LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029002.D
Acq On : 05 Mar 2021 18:53
Operator : CG/JU
Sample : M1575-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW803-AQ-030321

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: BM029002.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.358	60	63	70	rBV	18744	25175	4.50%	1.075%
2	5.240	378	383	394	rVB	85112	122397	21.90%	5.227%
3	5.722	461	465	471	rBV	12288	16880	3.02%	0.721%
4	6.863	654	659	670	rVB	48644	76558	13.70%	3.269%
5	7.675	792	797	804	rBV	35240	51828	9.27%	2.213%
6	8.310	899	905	911	rVB2	5962	9370	1.68%	0.400%
7	8.851	990	997	1006	rVB	101473	161392	28.88%	6.892%
8	10.469	1266	1272	1279	rVB	42051	66722	11.94%	2.849%
9	12.957	1689	1695	1702	rVB	224787	314688	56.31%	13.438%
10	14.345	1926	1931	1936	rBV	56572	78144	13.98%	3.337%
11	15.845	2180	2186	2193	rVB	197795	269067	48.15%	11.490%
12	17.092	2393	2398	2404	rBV	65623	86975	15.56%	3.714%
13	17.992	2544	2551	2558	rBV	29820	41677	7.46%	1.780%
14	18.462	2627	2631	2636	rBV2	3004	5675	1.02%	0.242%
15	18.733	2671	2677	2681	rBV	16751	20969	3.75%	0.895%
16	18.821	2688	2692	2699	rVB	4689	6538	1.17%	0.279%
17	19.274	2762	2769	2776	rBV	20512	28404	5.08%	1.213%
18	19.721	2839	2845	2850	rBV	487815	558858	100.00%	23.865%
19	20.227	2926	2931	2946	rBV	74635	118596	21.22%	5.064%
20	20.980	3055	3059	3066	rBV	37169	47115	8.43%	2.012%
21	21.268	3103	3108	3113	rBV	96608	113901	20.38%	4.864%
22	23.433	3470	3476	3482	rVB	70368	120852	21.62%	5.161%

Sum of corrected areas: 2341781

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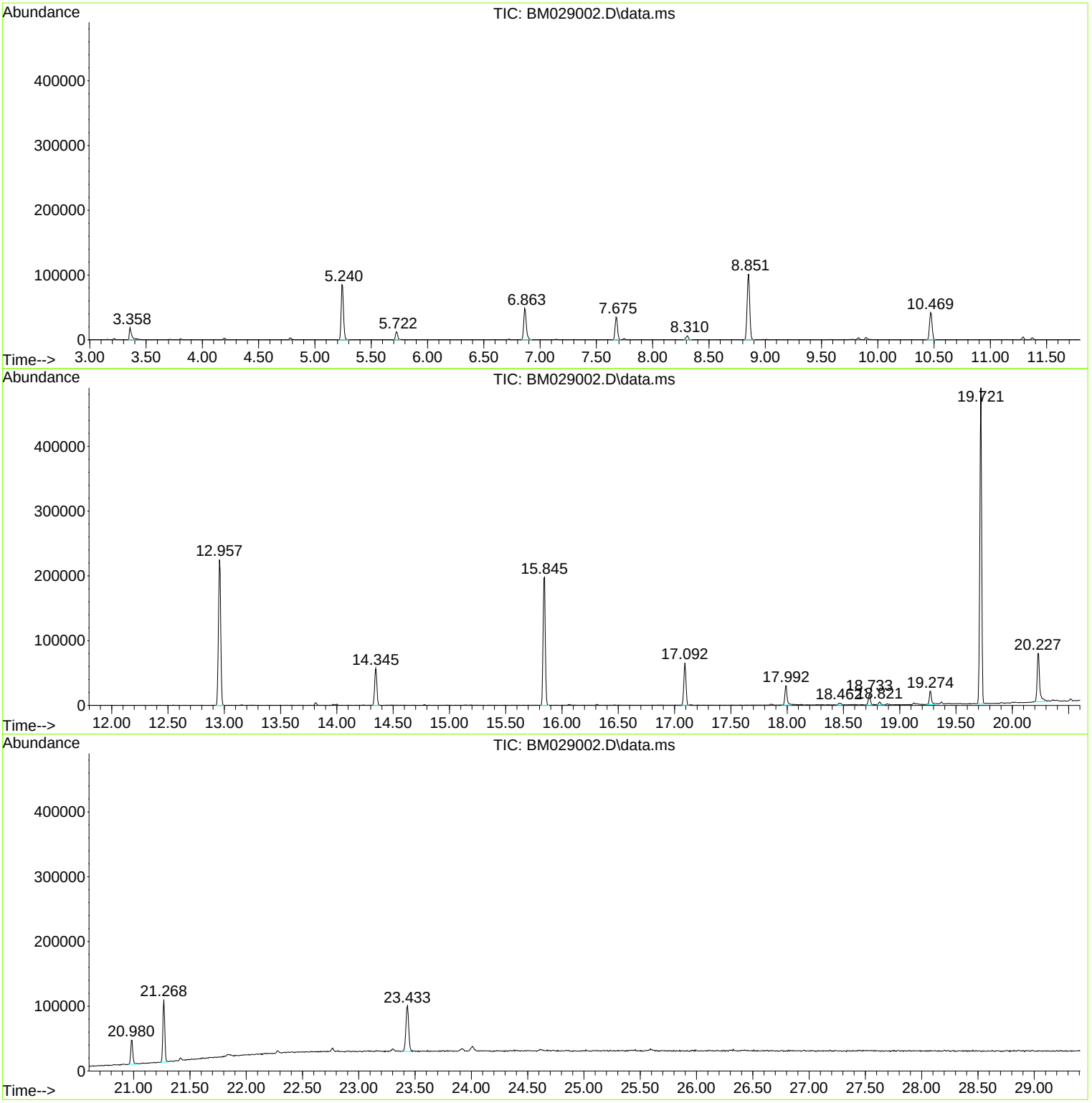
Instrument :
BNA_M
ClientSampleId :
IDW-GW803-AQ-030321

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 : BM029002.D
Acq On : 05 Mar 2021 18:53
Operator : CG/JU
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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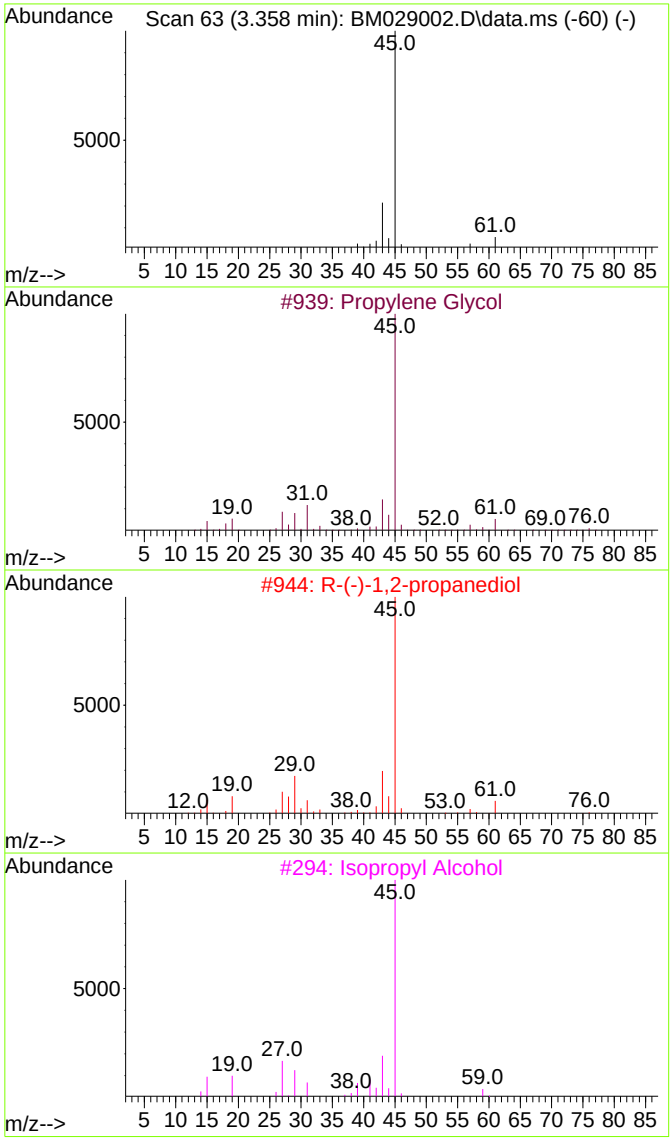
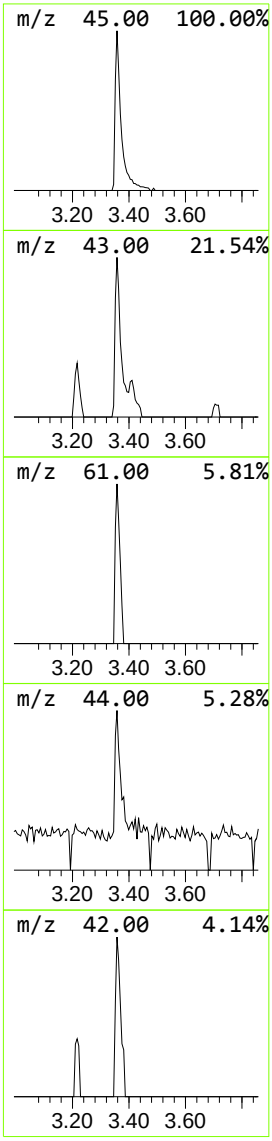
Peak Number 1 unknown3.358 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.358	9.71 ng	25175	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Formamide	45	CH3NO	000075-12-7	5
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	4





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IDW-GW803-AQ-030321

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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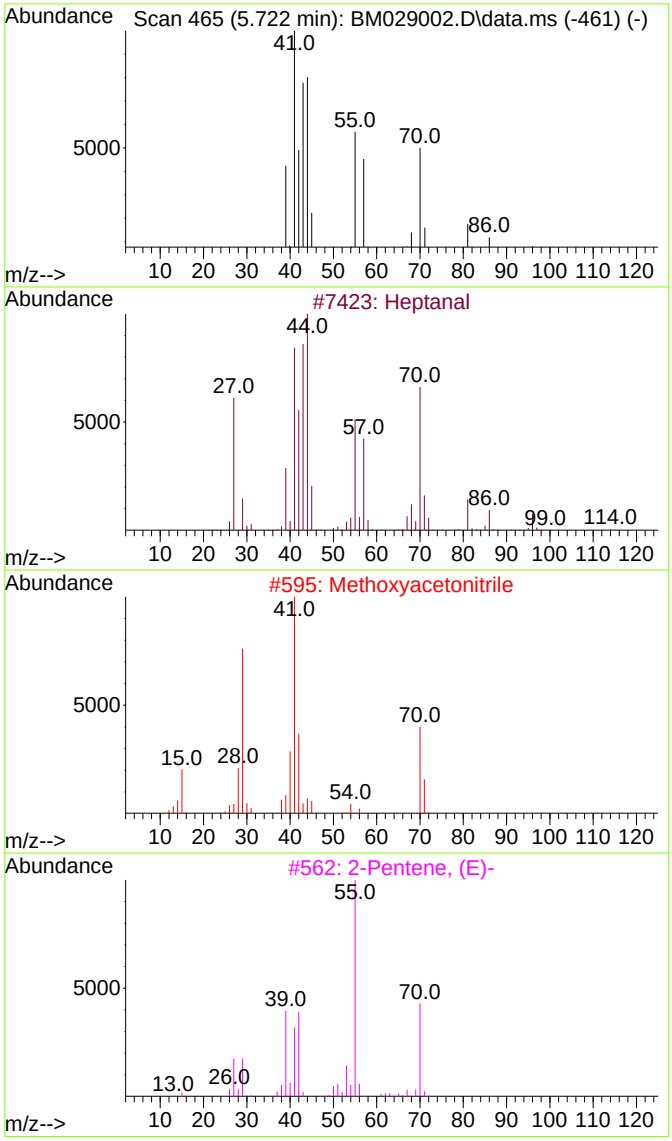
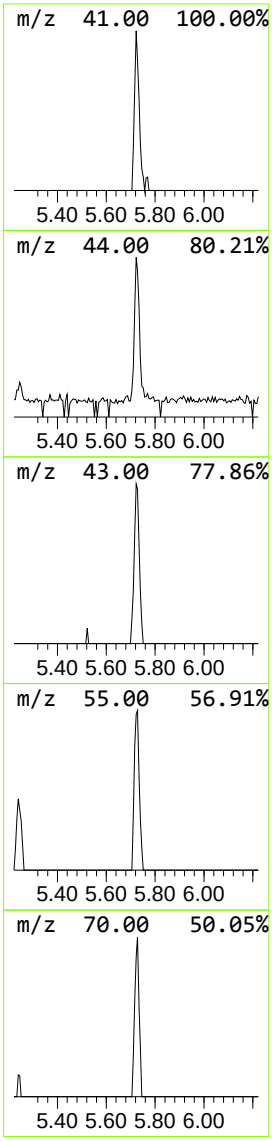
Peak Number 2 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.722	6.51 ng	16880	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	80
2	Methoxyacetonitrile	71	C3H5NO	001738-36-9	22
3	2-Pentene, (E)-	70	C5H10	000646-04-8	17
4	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	17
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	9





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Operator : CG/JU
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Misc :
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Instrument : BNA_M
ClientSampleId : IDW-GW803-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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TIC Library : C:\DATABASE\NIST11.L
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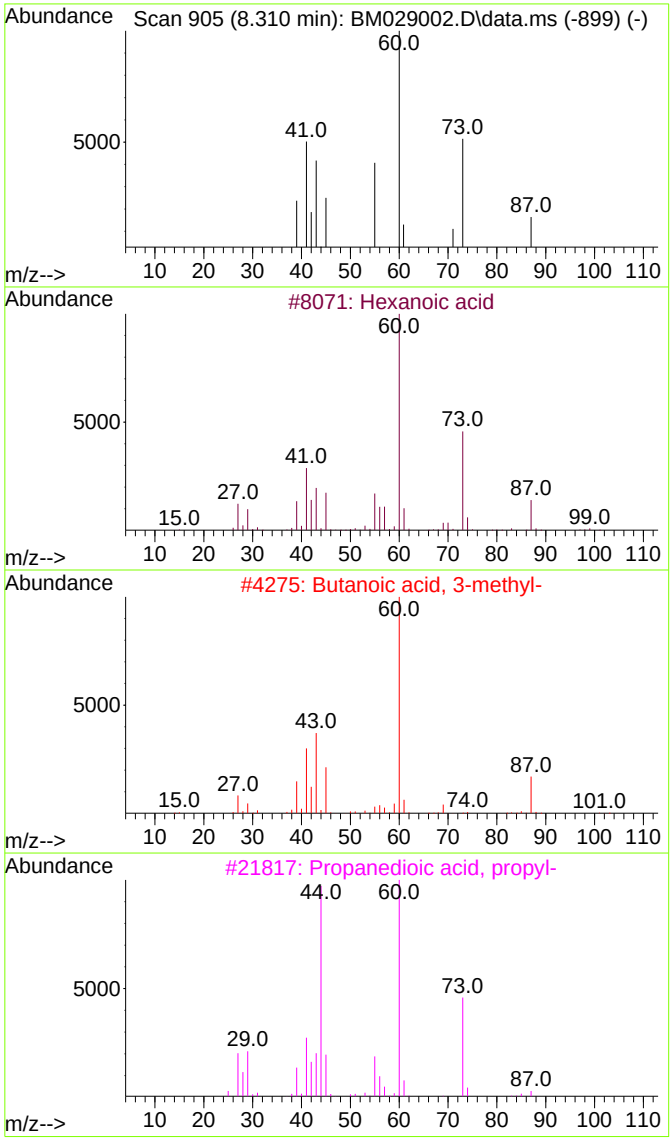
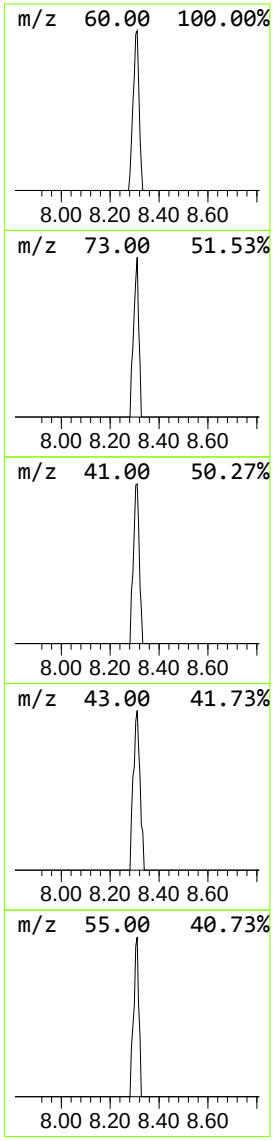
Peak Number 3 Hexanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.310	3.62 ng	9370	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	78
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	39
4	Formic acid hydrazide	60	CH4N2O	000624-84-0	7
5	Thiirane	60	C2H4S	000420-12-2	4





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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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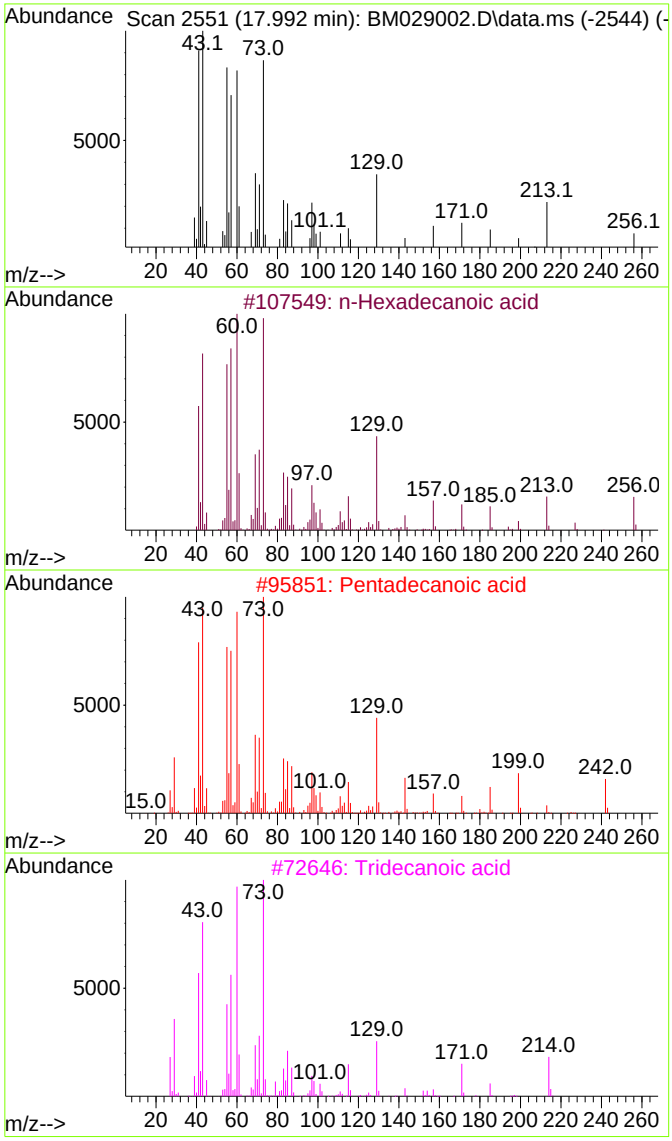
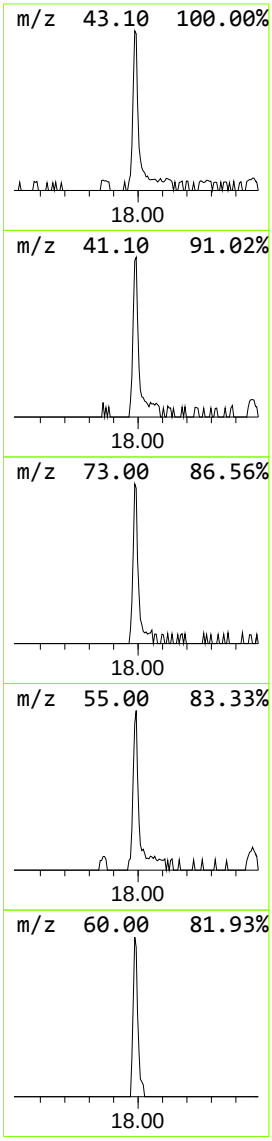
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	9.58 ng	41677	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Operator : CG/JU
Sample : M1575-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW803-AQ-030321

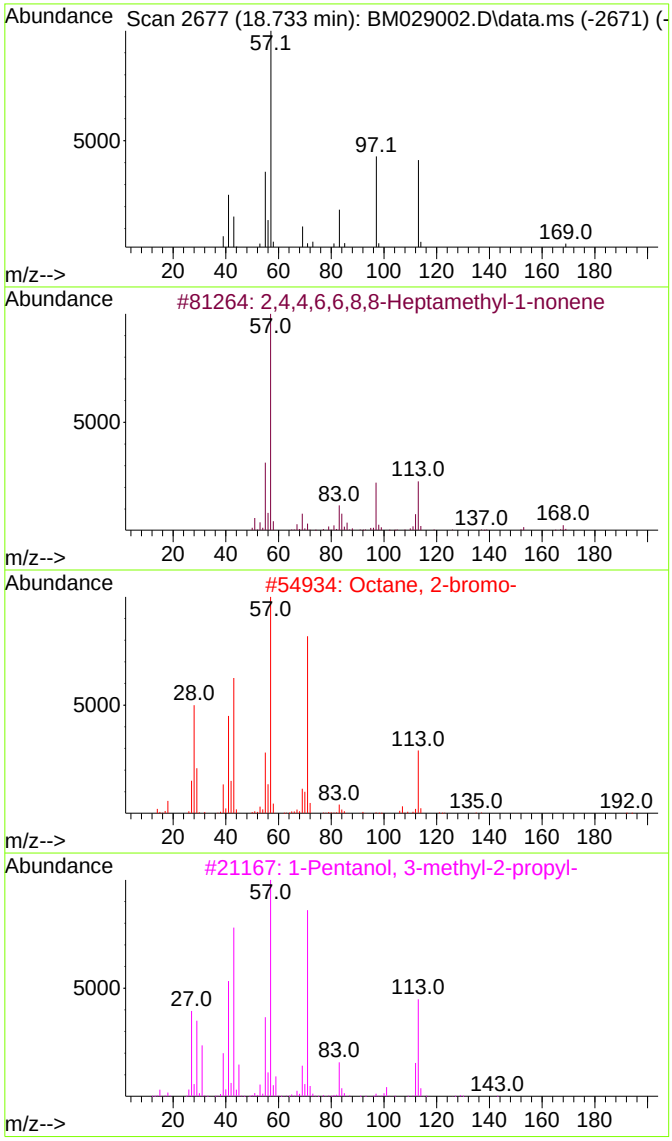
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

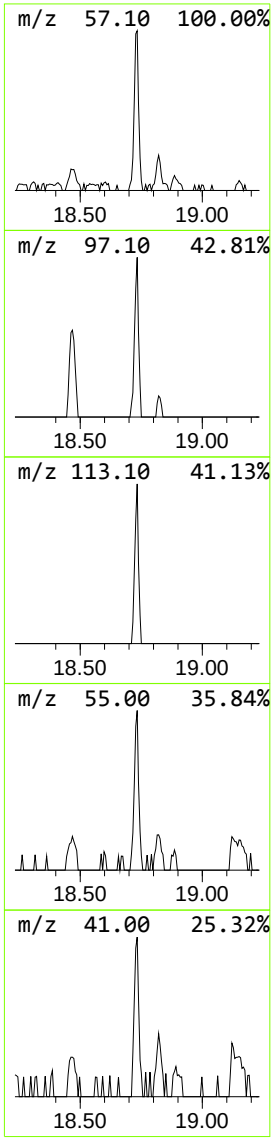
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.733	4.82 ng	20969	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	56
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	47
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	37





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

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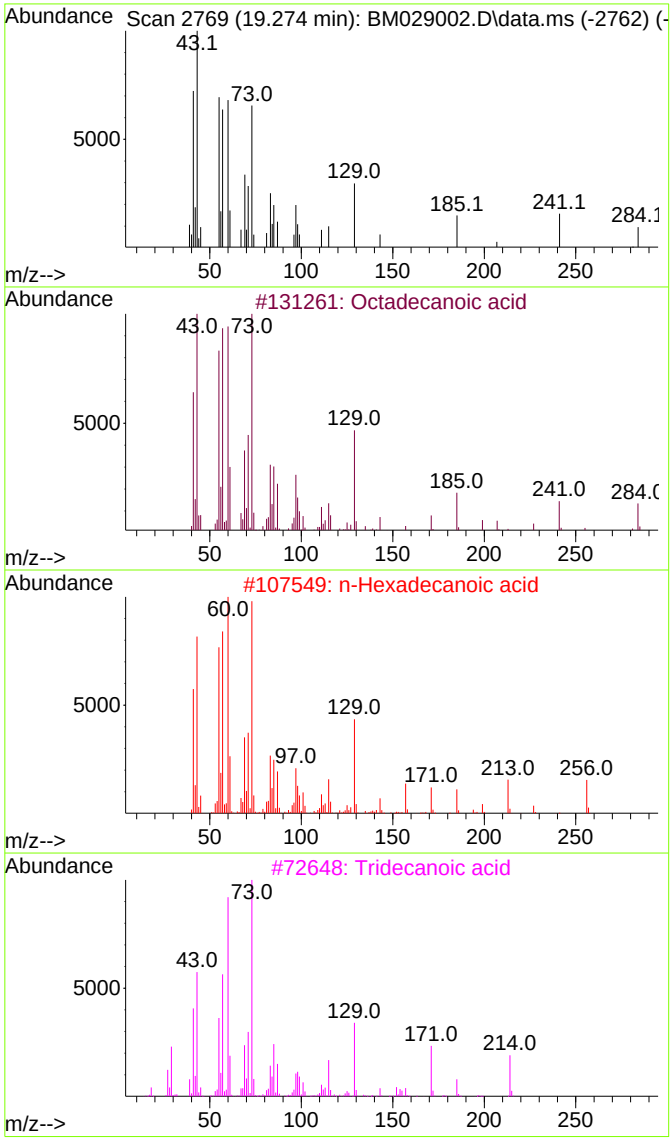
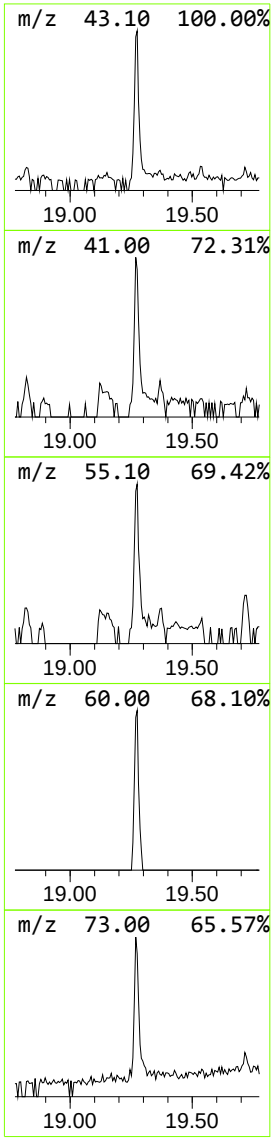
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	4.99 ng	28404	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





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BNA_M
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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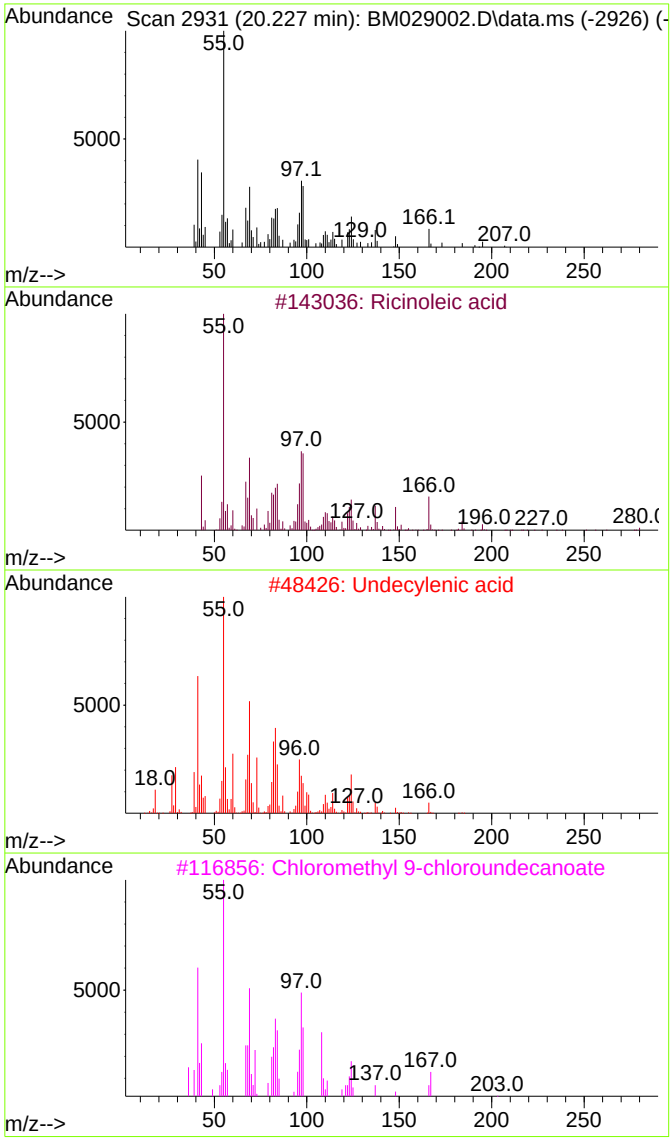
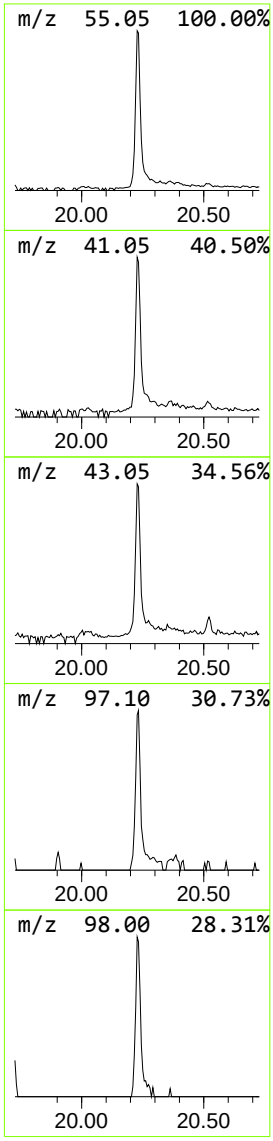
Peak Number 7 Ricinoleic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.227	20.82 ng	118596	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ricinoleic acid	298	C18H34O3	000141-22-0	91
2	Undecylenic acid	184	C11H20O2	000112-38-9	55
3	Chloromethyl 9-chloroundecanoate	268	C12H22Cl2O2	080418-95-7	50
4	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	46
5	Oxacyclotetradecan-2-one	212	C13H24O2	001725-04-8	43





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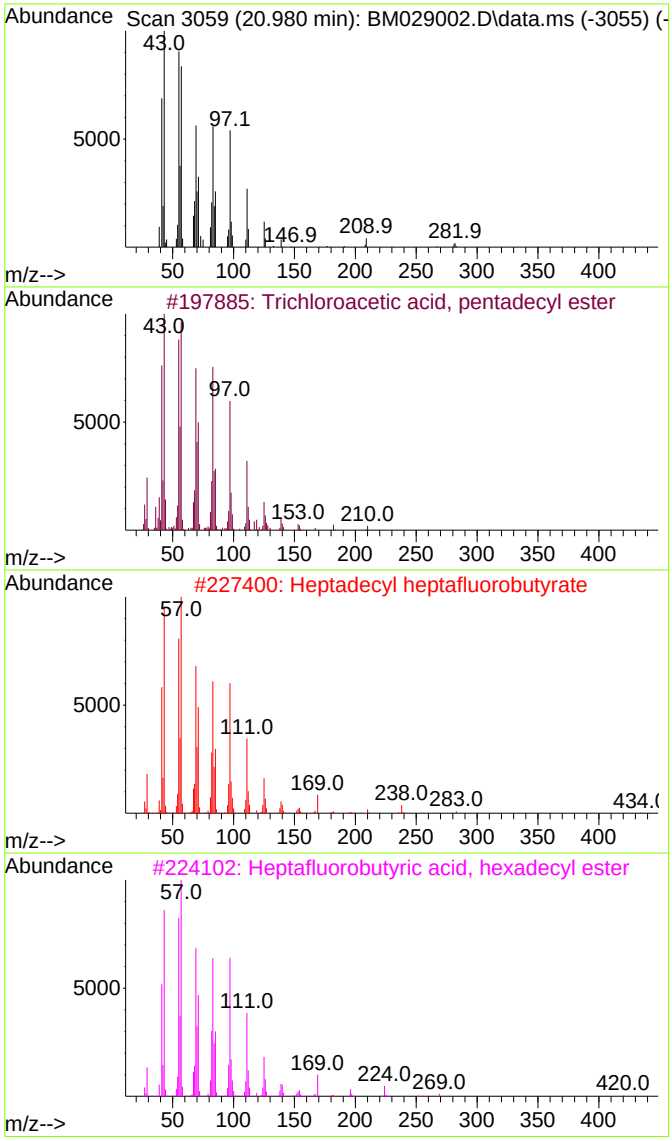
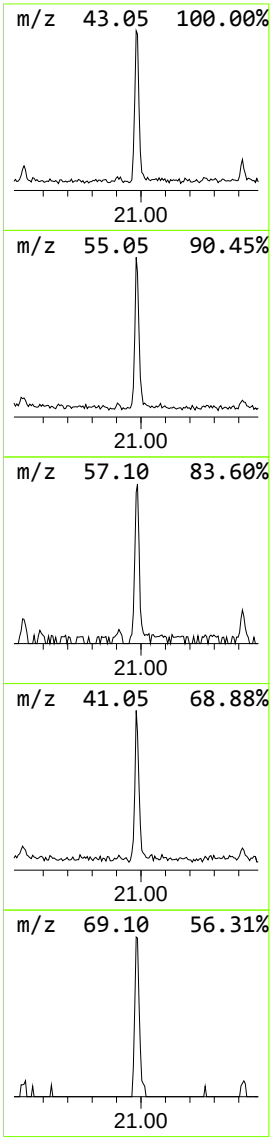
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	8.27 ng	47115	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Tentatively Identified Compound (LSC) summary

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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
unknown3.358	3.358	9.7	ng	25175	1	7.675	51828	20.0
Heptanal	5.722	6.5	ng	16880	1	7.675	51828	20.0
Hexanoic acid	8.310	3.6	ng	9370	1	7.675	51828	20.0
n-Hexadecanoic ...	17.992	9.6	ng	41677	4	17.092	86975	20.0
2,4,4,6,6,8,8-H...	18.733	4.8	ng	20969	4	17.092	86975	20.0
Octadecanoic acid	19.274	5.0	ng	28404	5	21.268	113901	20.0
Ricinoleic acid	20.227	20.8	ng	118596	5	21.268	113901	20.0
Trichloroacetic...	20.980	8.3	ng	47115	5	21.268	113901	20.0