LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057915.D
Acq On : 29 Jun 2023 22:20
Operator : CG/JU
Sample : 03368-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-29

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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057915.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.020	322	329	335	rBV	34330	53458	2.29%	0.345%
2	5.490	402	409	423	rBV	887752	1424654	61.04%	9.206%
3	7.082	672	680	690	rBV	902878	1520553	65.15%	9.826%
4	7.911	814	821	828	rBV	218879	368211	15.78%	2.379%
5	9.074	1011	1019	1031	rBV	532561	935681	40.09%	6.046%
6	10.713	1288	1298	1308	rBV	306907	544182	23.32%	3.516%
7	13.175	1709	1717	1725	rBV	1237439	1972207	84.50%	12.744%
8	14.550	1941	1951	1958	rBV	455591	721324	30.90%	4.661%
9	15.901	2175	2181	2187	rBV	187901	274712	11.77%	1.775%
10	16.037	2197	2204	2217	rBV	982145	1475171	63.20%	9.532%
11	17.294	2412	2418	2423	rBV	536808	803941	34.44%	5.195%
12	17.470	2443	2448	2455	rVB3	22757	39633	1.70%	0.256%
13	18.122	2555	2559	2564	rBV7	12155	26624	1.14%	0.172%
14	18.181	2564	2569	2579	rBV	343527	520819	22.31%	3.365%
15	18.910	2689	2693	2698	rVB6	30224	49317	2.11%	0.319%
16	19.344	2763	2767	2772	rBV	65084	91563	3.92%	0.592%
17	19.397	2773	2776	2781	rVB	92582	118584	5.08%	0.766%
18	19.456	2782	2786	2797	rBV	131211	204714	8.77%	1.323%
19	19.709	2826	2829	2837	rVB	63217	92513	3.96%	0.598%
20	19.908	2858	2863	2869	rBV	1783141	2334010	100.00%	15.082%
21	21.195	3078	3082	3092	rVB2	237101	342365	14.67%	2.212%
22	21.548	3136	3142	3147	rVB	464632	746711	31.99%	4.825%
23	24.703	3673	3679	3691	rVB	286661	814622	34.90%	5.264%

Sum of corrected areas: 15475569

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Misc :
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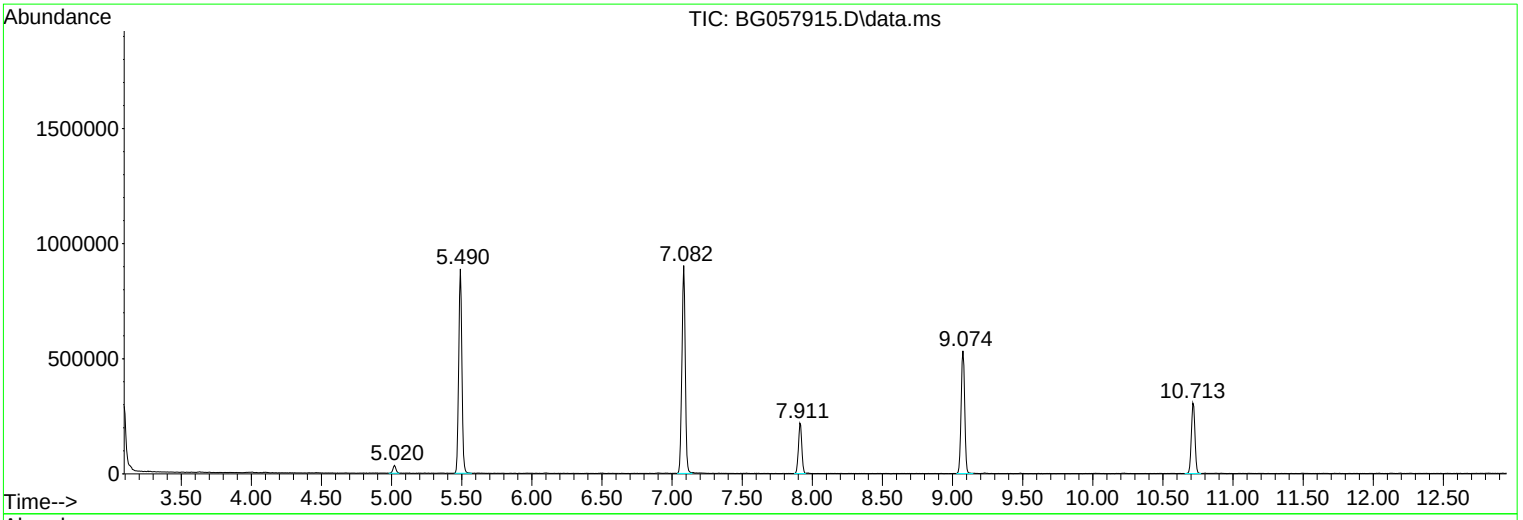
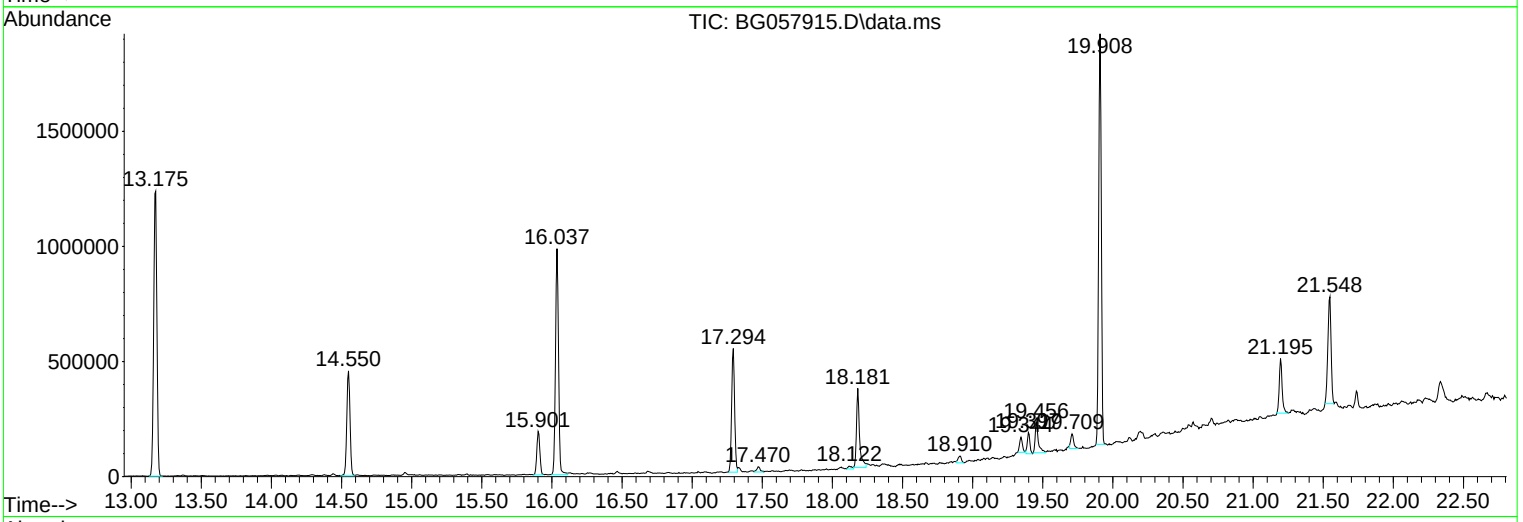
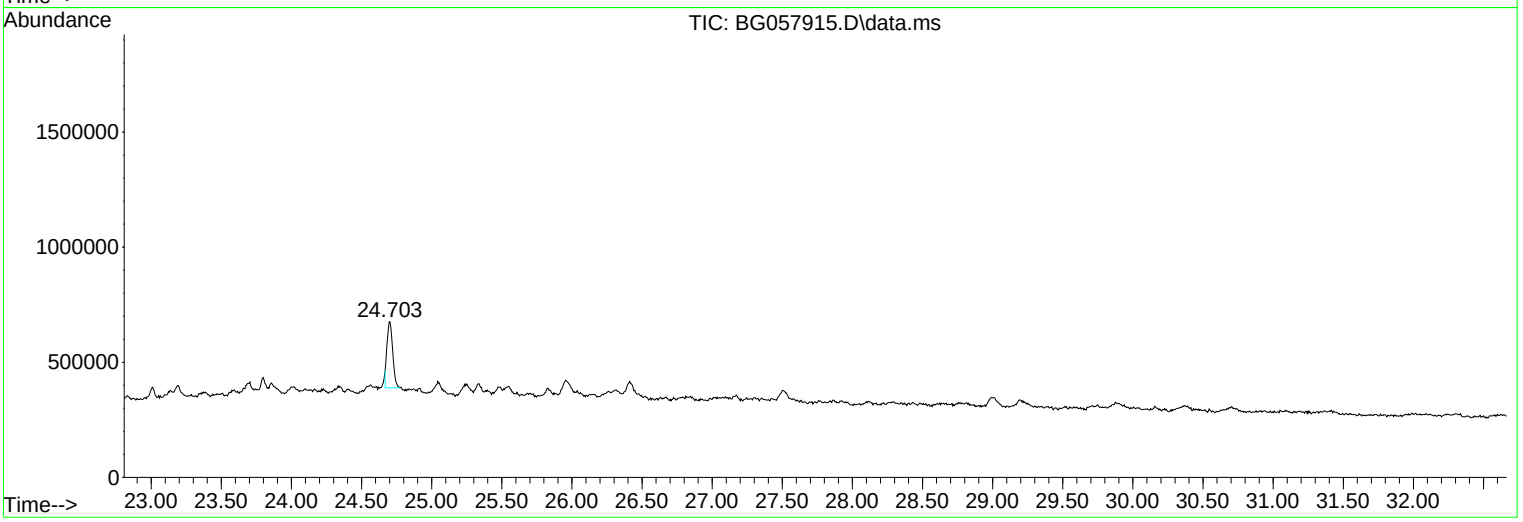
Instrument :
BNA_G
ClientSampleId :
CF-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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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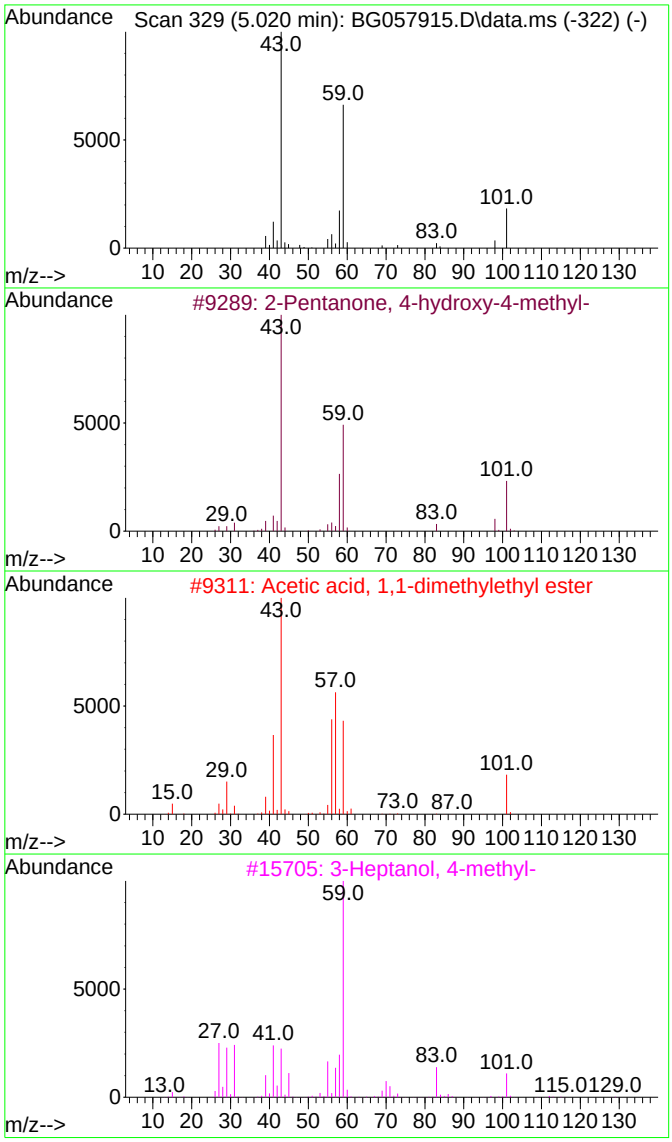
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

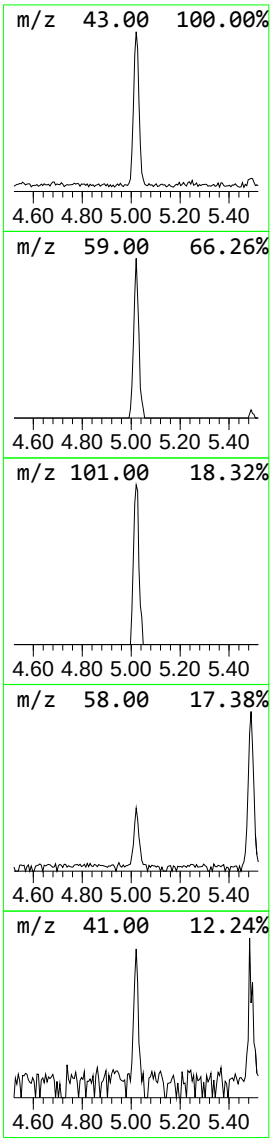
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.020	2.90 ng	53458	1,4-Dichlorobenzene-d4	7.911

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	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	23





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

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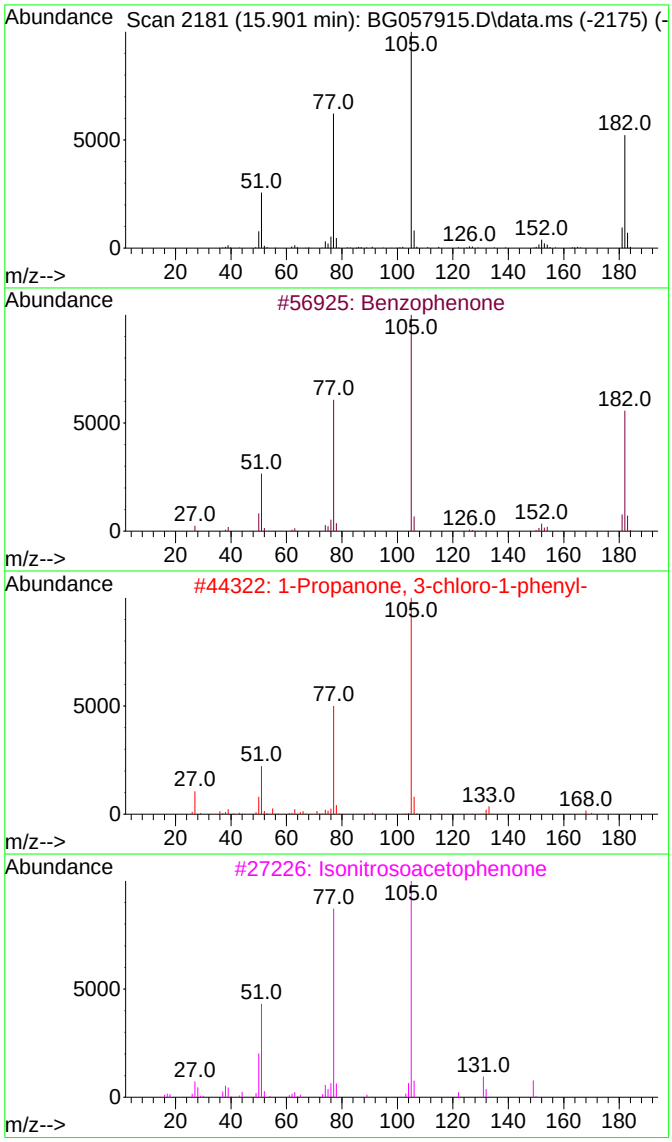
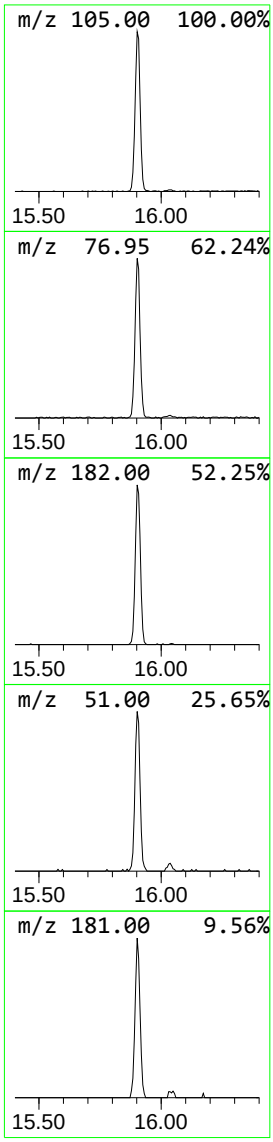
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.901	7.62 ng	274712	Acenaphthene-d10	14.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3	Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	47
4	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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Operator : CG/JU
Sample : 03368-02
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
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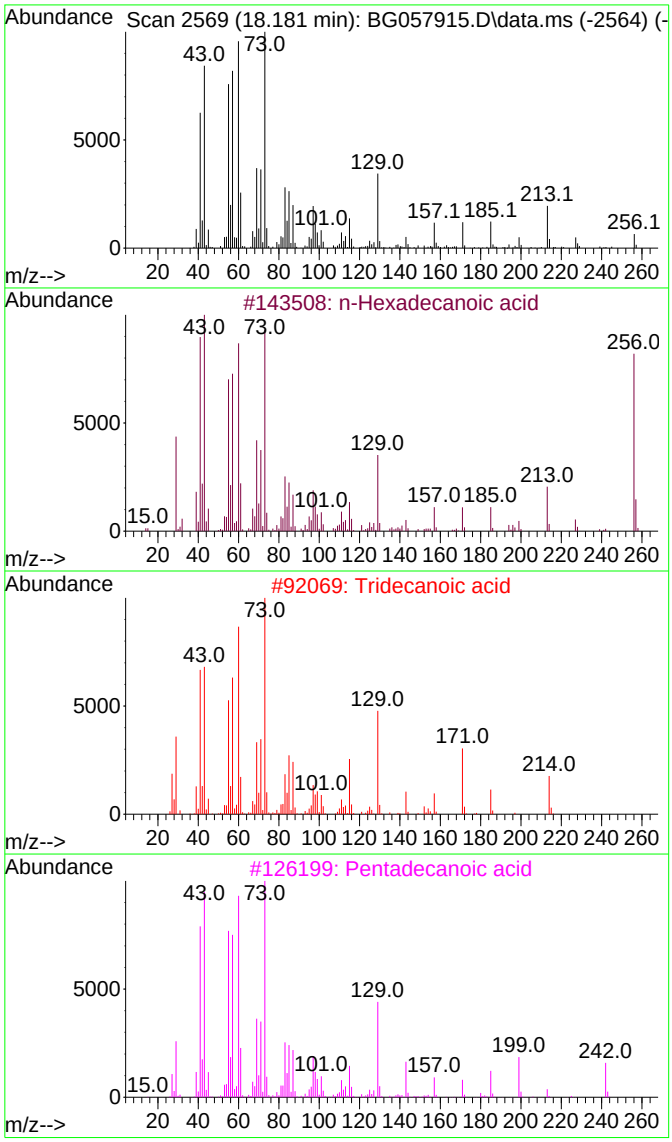
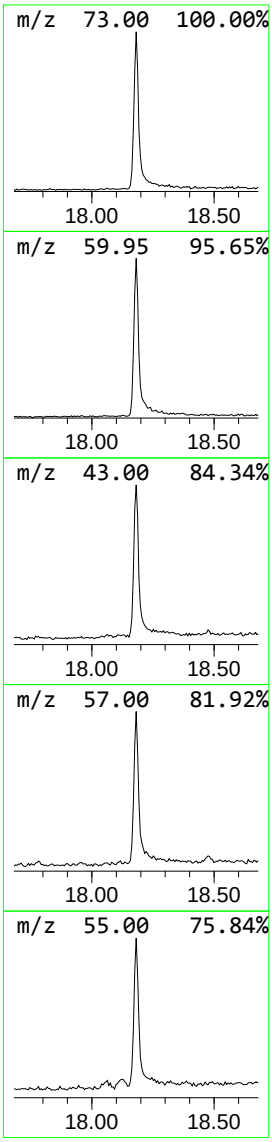
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.181	12.96 ng	520819	Phenanthrene-d10	17.294

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	49





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Misc :
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Instrument :
BNA_G
ClientSampleId :
CF-29

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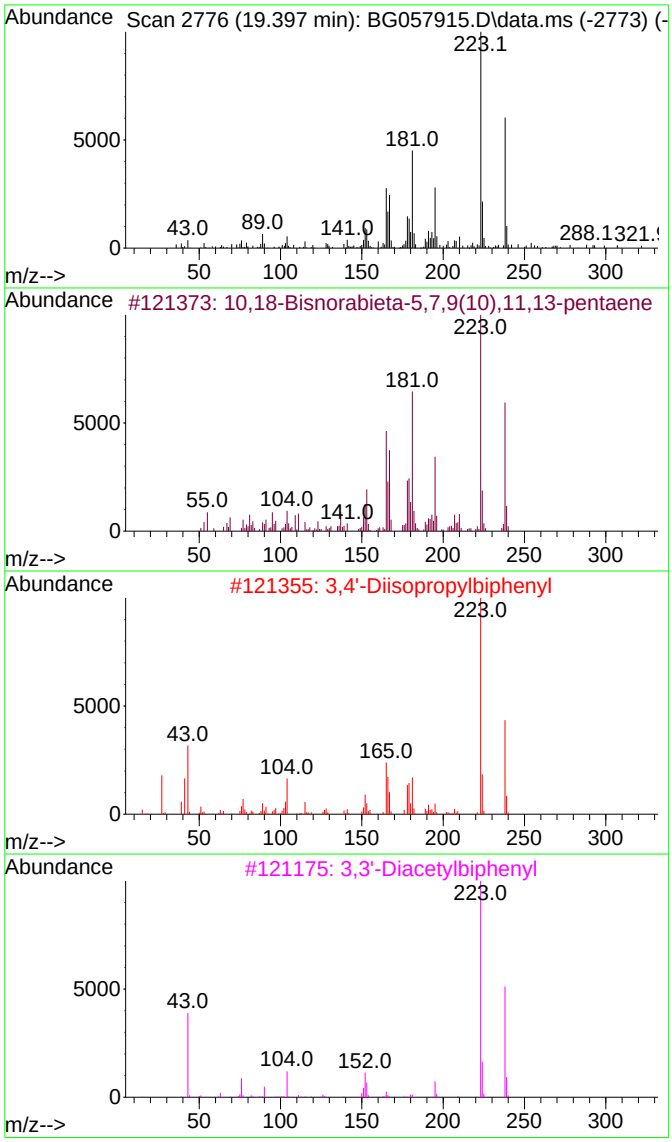
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

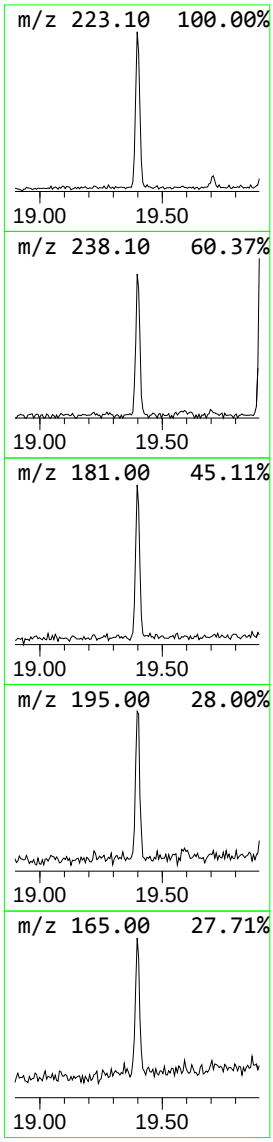
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.397	2.95 ng	118584	Phenanthrene-d10	17.294

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	98
2	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	93
3	3,3'-Diacetylbiphenyl	238	C16H14O2	094113-07-2	53
4	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	49
5	Anthracene, 9,10-dimethoxy-	238	C16H14O2	002395-97-3	49





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BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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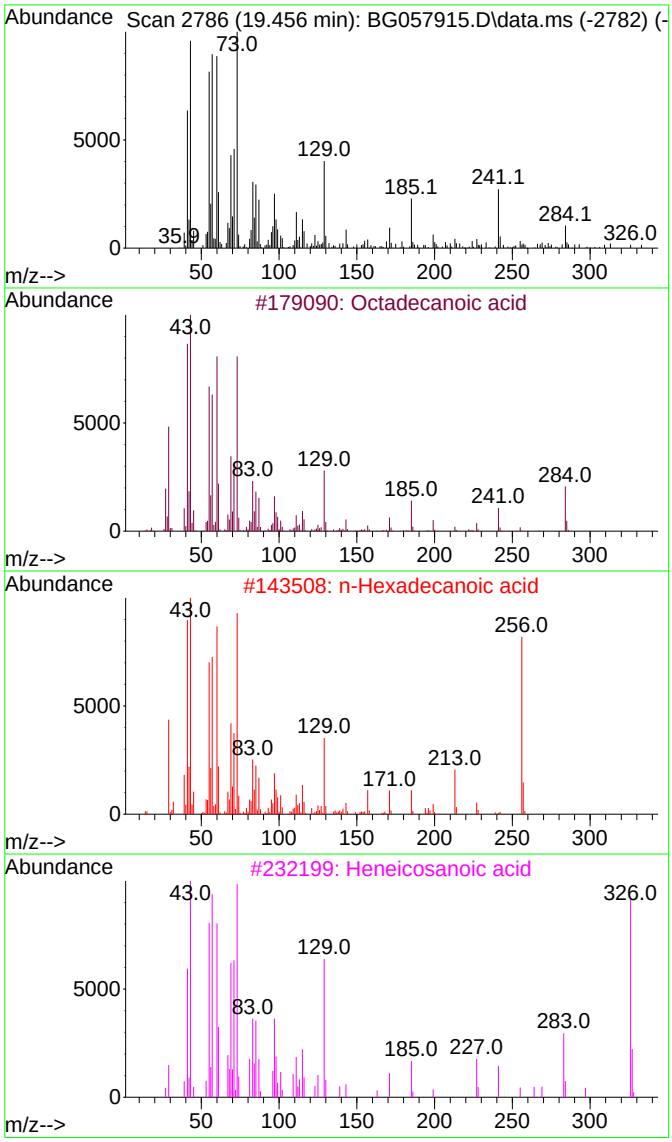
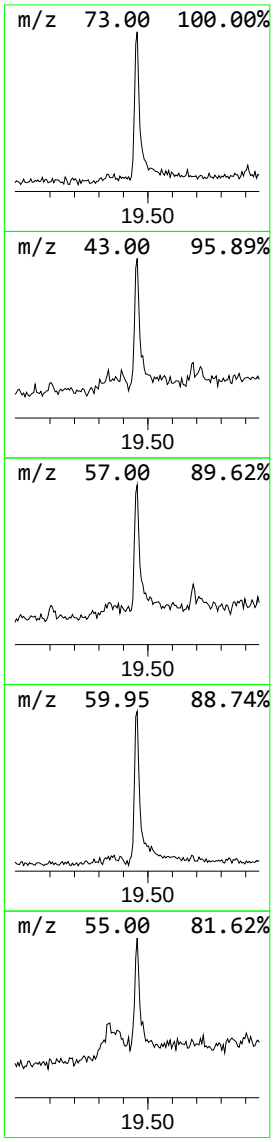
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.456	5.48 ng	204714	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Heneicosanoic acid	326	C21H42O2	002363-71-5	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87





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BNA_G
ClientSampleId :
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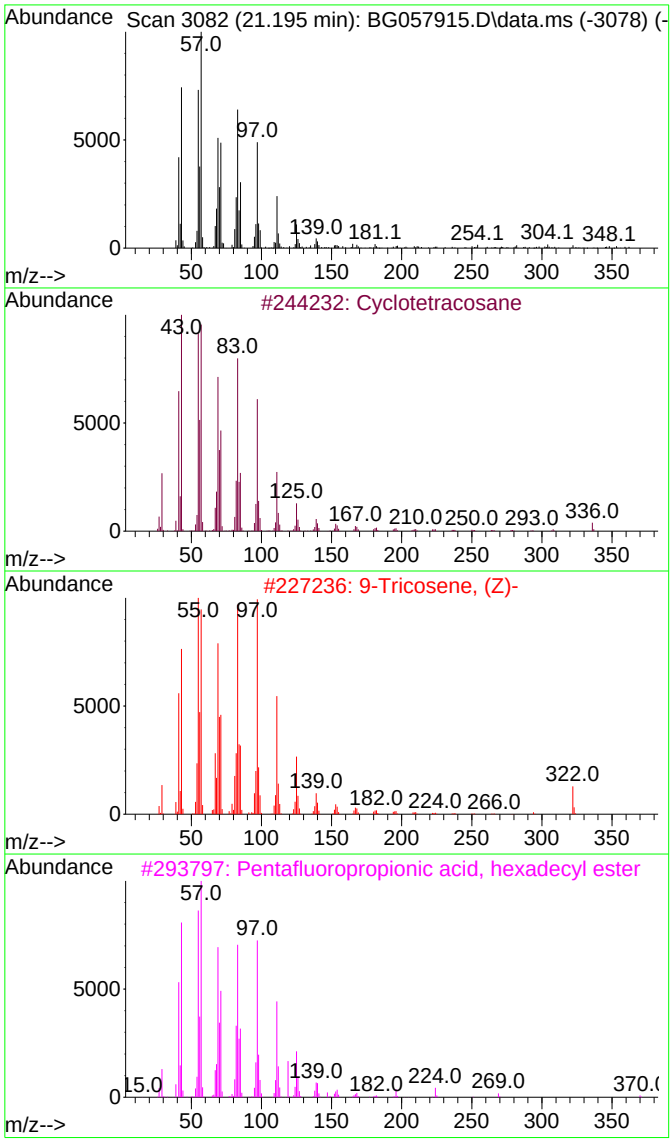
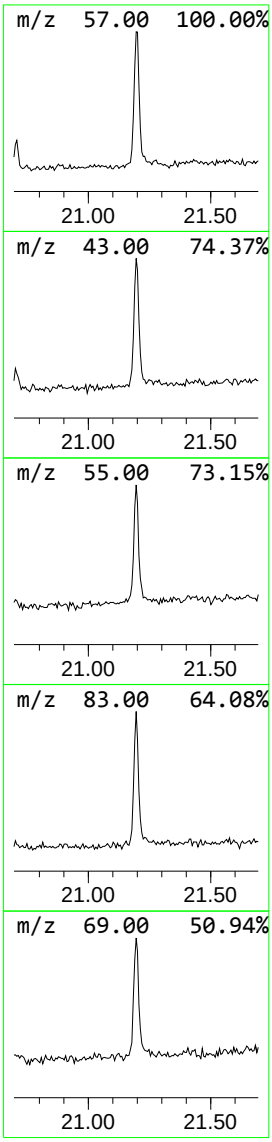
Peak Number 8 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.195	9.17 ng	342365	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91





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-...	5.020	2.9	ng	53458	1	7.911	368211	20.0
Benzophenone	15.901	7.6	ng	274712	3	14.550	721324	20.0
n-Hexadecanoic ...	18.181	13.0	ng	520819	4	17.294	803941	20.0
10,18-Bisnorabi...	19.397	3.0	ng	118584	4	17.294	803941	20.0
Octadecanoic acid	19.456	5.5	ng	204714	5	21.548	746711	20.0
Cyclotetracosane	21.195	9.2	ng	342365	5	21.548	746711	20.0