LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029323.D
Acq On : 02 Apr 2021 16:34
Operator : CG/JU
Sample : M1874-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB18(39-40)

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-BM040121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029323.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.940	5	9	14	rBV	525088	610506	10.36%	1.859%
2	2.981	14	16	29	rVB	115295	164089	2.78%	0.500%
3	5.298	403	410	423	rBV	1824739	2639439	44.79%	8.036%
4	6.875	670	678	693	rBV	1807881	2823746	47.92%	8.597%
5	7.698	812	818	825	rBV	435243	669508	11.36%	2.038%
6	8.851	1006	1014	1025	rBV	1095015	1775115	30.13%	5.405%
7	10.480	1283	1291	1298	rBV	528965	856626	14.54%	2.608%
8	12.957	1704	1712	1720	rBV	2488695	3608636	61.24%	10.987%
9	13.792	1849	1854	1863	rBV	65810	102117	1.73%	0.311%
10	14.333	1939	1946	1952	rBV	720305	1071842	18.19%	3.263%
11	15.821	2192	2199	2213	rBV	2025330	2854753	48.45%	8.692%
12	17.074	2404	2412	2418	rBV	893208	1276227	21.66%	3.886%
13	17.980	2560	2566	2582	rBV	561517	905264	15.36%	2.756%
14	19.133	2755	2762	2767	rBV9	31107	72442	1.23%	0.221%
15	19.256	2778	2783	2796	rBV	221928	359799	6.11%	1.095%
16	19.698	2852	2858	2868	rBV	4890227	5892419	100.00%	17.940%
17	20.392	2969	2976	2989	rBV	1152758	1529659	25.96%	4.657%
18	20.968	3070	3074	3084	rBV	990978	1244687	21.12%	3.790%
19	21.244	3116	3121	3127	rBV	1311602	1632006	27.70%	4.969%
20	22.286	3295	3298	3303	rBV2	175834	232815	3.95%	0.709%
21	22.421	3318	3321	3326	rVB	128008	168694	2.86%	0.514%
22	23.456	3491	3497	3510	rVB2	948278	1798157	30.52%	5.475%
23	24.080	3598	3603	3618	rVB2	251207	556189	9.44%	1.693%

Sum of corrected areas: 32844735

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
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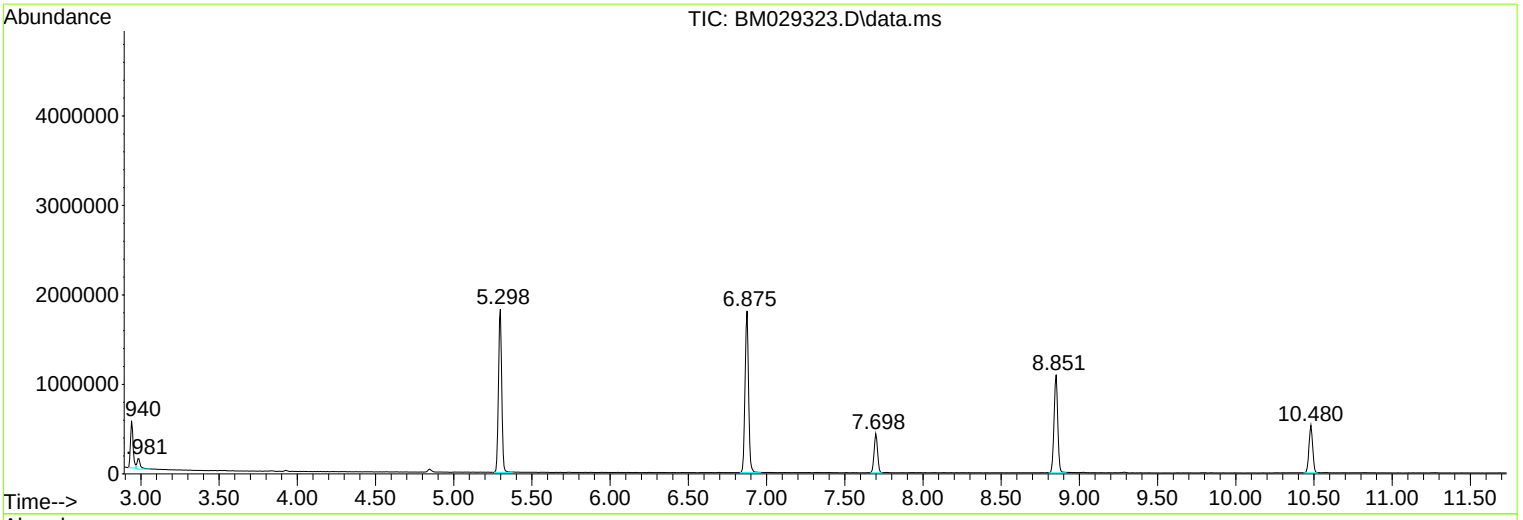
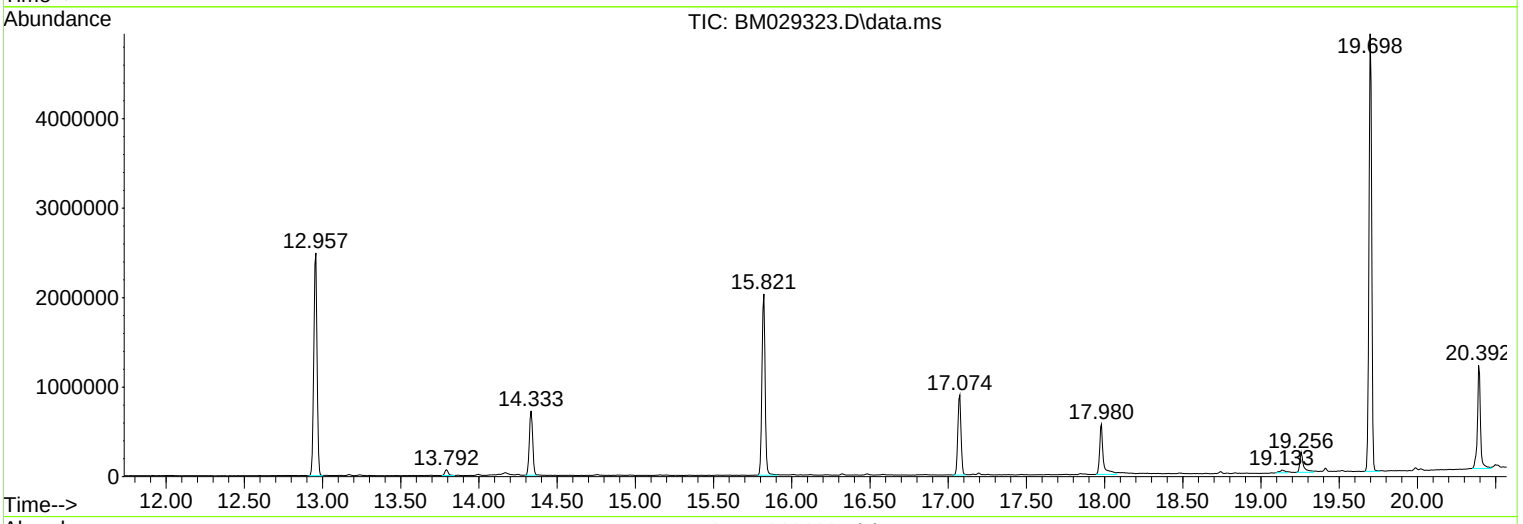
Misc :
ALS Vial : 13 Sample Multiplier: 1

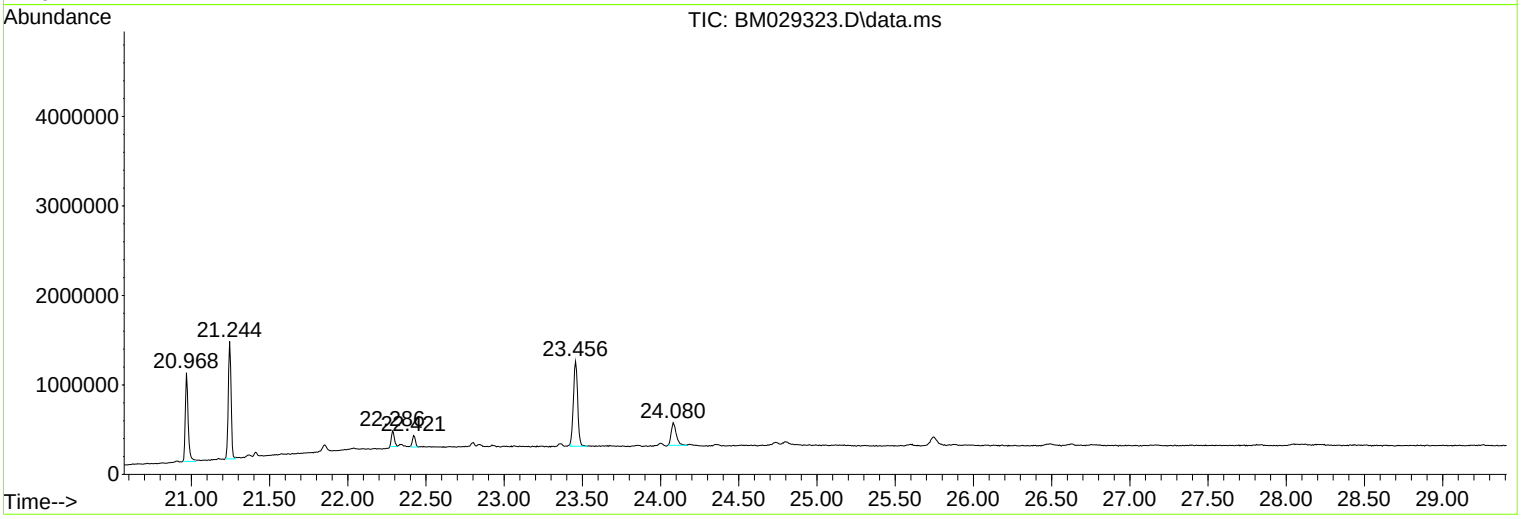
Instrument :
BNA_M
ClientSampleId :
FS-SB18(39-40)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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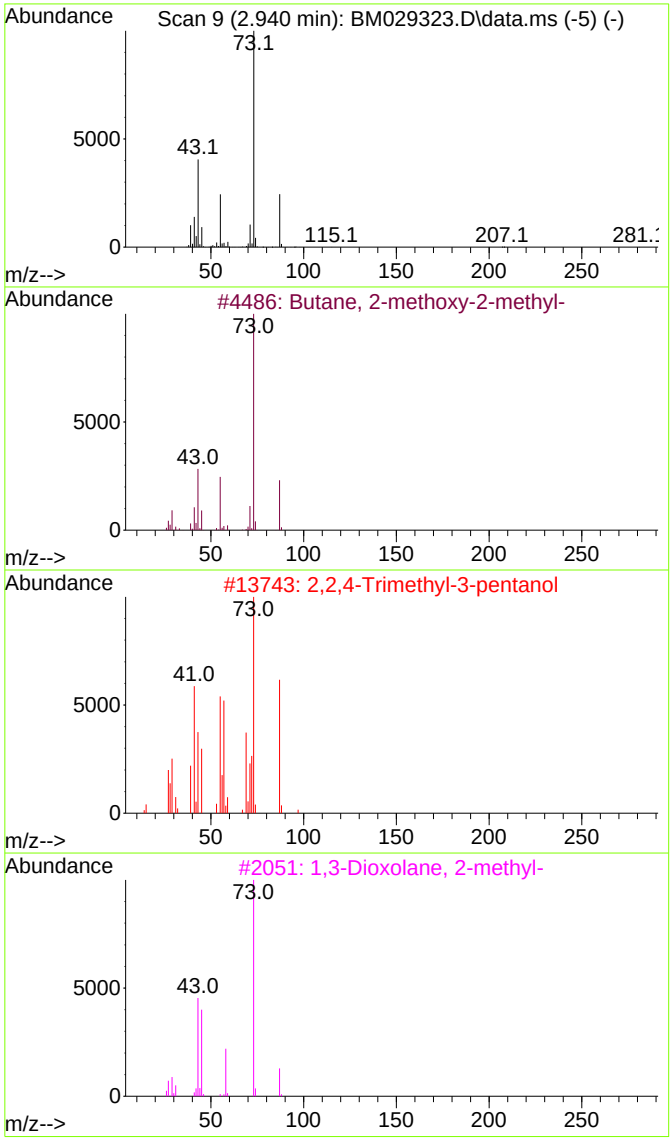
TIC Integration Parameters: LSCINT.P

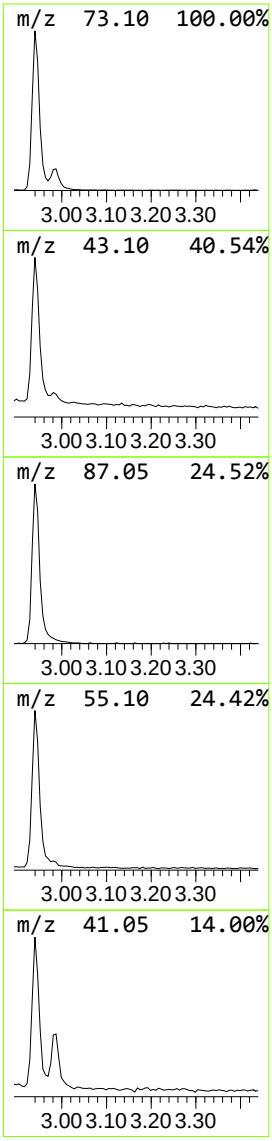
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.940	18.24 ng	610506	1,4-Dichlorobenzene-d4	7.698

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	64
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Acq On : 02 Apr 2021 16:34
Operator : CG/JU
Sample : M1874-03
Misc :
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Instrument :
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ClientSampleId :
FS-SB18(39-40)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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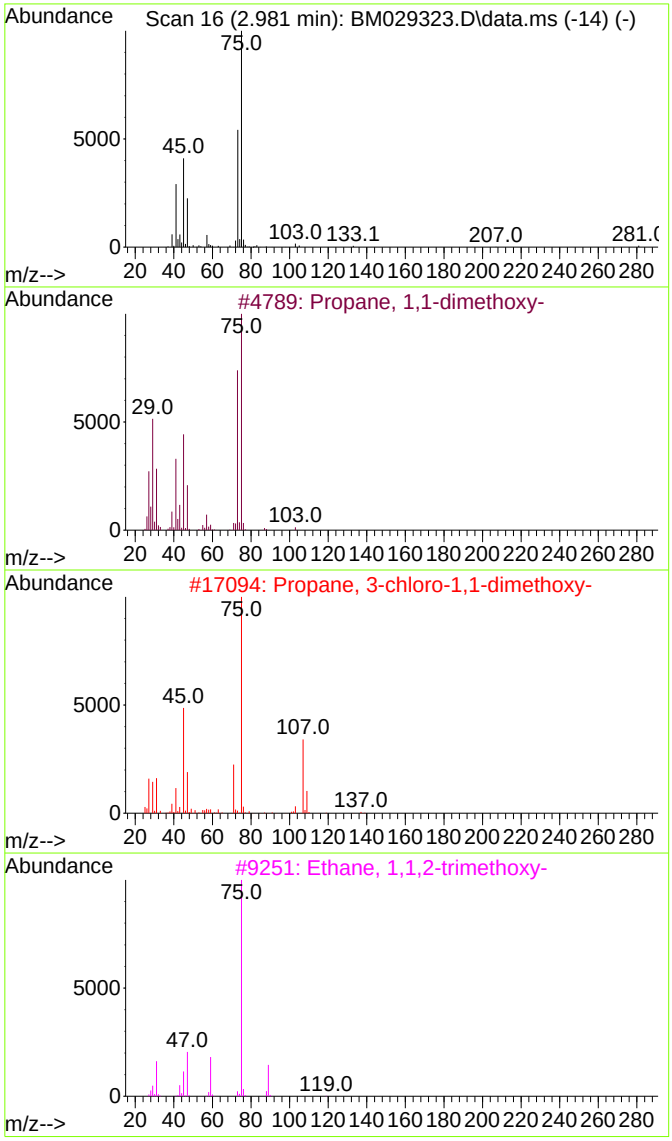
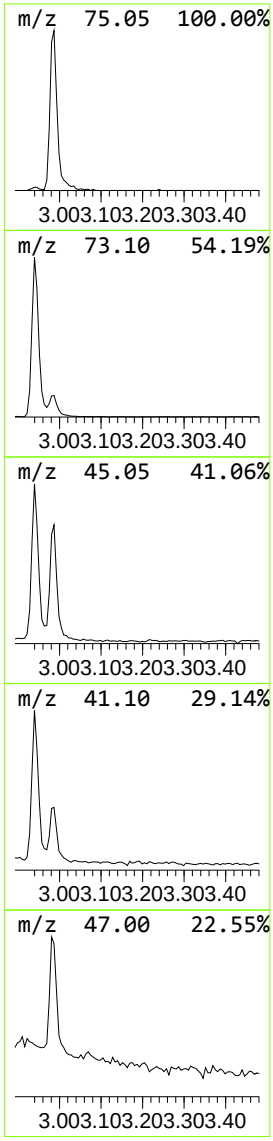
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.981	4.90 ng	164089	1,4-Dichlorobenzene-d4	7.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	40
3	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	40
4	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	38
5	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36





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Misc :
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Instrument :
BNA_M
ClientSampleId :
FS-SB18(39-40)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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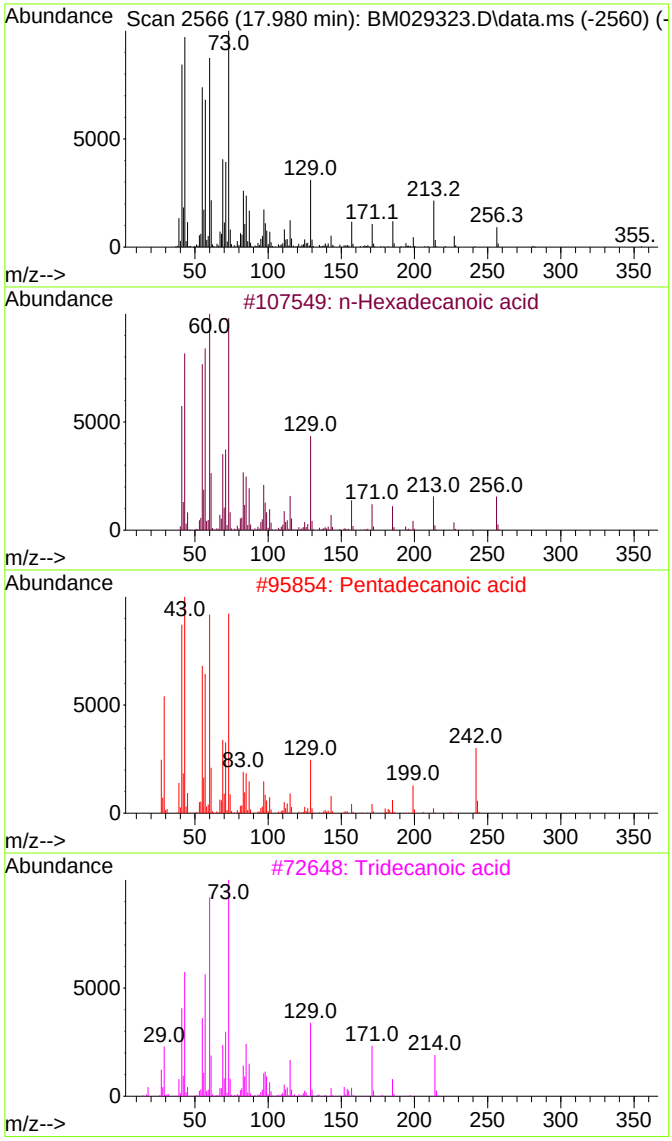
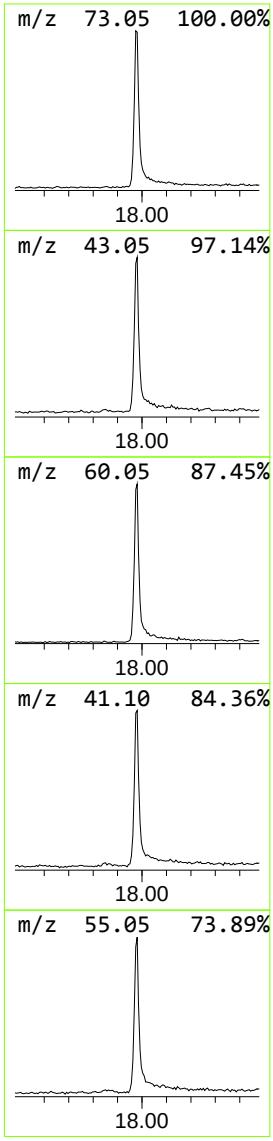
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	14.19 ng	905264	Phenanthrene-d10	17.074

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	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Sample : M1874-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB18(39-40)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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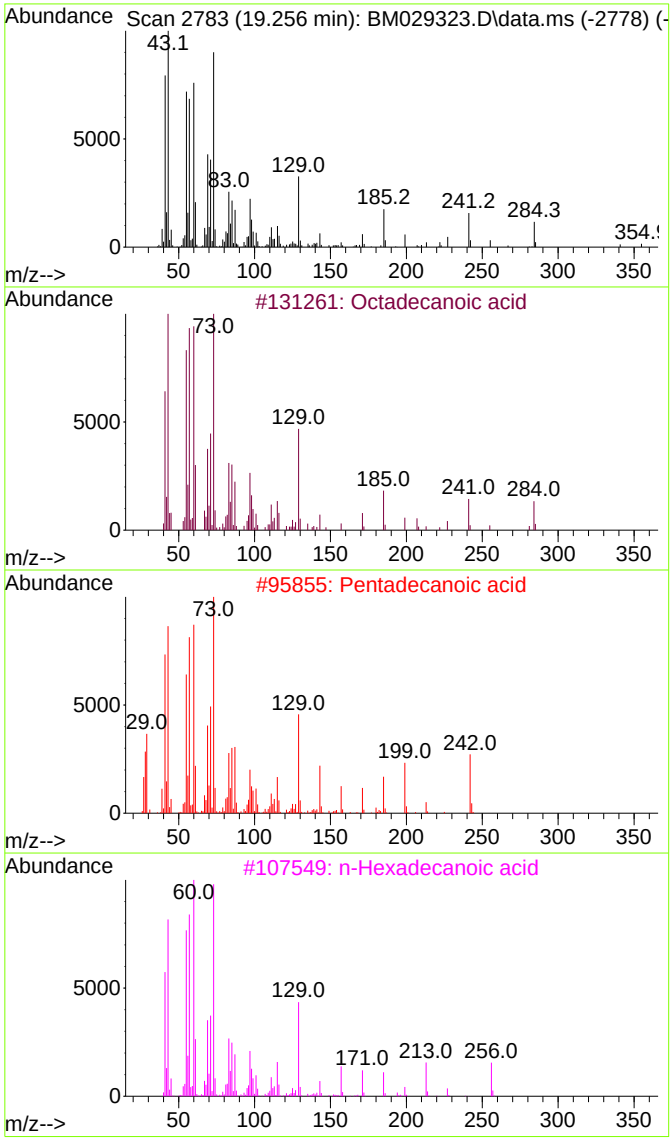
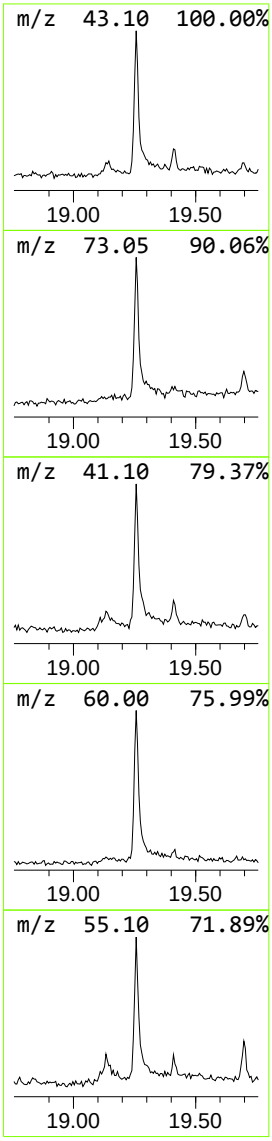
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.256	4.41 ng	359799	Chrysene-d12	21.244

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	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Data File : BM029323.D
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Operator : CG/JU
Sample : M1874-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB18(39-40)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

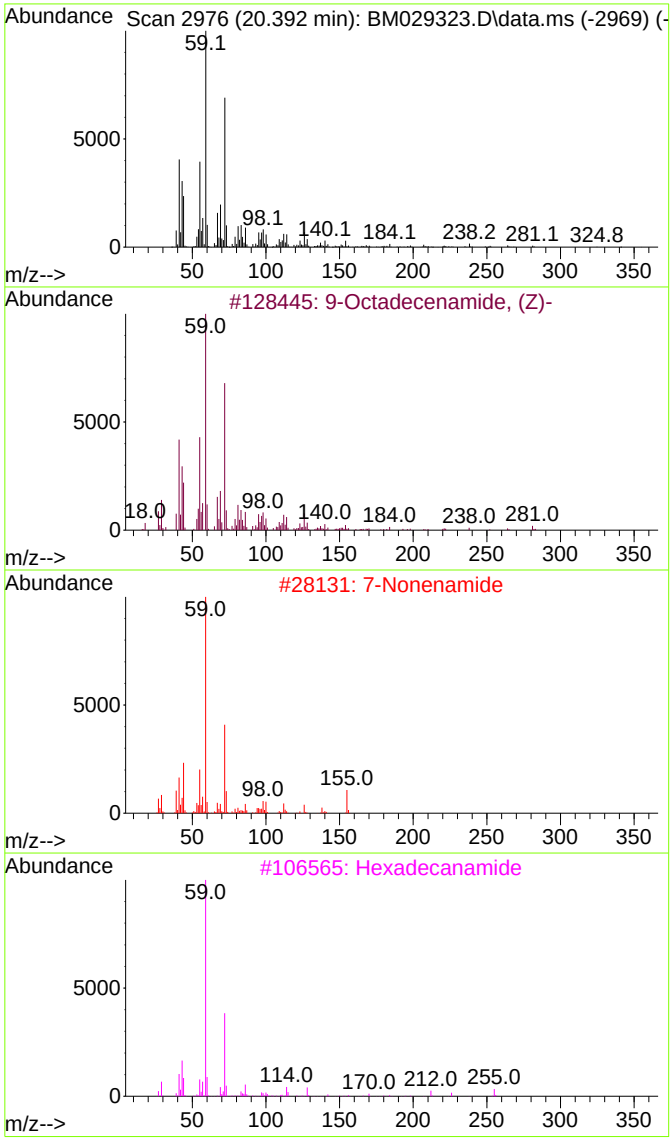
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

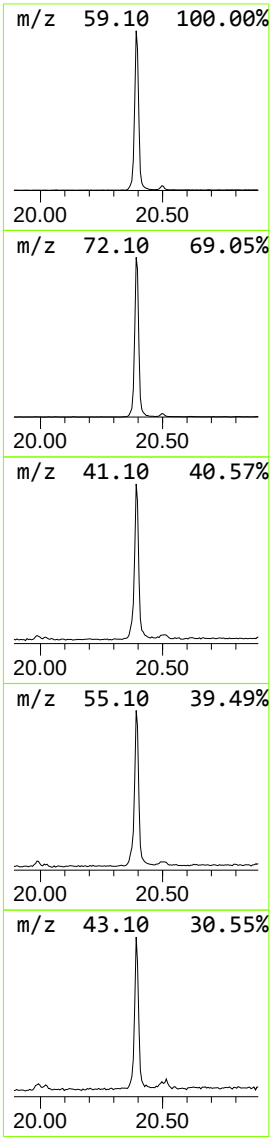
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.392	18.75 ng	1529660	Chrysene-d12	21.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	7-Nonenamide	155	C9H17NO	090949-53-4	64
3	Hexadecanamide	255	C16H33NO	000629-54-9	64
4	Octanamide	143	C8H17NO	000629-01-6	64
5	Dodecanamide	199	C12H25NO	001120-16-7	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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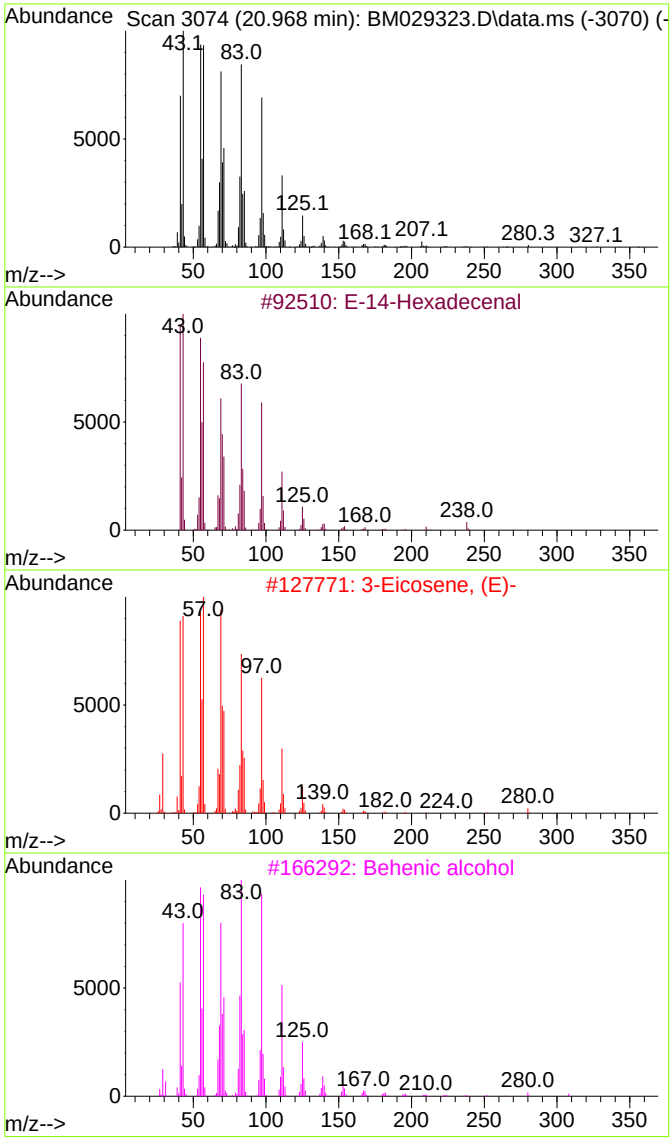
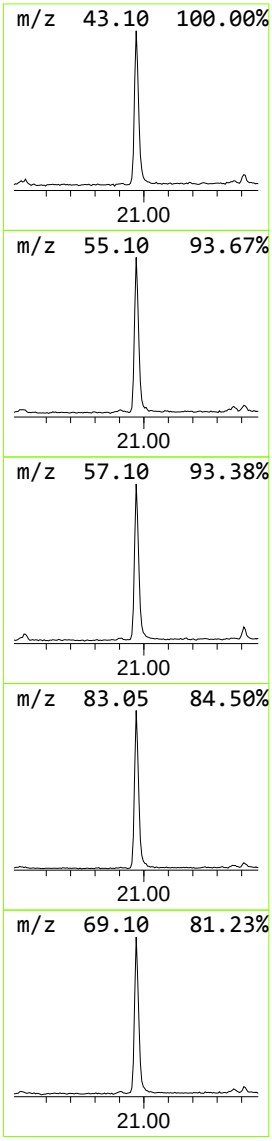
Peak Number 6 E-14-Hexadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.968	15.25 ng	1244690	Chrysene-d12	21.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Docosene	308	C22H44	001599-67-3	93
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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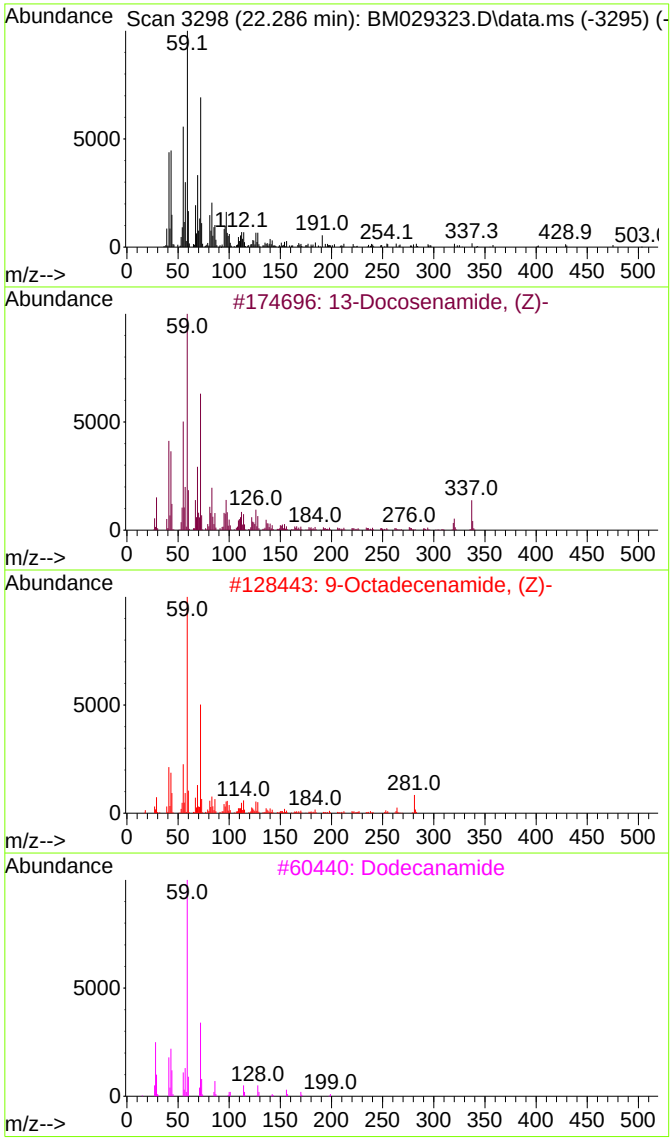
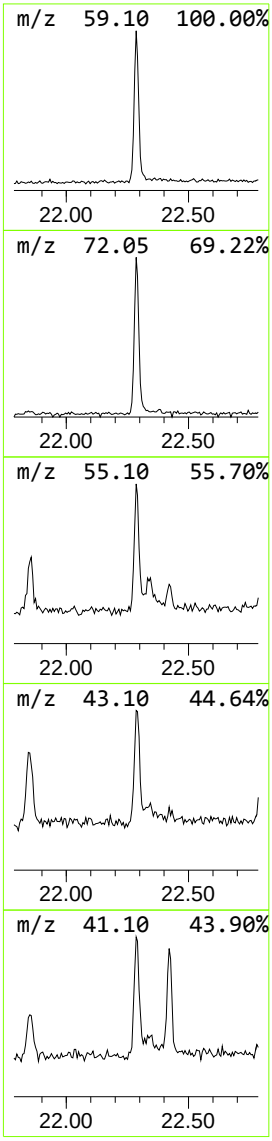
Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.286	2.85 ng	232815	Chrysene-d12	21.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	76
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
3	Dodecanamide	199	C12H25NO	001120-16-7	60
4	Octadecanamide	283	C18H37NO	000124-26-5	59
5	d-Glucosamine	179	C6H13NO5	000090-77-7	50





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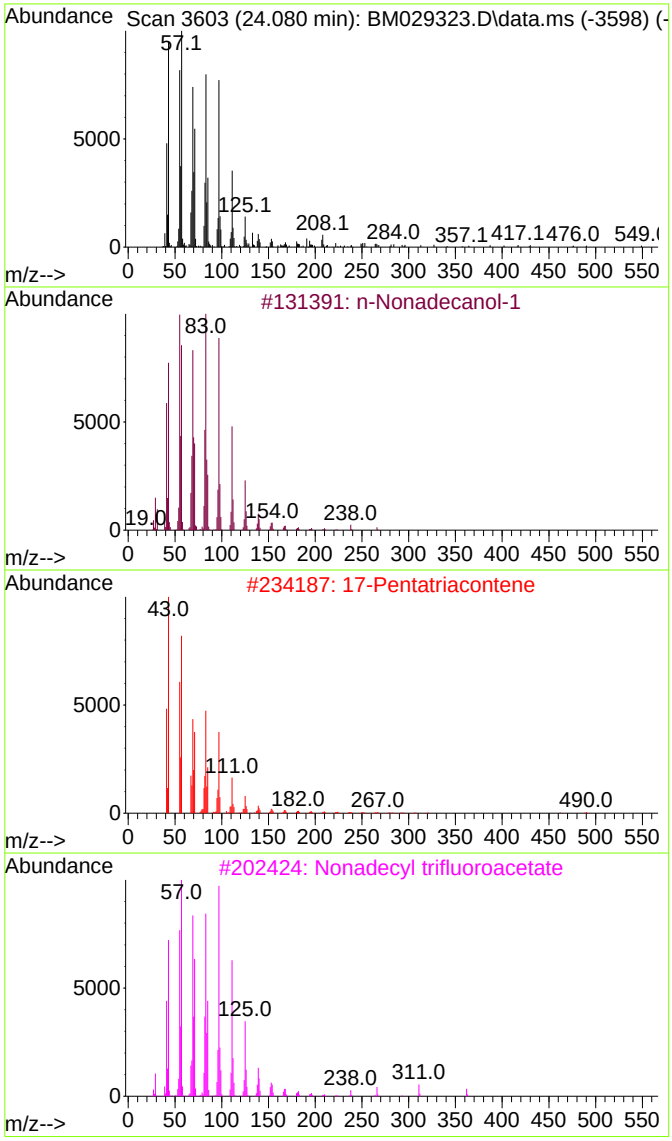
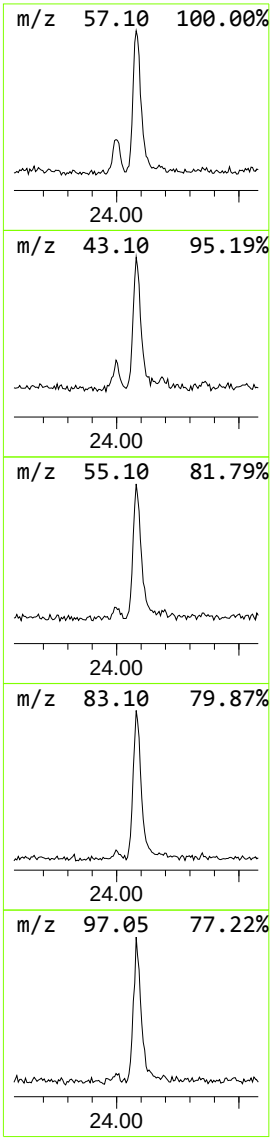
Peak Number 8 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.080	6.19 ng	556189	Perylene-d12	23.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	90





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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
Butane, 2-metho...	2.940	18.2	ng	610506	1	7.698	669508	20.0
Propane, 1,1-di...	2.981	4.9	ng	164089	1	7.698	669508	20.0
n-Hexadecanoic ...	17.980	14.2	ng	905264	4	17.074	1276230	20.0
Octadecanoic acid	19.256	4.4	ng	359799	5	21.244	1632010	20.0
9-Octadecenamid...	20.392	18.8	ng	1529660	5	21.244	1632010	20.0
E-14-Hexadecenal	20.968	15.3	ng	1244690	5	21.244	1632010	20.0
13-Docosenamide...	22.286	2.9	ng	232815	5	21.244	1632010	20.0
n-Nonadecanol-1	24.080	6.2	ng	556189	6	23.456	1798160	20.0