LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
Data File : BM039949.D
Acq On : 18 May 2023 15:10
Operator : CG/JU
Sample : 02828-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-6

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-BM051223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039949.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.125	11	15	20	rVB	2591906	2792227	11.07%	2.260%
2	5.096	344	350	360	rVB	1716689	2331719	9.24%	1.887%
3	5.566	423	430	440	rBV	8720448	11952194	47.38%	9.674%
4	7.172	695	703	714	rBV	7933460	12011868	47.61%	9.722%
5	8.019	840	847	854	rBV	1552258	2366426	9.38%	1.915%
6	9.190	1038	1046	1056	rBV	4633372	7341153	29.10%	5.942%
7	10.836	1319	1326	1334	rBV	2033363	3263409	12.94%	2.641%
8	13.289	1735	1743	1749	rBV	12422630	16916405	67.06%	13.692%
9	14.660	1969	1976	1986	rVB	2548388	3751561	14.87%	3.036%
10	16.013	2200	2206	2211	rBV	464611	628868	2.49%	0.509%
11	16.142	2221	2228	2241	rBV	9555190	12670918	50.23%	10.256%
12	17.401	2436	2442	2448	rBV	2882919	4040059	16.01%	3.270%
13	18.295	2586	2594	2603	rBV	1999235	3423384	13.57%	2.771%
14	18.365	2603	2606	2622	rVB	281273	637721	2.53%	0.516%
15	18.565	2635	2640	2644	rBV	192621	283599	1.12%	0.230%
16	18.607	2644	2647	2664	rVB4	151923	284057	1.13%	0.230%
17	19.565	2805	2810	2829	rBV	1371111	2590611	10.27%	2.097%
18	19.824	2850	2854	2861	rBV3	167979	354799	1.41%	0.287%
19	20.018	2881	2887	2892	rVB	23389127	25227176	100.00%	20.418%
20	21.283	3098	3102	3114	rBV2	712461	1012848	4.01%	0.820%
21	21.571	3146	3151	3157	rBV	3462585	4363285	17.30%	3.532%
22	22.212	3256	3260	3265	rBV3	176454	285995	1.13%	0.231%
23	24.030	3562	3569	3583	rVB	2517156	5021112	19.90%	4.064%

Sum of corrected areas: 123551394

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
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Misc :
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Instrument :
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ClientSampleId :
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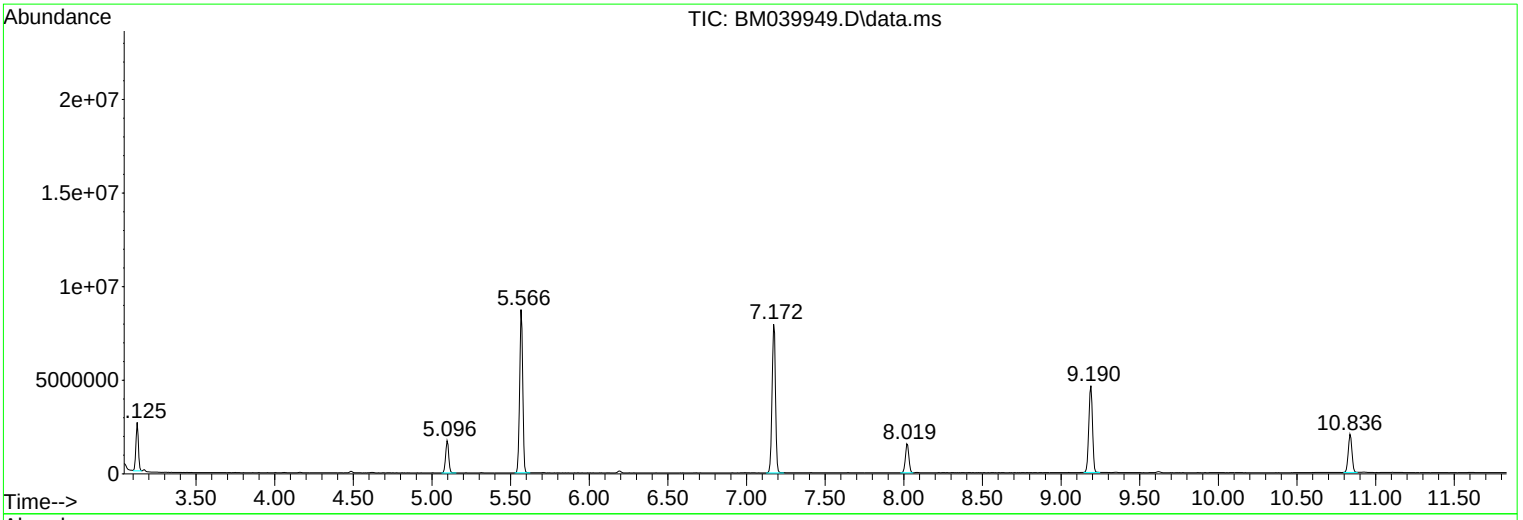
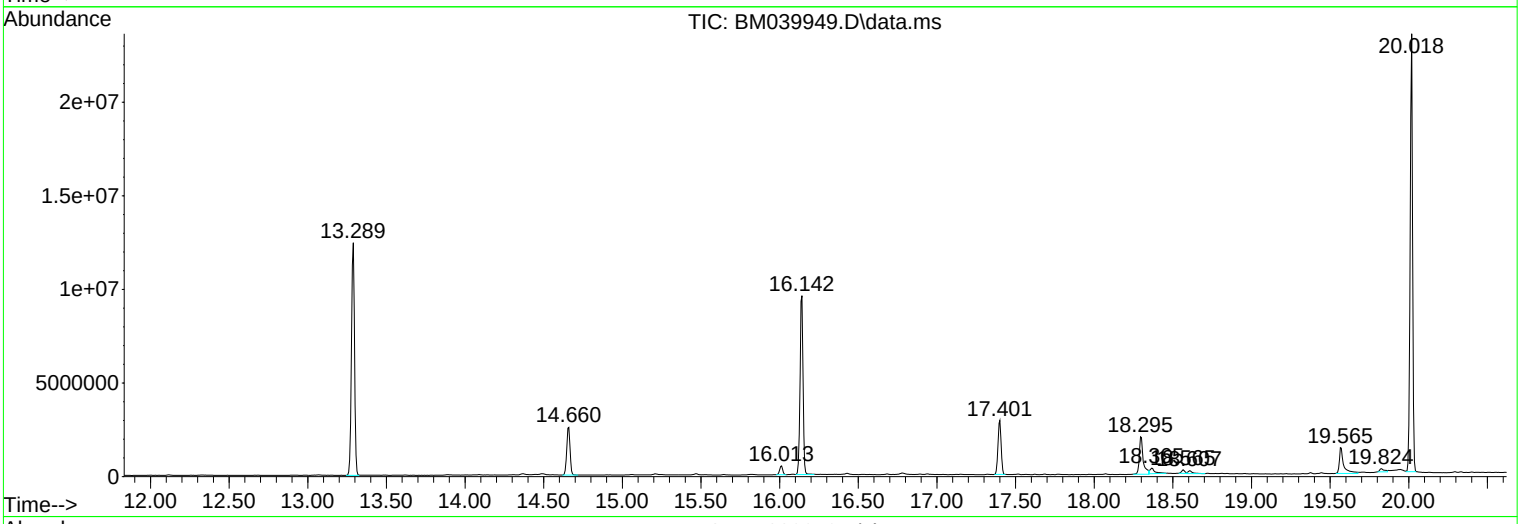
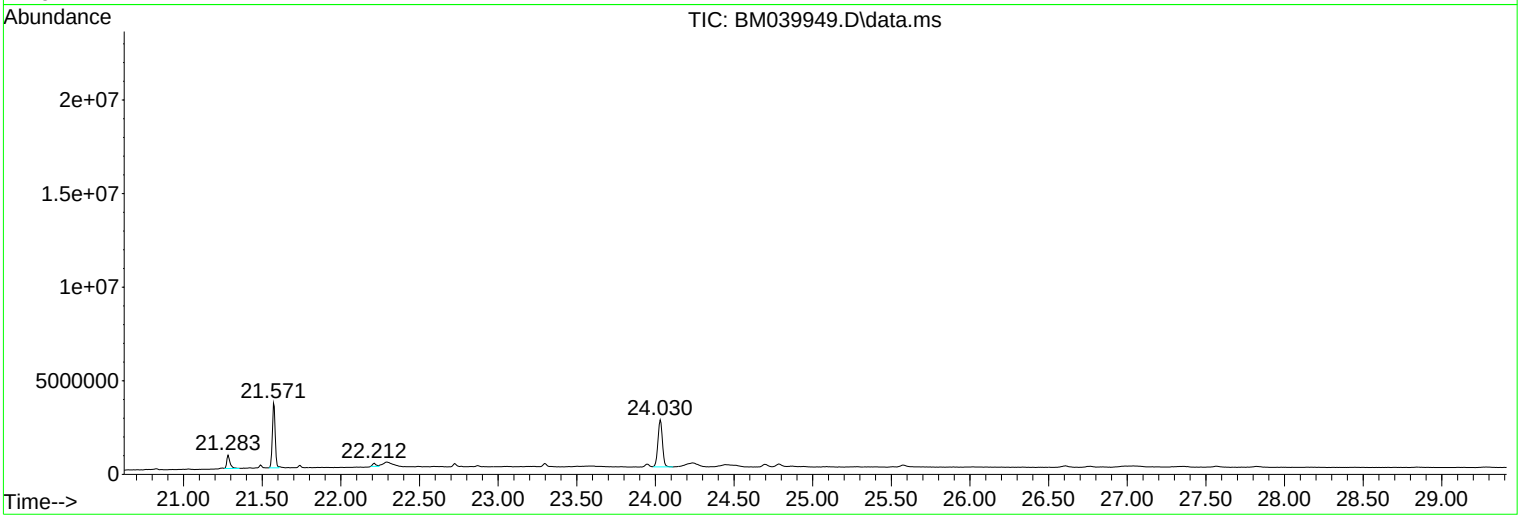
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM051223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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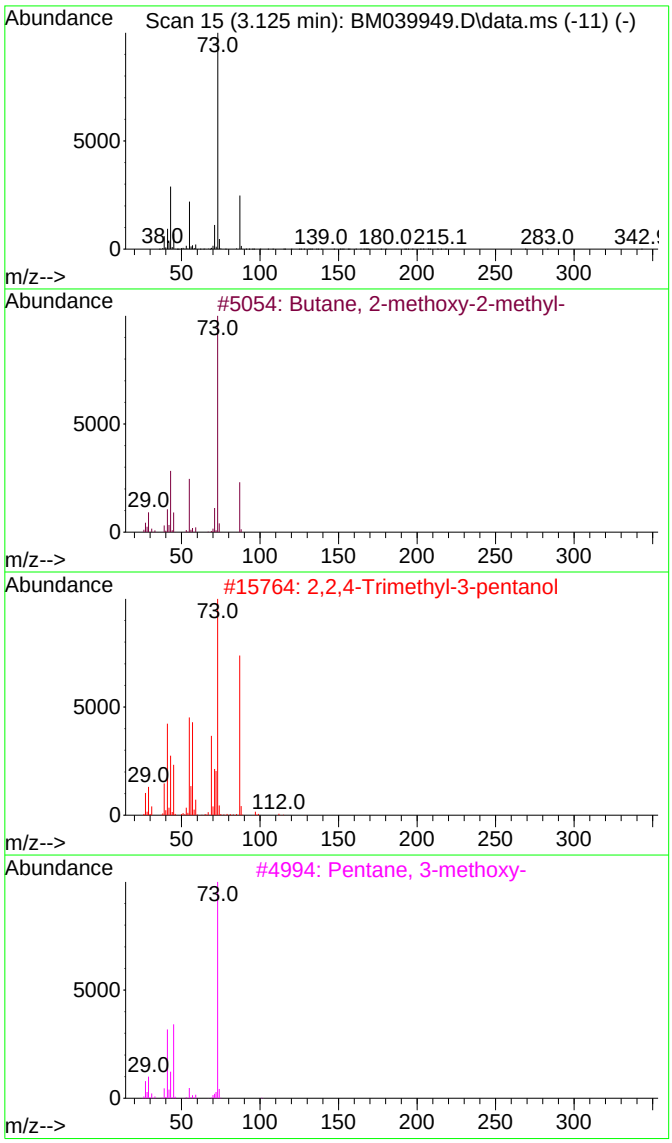
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

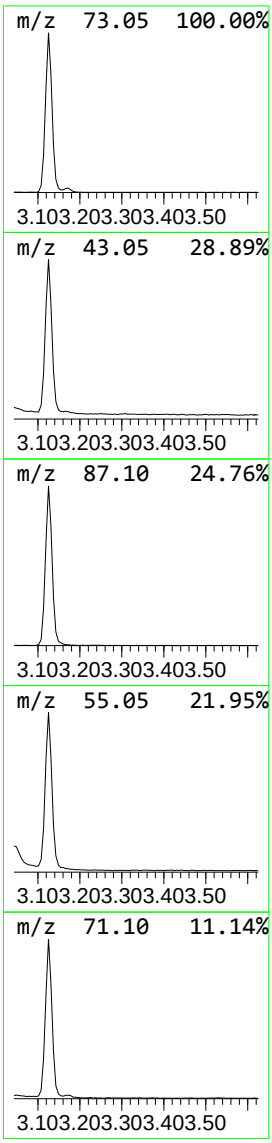
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.125	23.60 ng	2792230	1,4-Dichlorobenzene-d4	8.019

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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BM039949.D
Acq On : 18 May 2023 15:10
Operator : CG/JU
Sample : 02828-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-6

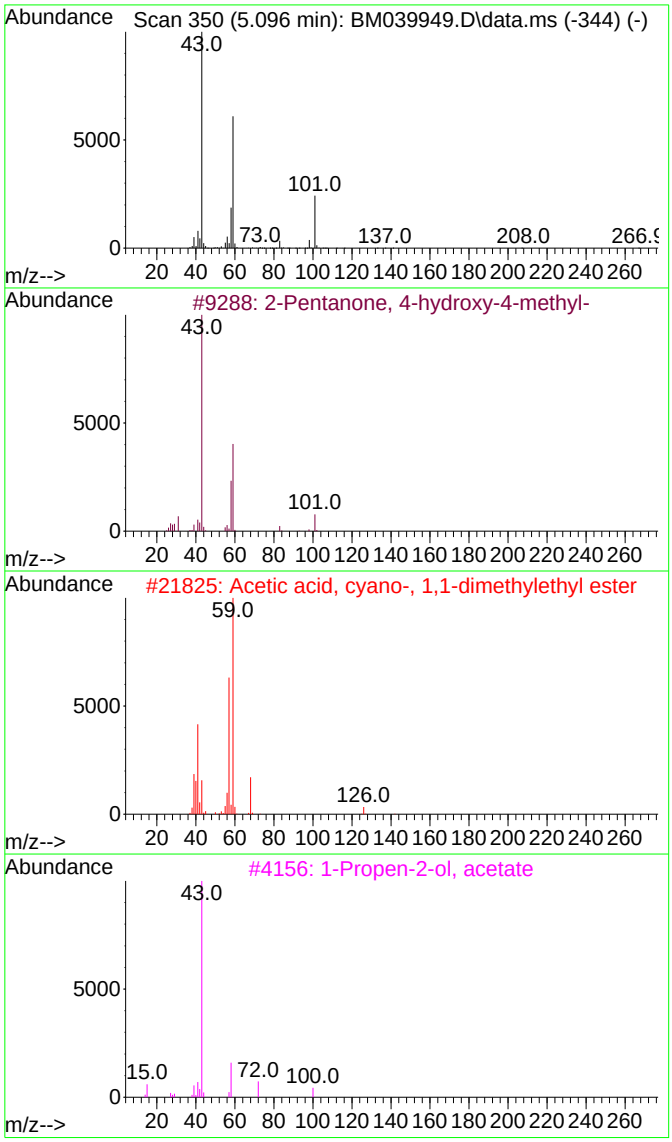
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM051223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

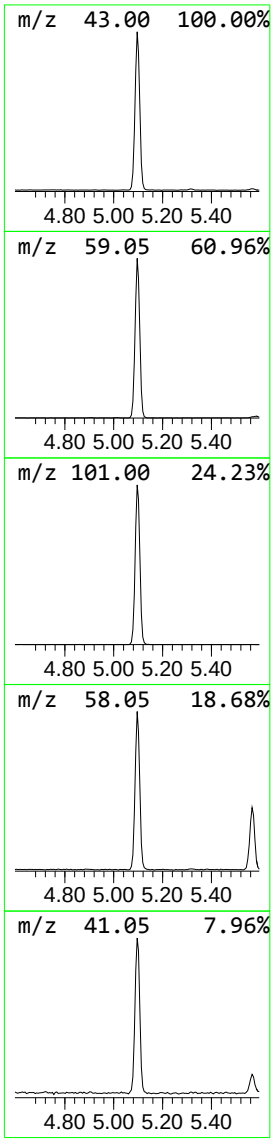
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.096	19.71 ng	2331720	1,4-Dichlorobenzene-d4	8.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
Data File : BM039949.D
Acq On : 18 May 2023 15:10
Operator : CG/JU
Sample : 02828-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM051223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

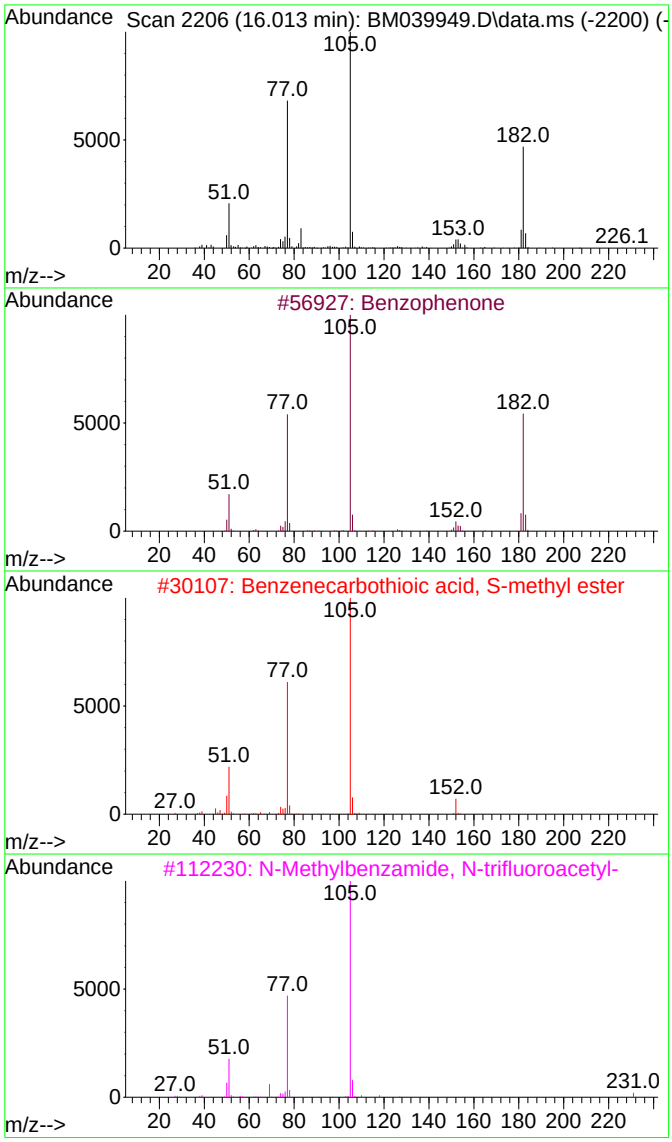
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

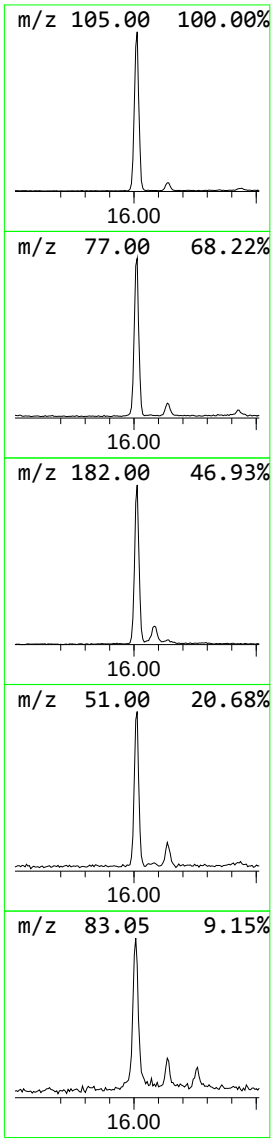
****

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.013	3.35 ng	628868	Acenaphthene-d10	14.660

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	43
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
5	N-Benzoylimidazole	172	C10H8N2O	010364-94-0	43





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Sample : 02828-06
Misc :
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Instrument :
BNA_M
ClientSampleId :
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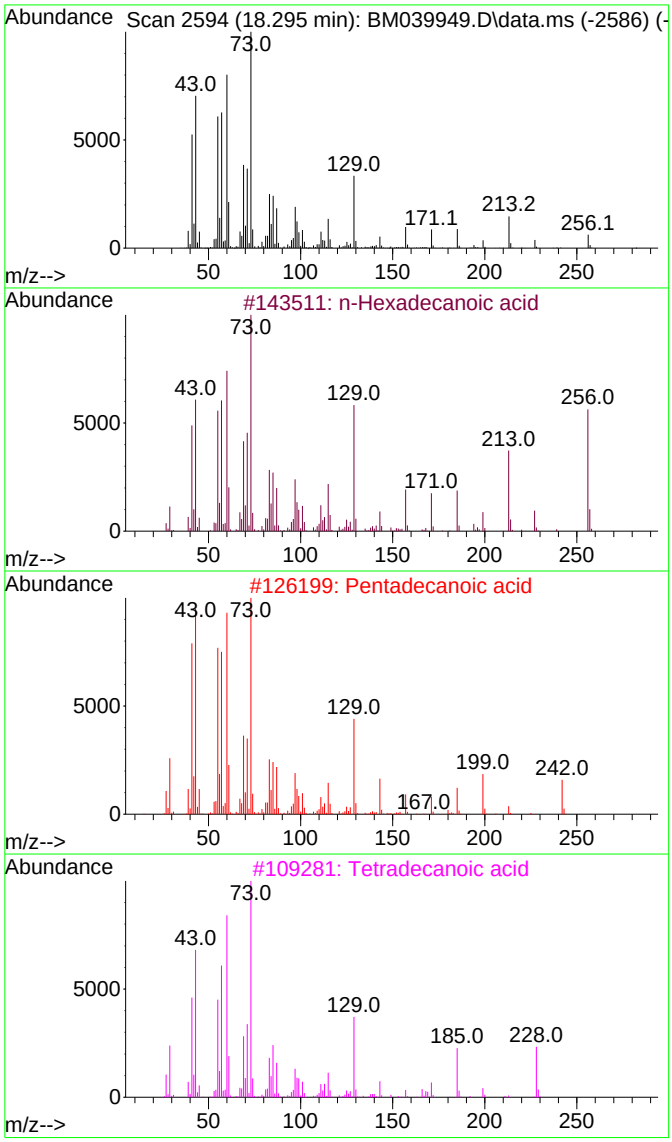
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM051223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

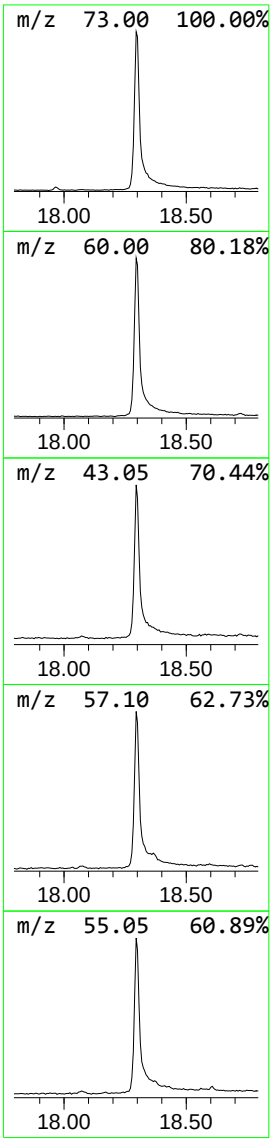
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.295	16.95 ng	3423380	Phenanthrene-d10	17.401

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





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Acq On : 18 May 2023 15:10
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Sample : 02828-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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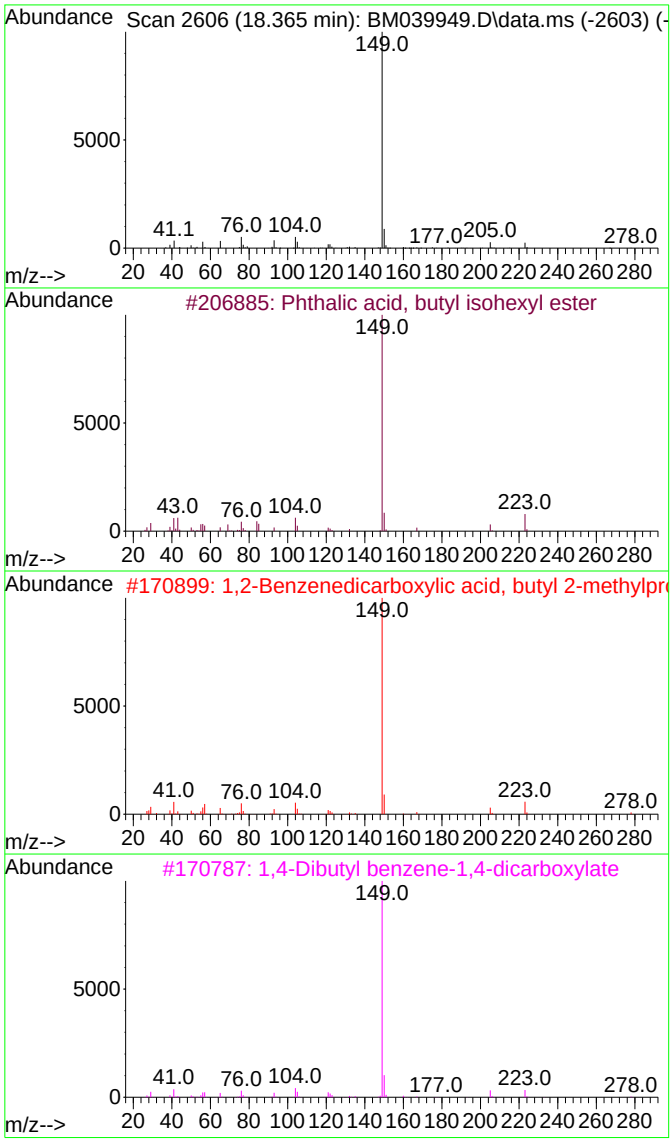
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM051223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

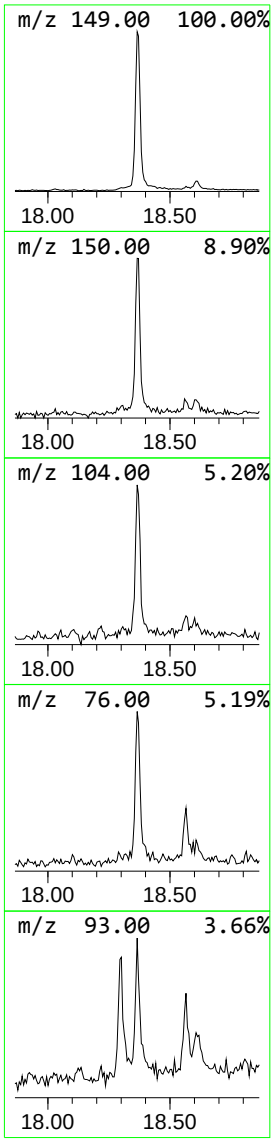
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phthalic acid, butyl isohex... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.365	3.16 ng	637721	Phenanthrene-d10	17.401

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, butyl isohexyl ester	306	C18H26O4	1000309-03-6	83
2	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	83
3	1,4-Dibutyl benzene-1,4-dicarbox...	278	C16H22O4	001962-75-0	83
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	83
5	Di-sec-butyl phthalate	278	C16H22O4	1000373-65-4	80





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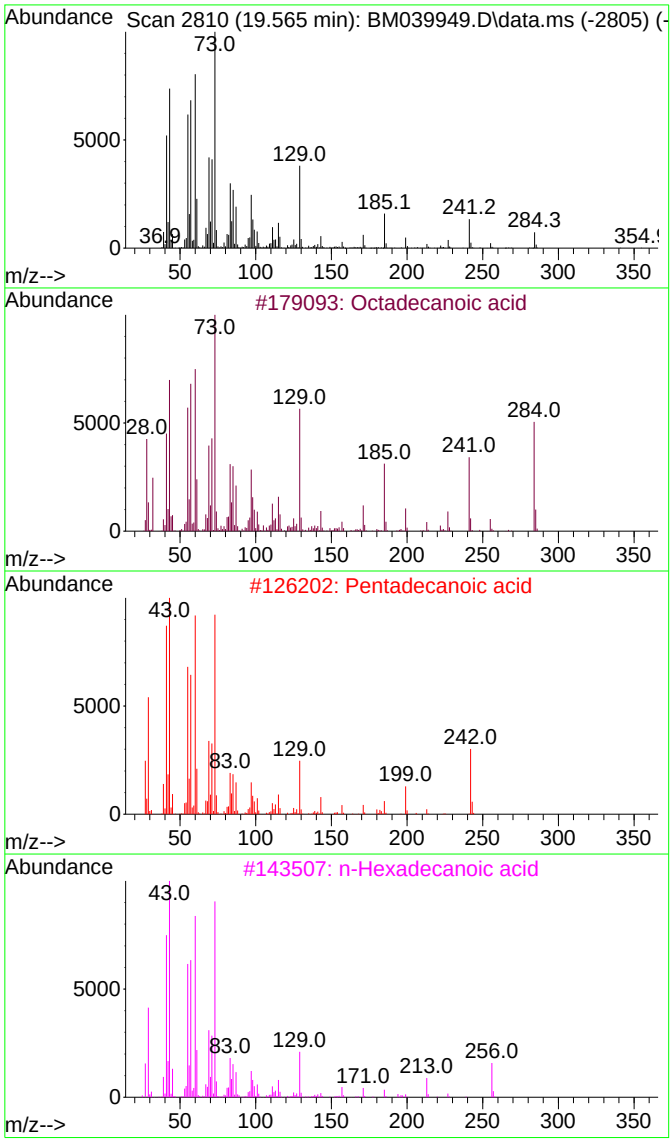
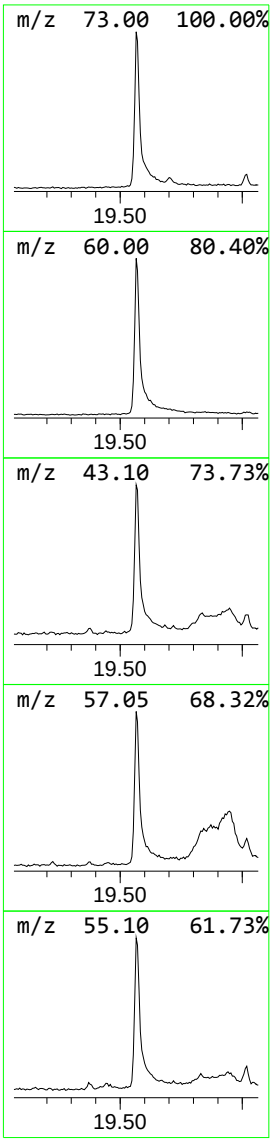
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.565	11.87 ng	2590610	Chrysene-d12	21.571

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	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

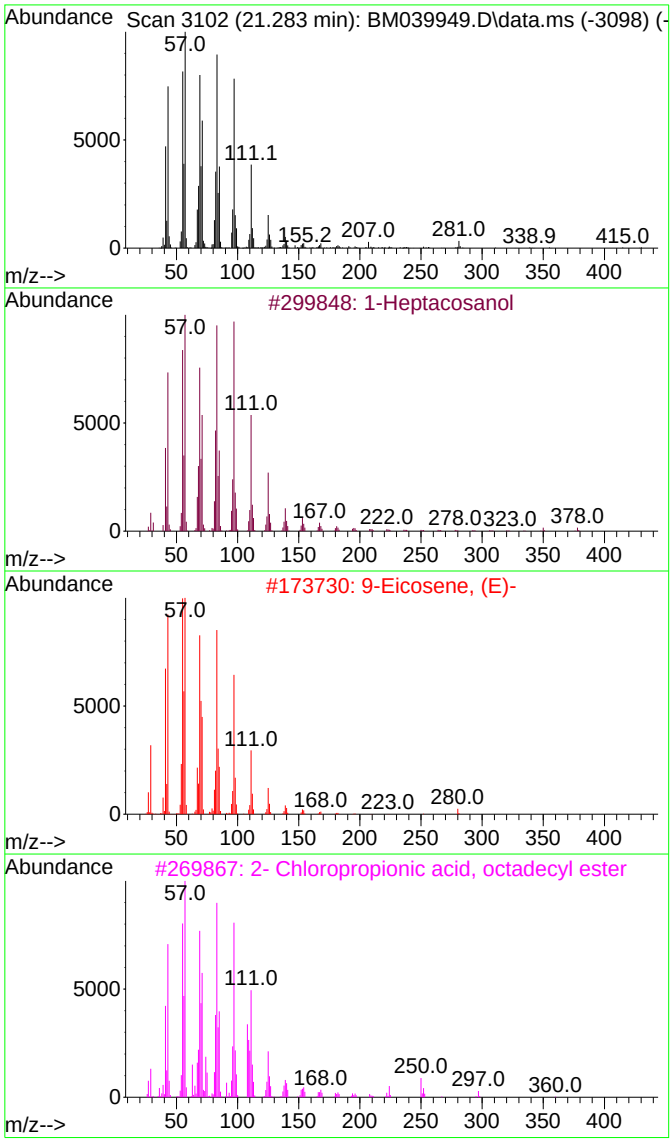
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

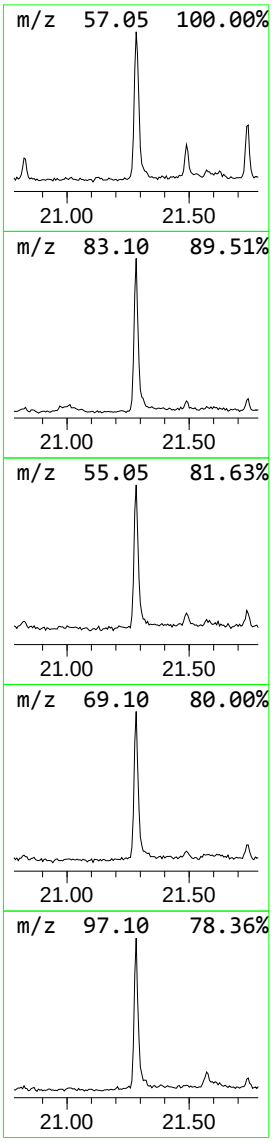
****

Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.283	4.64 ng	1012850	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.125	23.6	ng	2792230	1	8.019	2366430	20.0
2-Pentanone, 4-...	5.096	19.7	ng	2331720	1	8.019	2366430	20.0
Benzophenone	16.013	3.4	ng	628868	3	14.660	3751560	20.0
n-Hexadecanoic ...	18.295	16.9	ng	3423380	4	17.401	4040060	20.0
Phthalic acid, ...	18.365	3.2	ng	637721	4	17.401	4040060	20.0
Octadecanoic acid	19.565	11.9	ng	2590610	5	21.571	4363290	20.0
1-Heptacosanol	21.283	4.6	ng	1012850	5	21.571	4363290	20.0