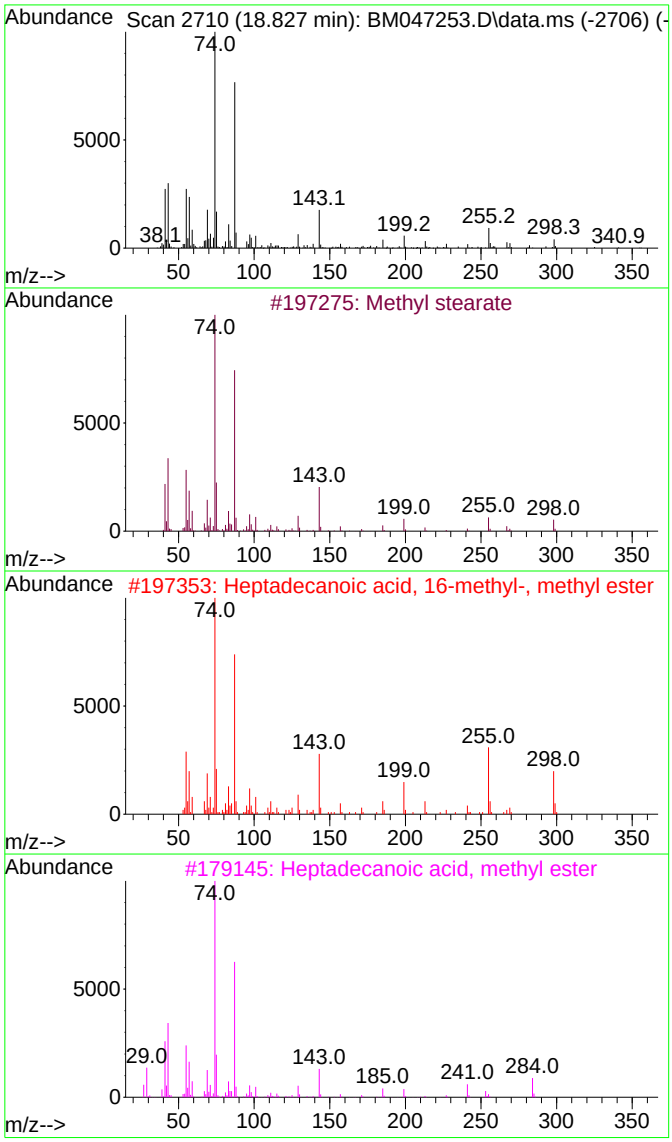
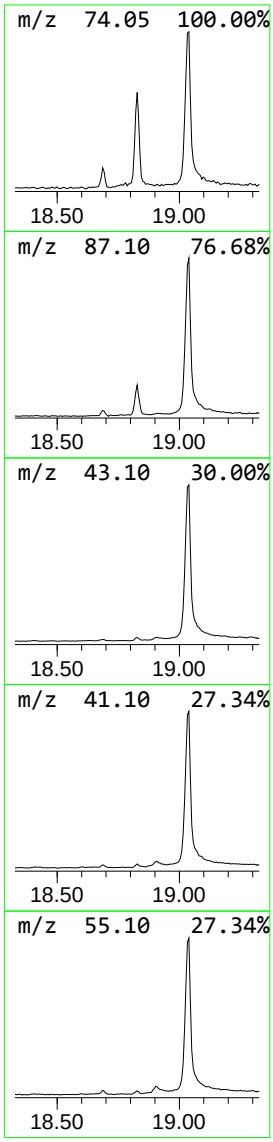
Peak Number 8 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.827	3.45 ng	239565	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047253.D
Acq On : 19 Aug 2024 15:28
Operator : RC/JU
Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

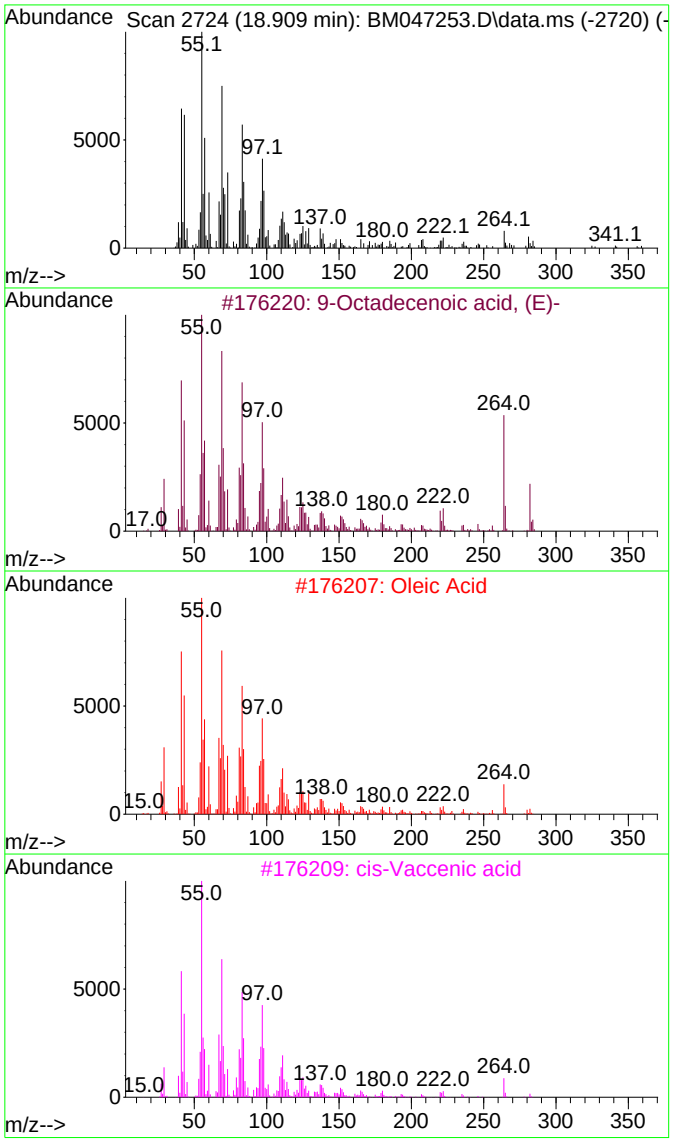
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

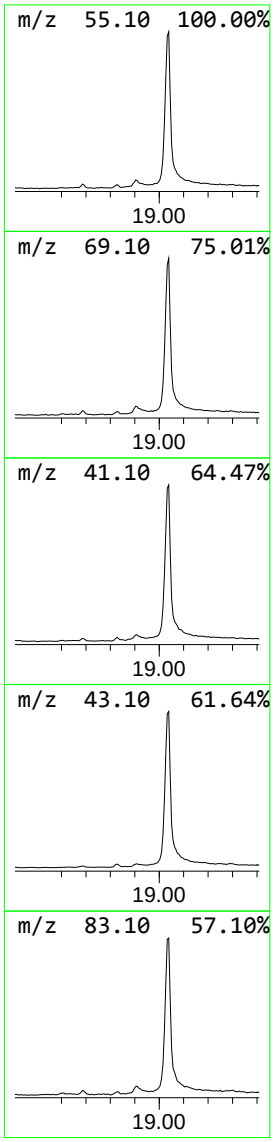
****

Peak Number 9 9-Octadecenoic acid, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.910	5.46 ng	379380	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
2	Oleic Acid	282	C18H34O2	000112-80-1	95
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
5	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047253.D
Acq On : 19 Aug 2024 15:28
Operator : RC/JU
Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

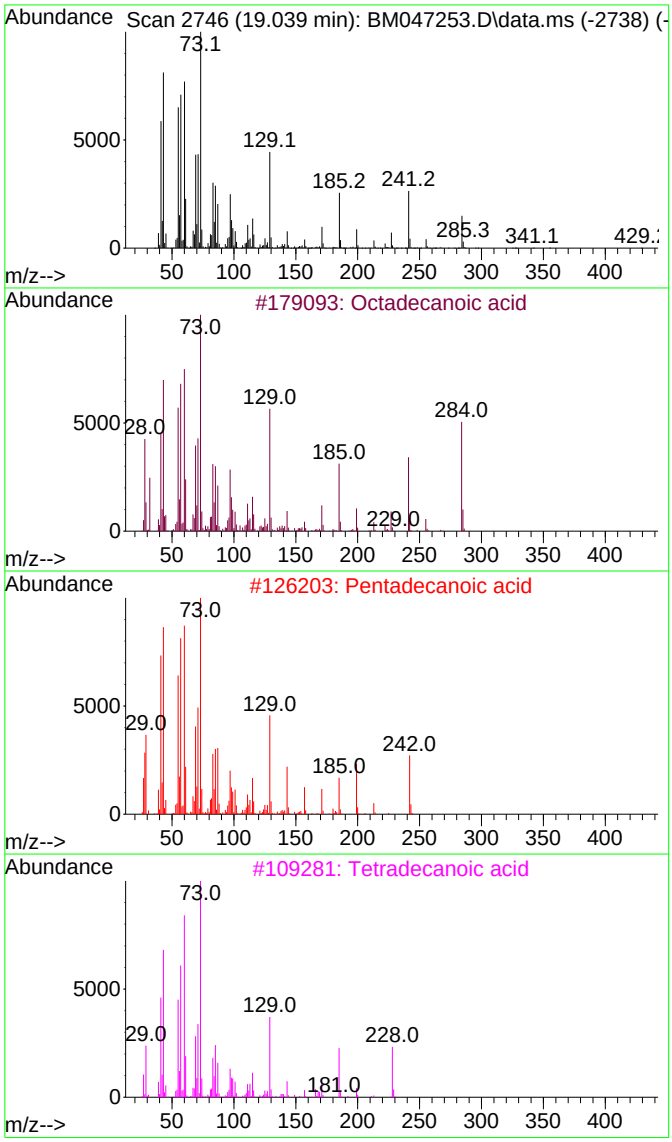
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

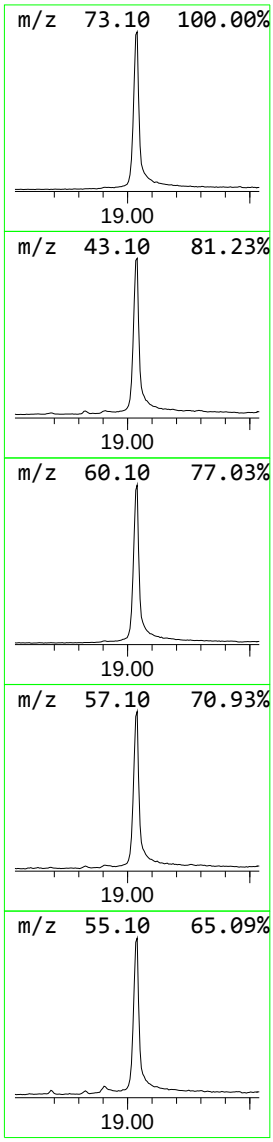
****

Peak Number 10 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.039	112.34 ng	11840900	Chrysene-d12	21.033

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047253.D
Acq On : 19 Aug 2024 15:28
Operator : RC/JU
Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

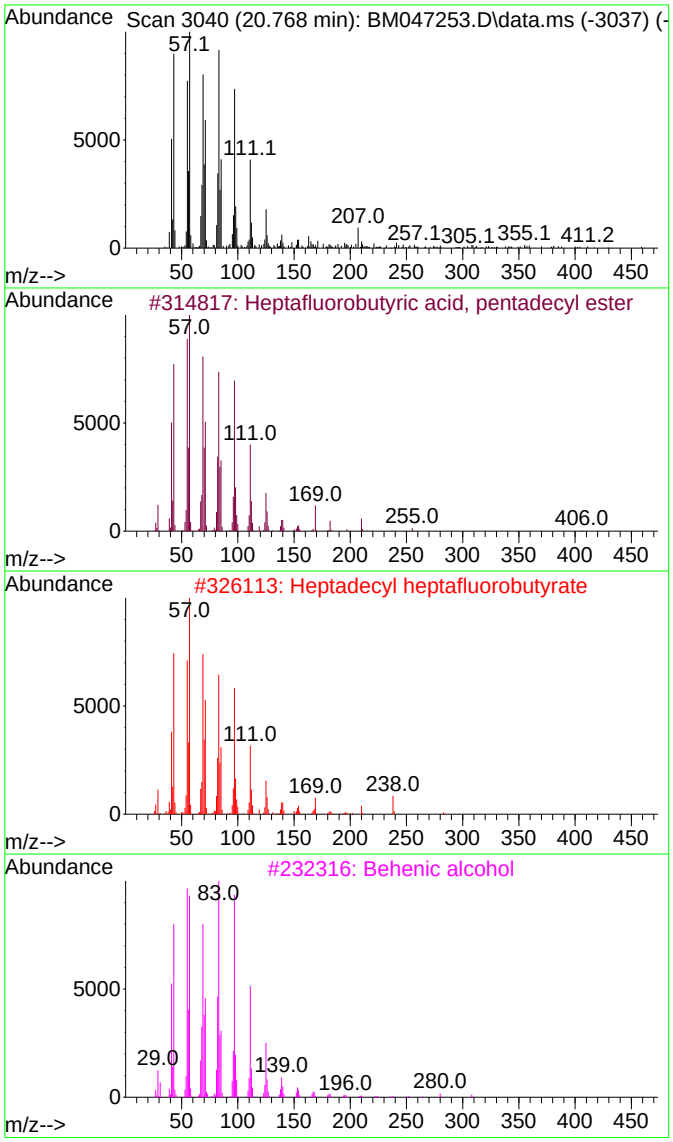
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

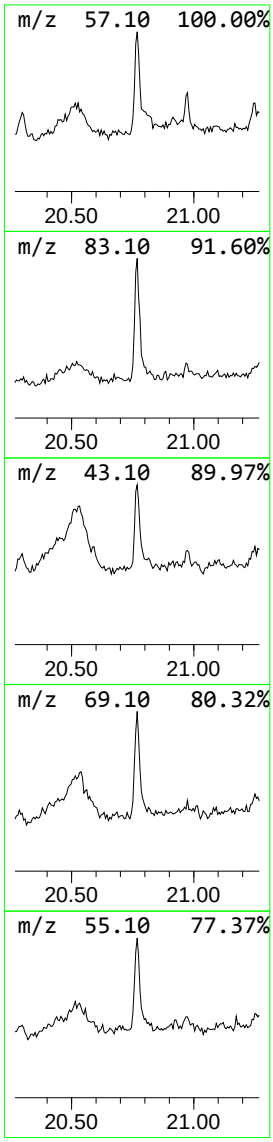
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptafluorobutyric acid, pe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.768	3.50 ng	368963	Chrysene-d12	21.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047253.D
Acq On : 19 Aug 2024 15:28
Operator : RC/JU
Sample : P3596-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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
1-Phenoxypropan...	10.881	3.4	ng	122768	2	10.122	715253	20.0
D-Allose	13.916	3.5	ng	183377	3	14.027	1046420	20.0
unknown14.263	14.263	20.4	ng	1067280	3	14.027	1046420	20.0
unknown14.280	14.280	24.4	ng	1278940	3	14.027	1046420	20.0
4-Methyleneproline	15.298	2.5	ng	133288	3	14.027	1046420	20.0
Neophytadiene	16.868	3.1	ng	217136	4	16.792	1388610	20.0
n-Hexadecanoic ...	17.727	47.6	ng	3302260	4	16.792	1388610	20.0
Methyl stearate	18.827	3.5	ng	239565	4	16.792	1388610	20.0
9-Octadecenoic ...	18.910	5.5	ng	379380	4	16.792	1388610	20.0
Octadecanoic acid	19.039	112.3	ng	11840900	5	21.033	2108080	20.0
Heptafluorobuty...	20.768	3.5	ng	368963	5	21.033	2108080	20.0