LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055677.D
Acq On : 17 Nov 2022 22:44
Operator : CG/JU
Sample : N5607-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-39

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_G\Methods\8270-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055677.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.304	335	343	352	rBV	96901	150701	7.37%	1.211%
2	5.786	418	425	439	rVB	664939	1082167	52.91%	8.694%
3	7.402	692	700	716	rVB	650388	1145164	55.99%	9.201%
4	8.254	837	845	852	rBV	191552	324444	15.86%	2.607%
5	9.423	1035	1044	1051	rBV	400990	721759	35.29%	5.799%
6	10.827	1274	1283	1293	rBV	44775	81559	3.99%	0.655%
7	11.080	1319	1326	1333	rBV	261620	468850	22.92%	3.767%
8	13.500	1727	1738	1745	rBV	1060611	1647072	80.53%	13.233%
9	14.875	1965	1972	1980	rVB	387122	627773	30.69%	5.044%
10	16.356	2217	2224	2234	rBV	782553	1227843	60.03%	9.865%
11	17.613	2431	2438	2444	rBV	470864	724540	35.42%	5.821%
12	18.254	2543	2547	2553	rVB	22685	29363	1.44%	0.236%
13	18.359	2559	2565	2570	rBV8	18319	38850	1.90%	0.312%
14	18.471	2579	2584	2591	rBV	164880	240430	11.75%	1.932%
15	18.765	2631	2634	2640	rBV6	12268	22090	1.08%	0.177%
16	19.593	2772	2775	2777	rBV2	32264	40184	1.96%	0.323%
17	19.646	2781	2784	2790	rVB	61401	98936	4.84%	0.795%
18	19.734	2795	2799	2805	rBV2	65356	98027	4.79%	0.788%
19	20.010	2844	2846	2851	rVB2	50182	67006	3.28%	0.538%
20	20.204	2873	2879	2884	rBV	1513453	2045383	100.00%	16.433%
21	21.515	3098	3102	3113	rVB3	97413	168440	8.24%	1.353%
22	21.914	3164	3170	3175	rBV	412405	707201	34.58%	5.682%
23	25.334	3745	3752	3764	rVB2	231249	688937	33.68%	5.535%

Sum of corrected areas: 12446719

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Misc :
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Instrument :
BNA_G
ClientSampleId :
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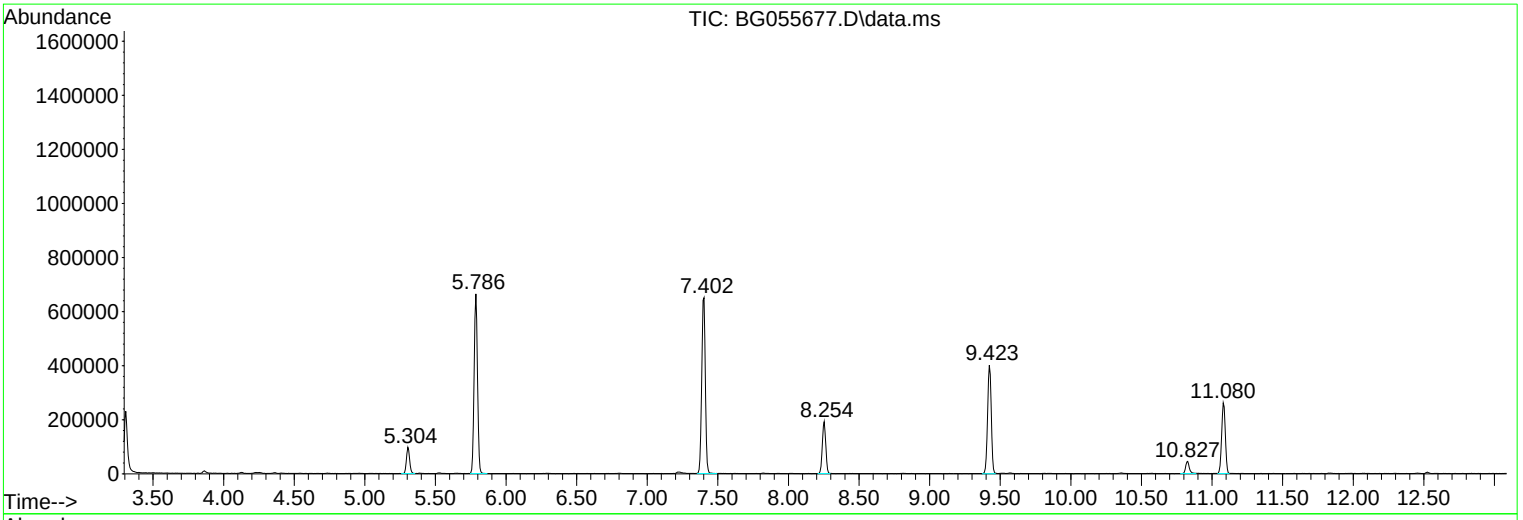
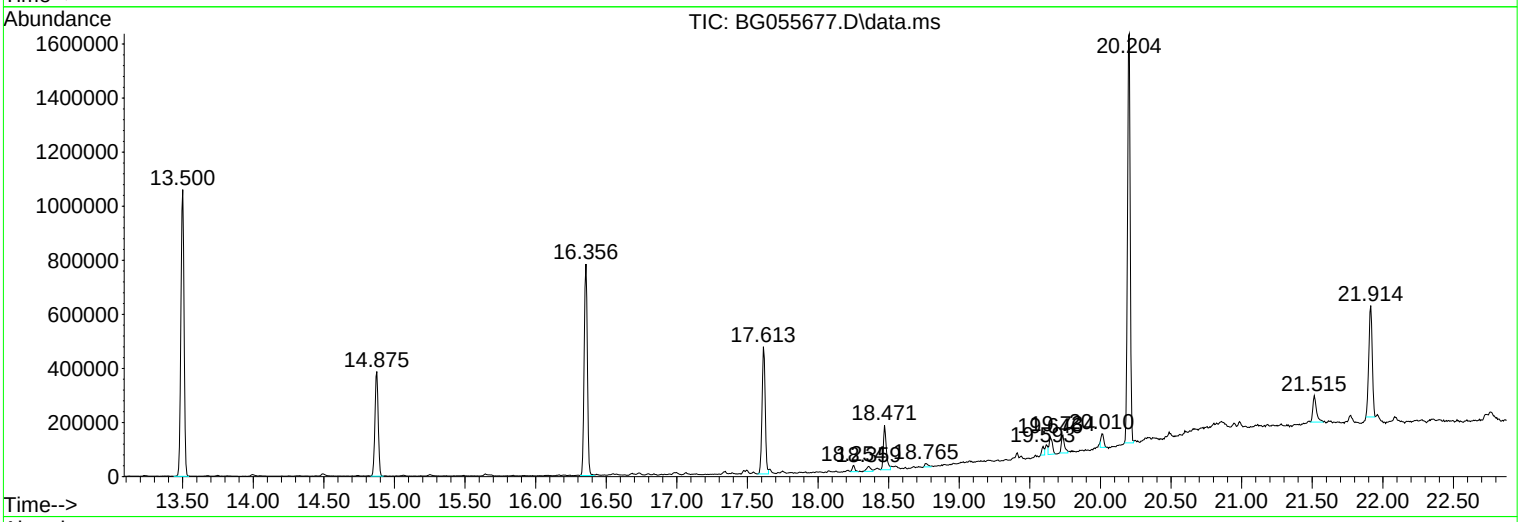
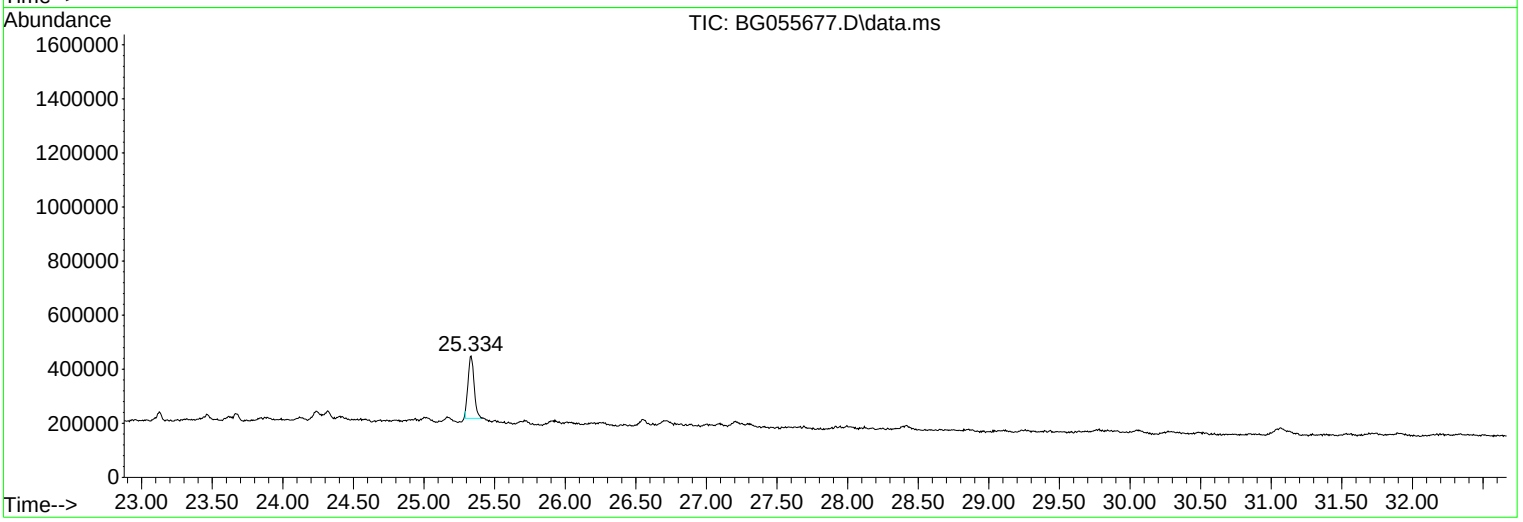
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BG055677.D
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Sample : N5607-09
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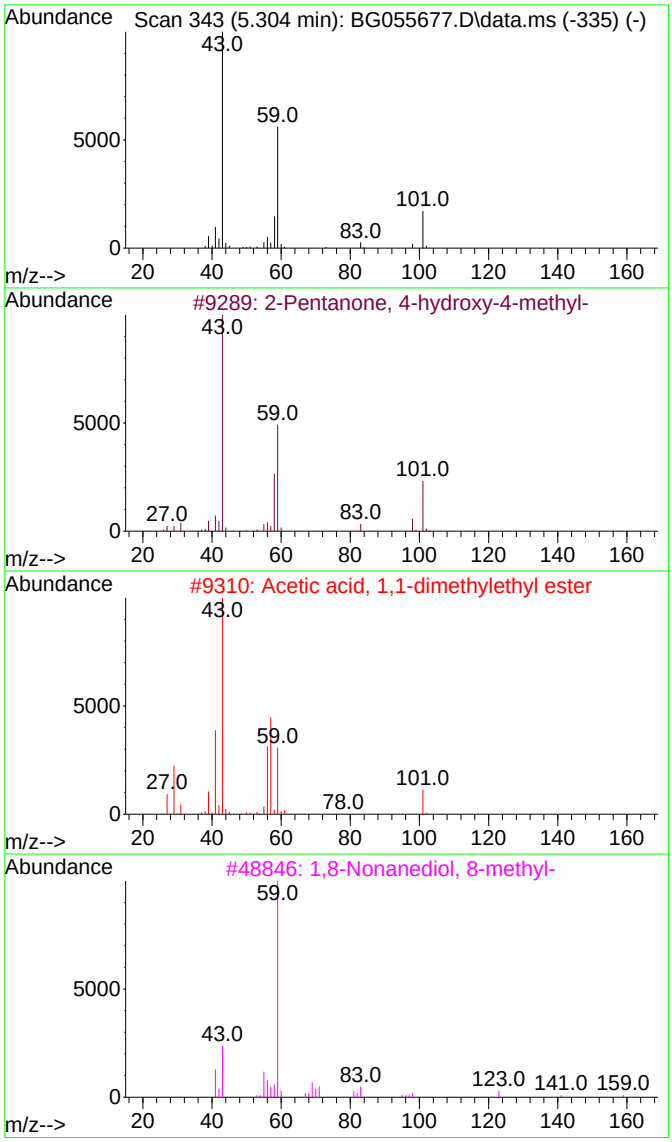
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

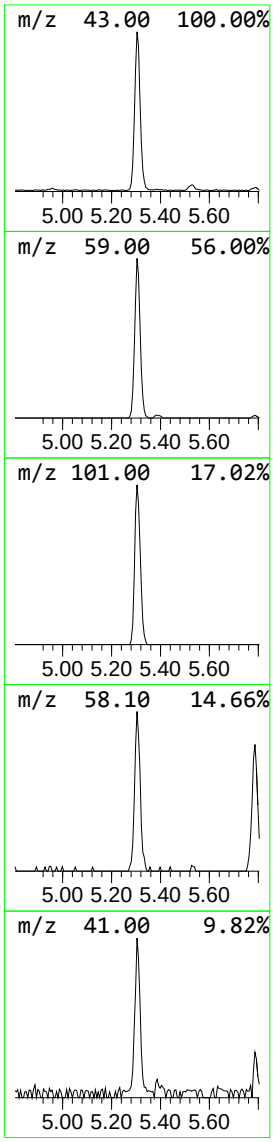
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.304	9.29 ng	150701	1,4-Dichlorobenzene-d4	8.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Sample : N5607-09
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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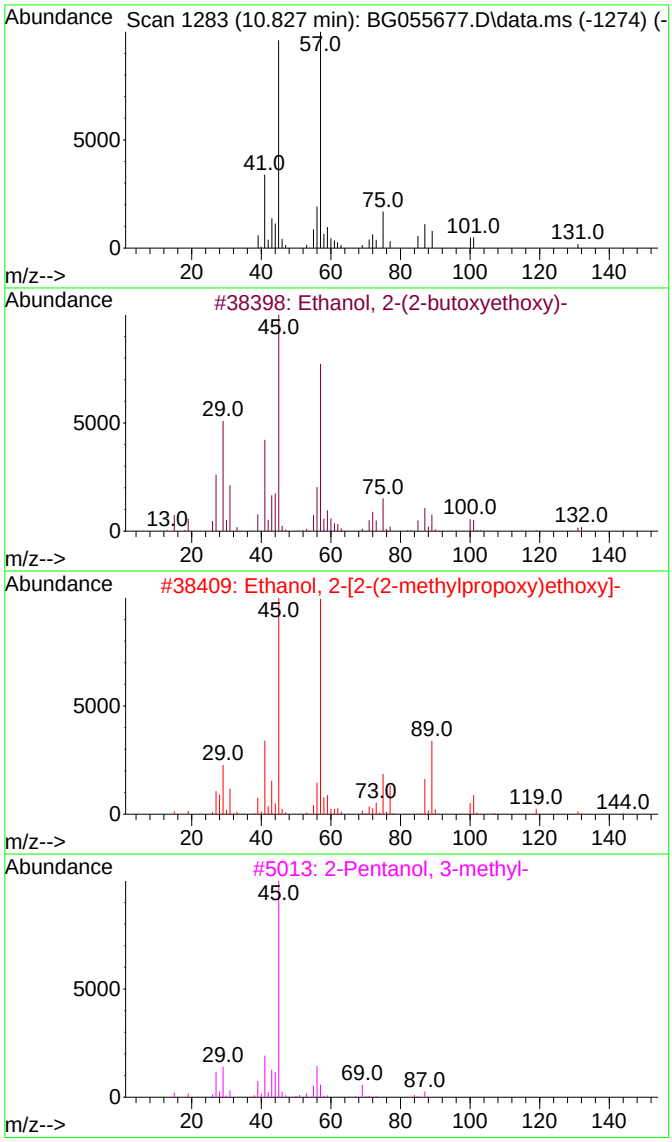
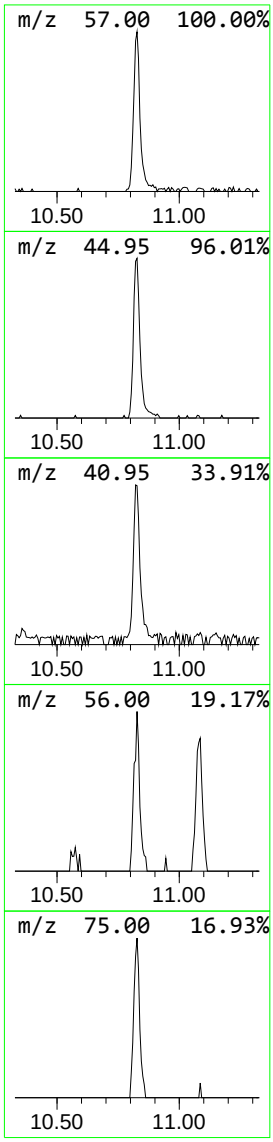
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.827	3.48 ng	81559	Naphthalene-d8	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	53
4	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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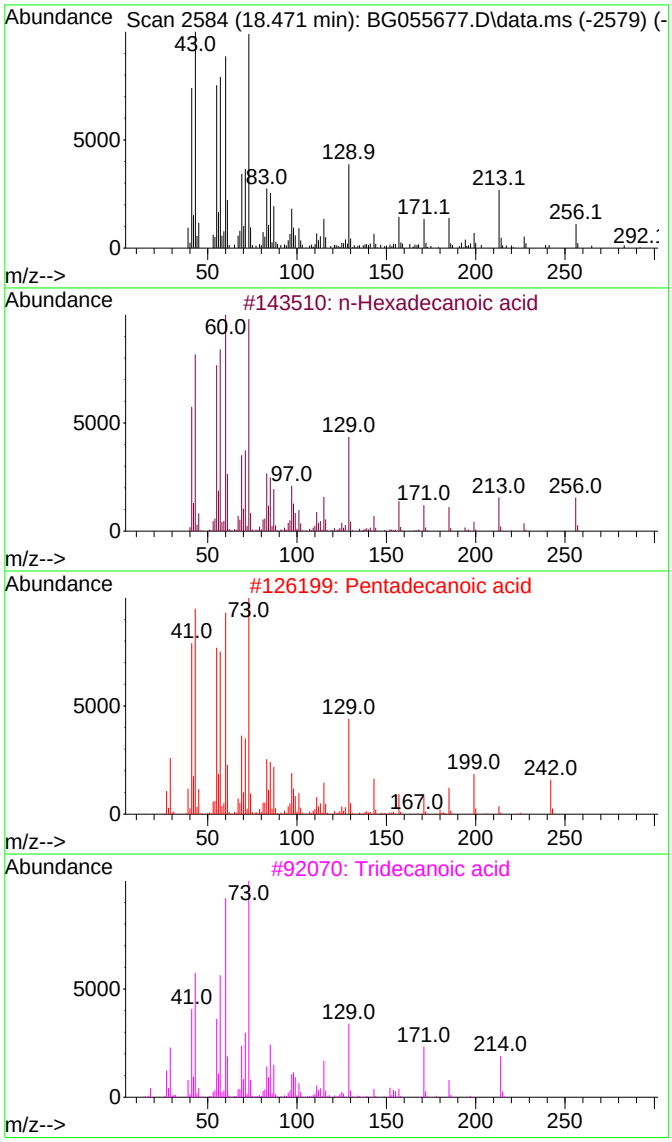
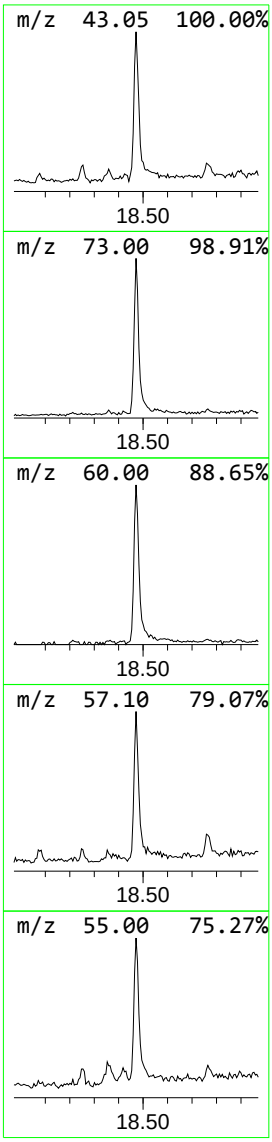
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.471	6.64 ng	240430	Phenanthrene-d10	17.613

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	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76





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Instrument :
BNA_G
ClientSampleId :
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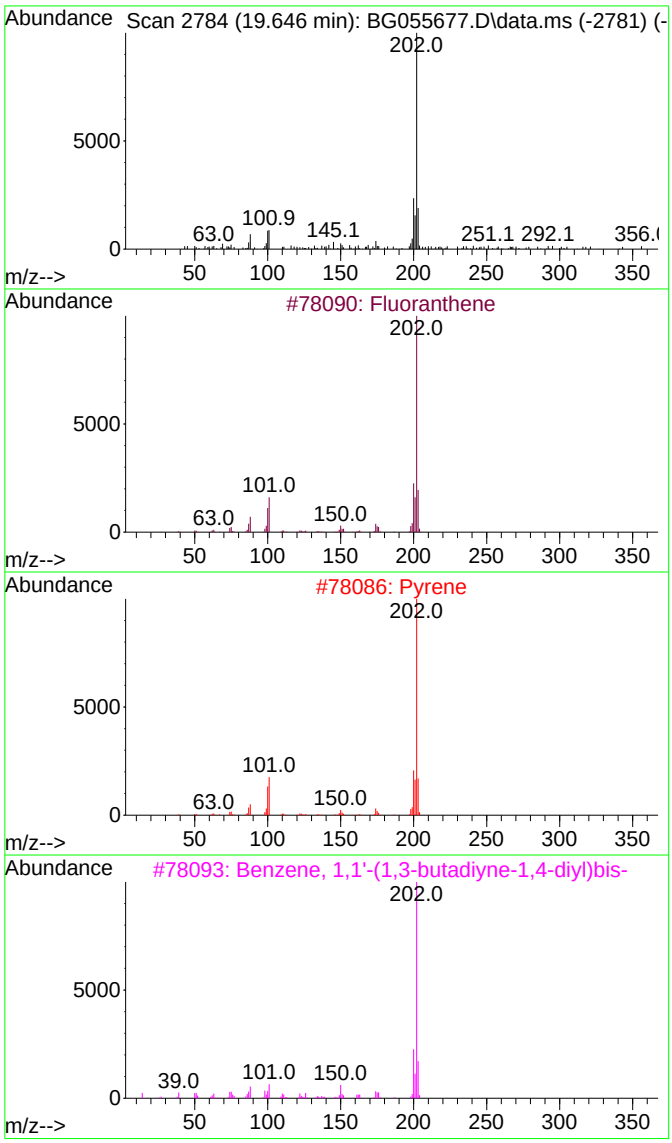
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

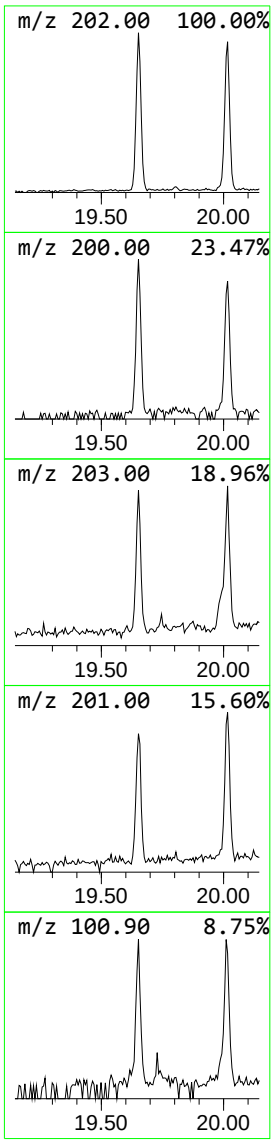
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.646	2.73 ng	98936	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	93
2	Pyrene	202	C16H10	000129-00-0	89
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4	7-(2-Butyl)amino-4-methylcoumarin	231	C14H17NO2	1000395-84-3	40
5	Succinic acid, di(4-cyanophenyl)...	320	C18H12N2O4	1000360-71-2	40





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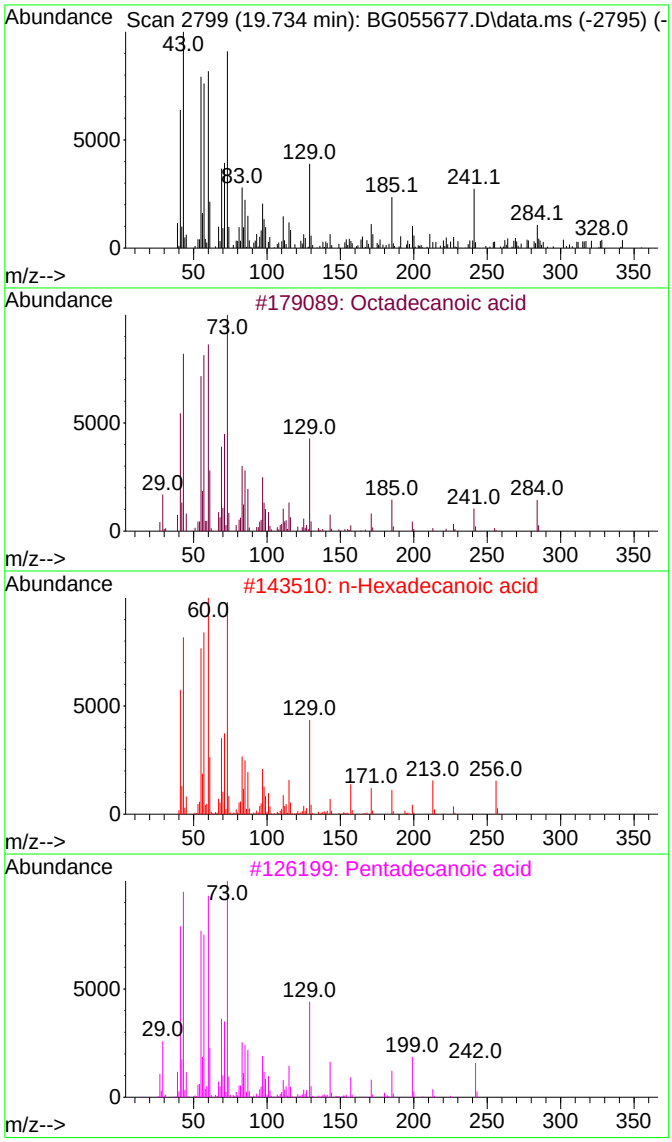
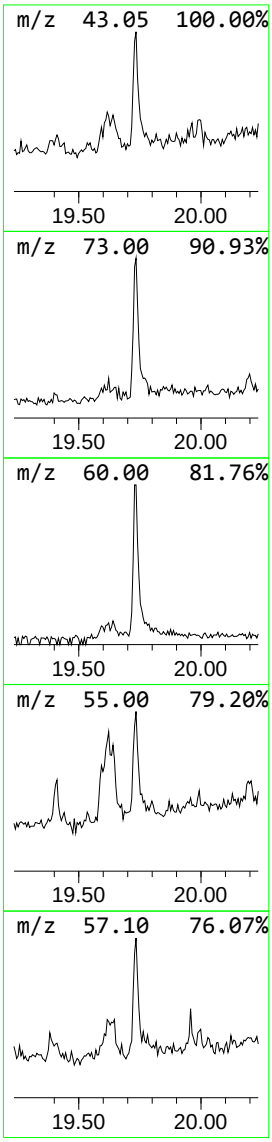
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.734	2.71 ng	98027	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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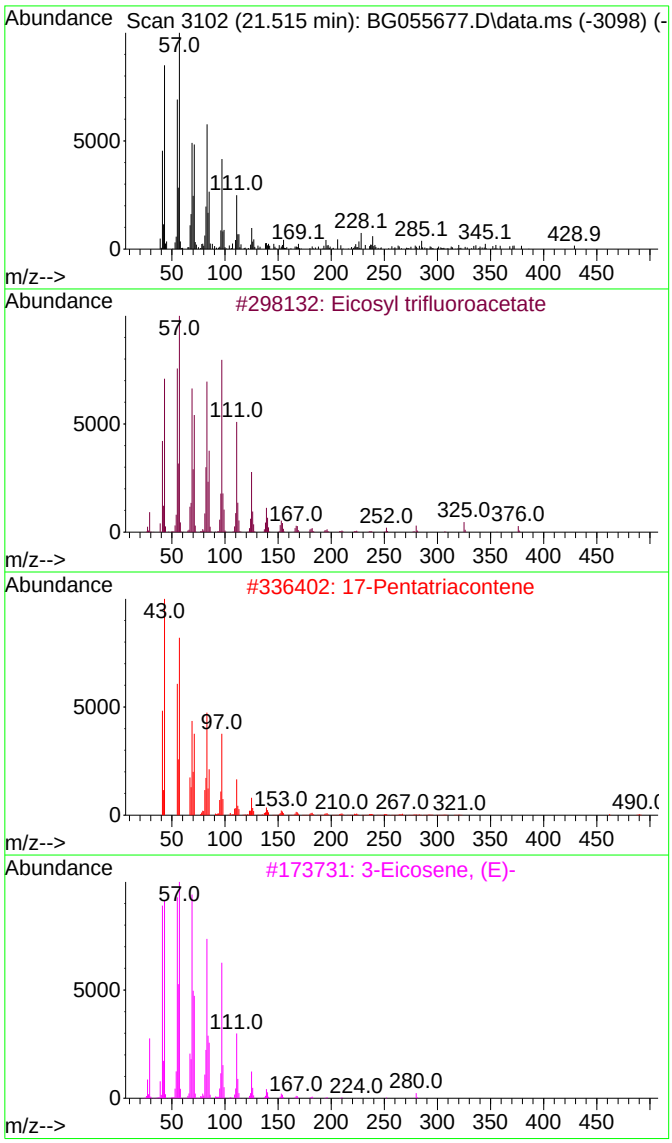
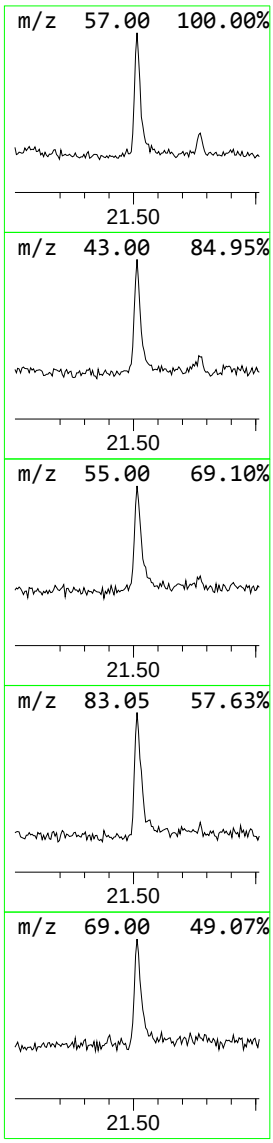
****

Peak Number 6 Eicosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.515	4.76 ng	168440	Chrysene-d12	21.914

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	1-Hexacosene	364	C26H52	018835-33-1	90





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-...	5.304	9.3	ng	150701	1	8.254	324444	20.0
Ethanol, 2-(2-b...	10.827	3.5	ng	81559	2	11.080	468850	20.0
n-Hexadecanoic ...	18.471	6.6	ng	240430	4	17.613	724540	20.0
Benzene, 1,1'-(...	19.646	2.7	ng	98936	4	17.613	724540	20.0
Octadecanoic acid	19.734	2.7	ng	98027	4	17.613	724540	20.0
Eicosyl trifluo...	21.515	4.8	ng	168440	5	21.914	707201	20.0