LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049889.D
Acq On : 10 Apr 2025 18:04
Operator : RC/JU
Sample : Q1749-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-14

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-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	319	324	338	rBV	1099711	1510114	9.62%	1.834%
2	5.363	397	404	418	rBV	4738703	6783996	43.20%	8.240%
3	5.975	502	508	516	rBV	171072	257524	1.64%	0.313%
4	6.951	666	674	691	rBV	4638510	7124874	45.37%	8.654%
5	7.775	805	814	823	rBV	1115739	1729329	11.01%	2.100%
6	8.933	1002	1011	1022	rBV	2775186	4455854	28.37%	5.412%
7	10.569	1281	1289	1302	rBV	1347070	2270008	14.46%	2.757%
8	13.039	1700	1709	1725	rBV	7671919	11059112	70.42%	13.432%
9	14.415	1936	1943	1951	rBV	2224283	3289833	20.95%	3.996%
10	15.774	2168	2174	2181	rBV	1727546	2420374	15.41%	2.940%
11	15.909	2190	2197	2212	rBV	7293431	10179856	64.82%	12.364%
12	16.339	2266	2270	2277	rVB	168837	238912	1.52%	0.290%
13	17.162	2404	2410	2422	rBV	2853079	3972471	25.30%	4.825%
14	18.062	2558	2563	2571	rBV	569469	888568	5.66%	1.079%
15	19.339	2777	2780	2786	rBV	188322	302453	1.93%	0.367%
16	19.786	2851	2856	2862	rBV	13388493	15703795	100.00%	19.074%
17	21.397	3125	3130	3144	rVB	3307976	5298615	33.74%	6.436%
18	24.391	3633	3639	3651	rVB	1858864	4847358	30.87%	5.887%

Sum of corrected areas: 82333046

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Instrument :
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ClientSampleId :
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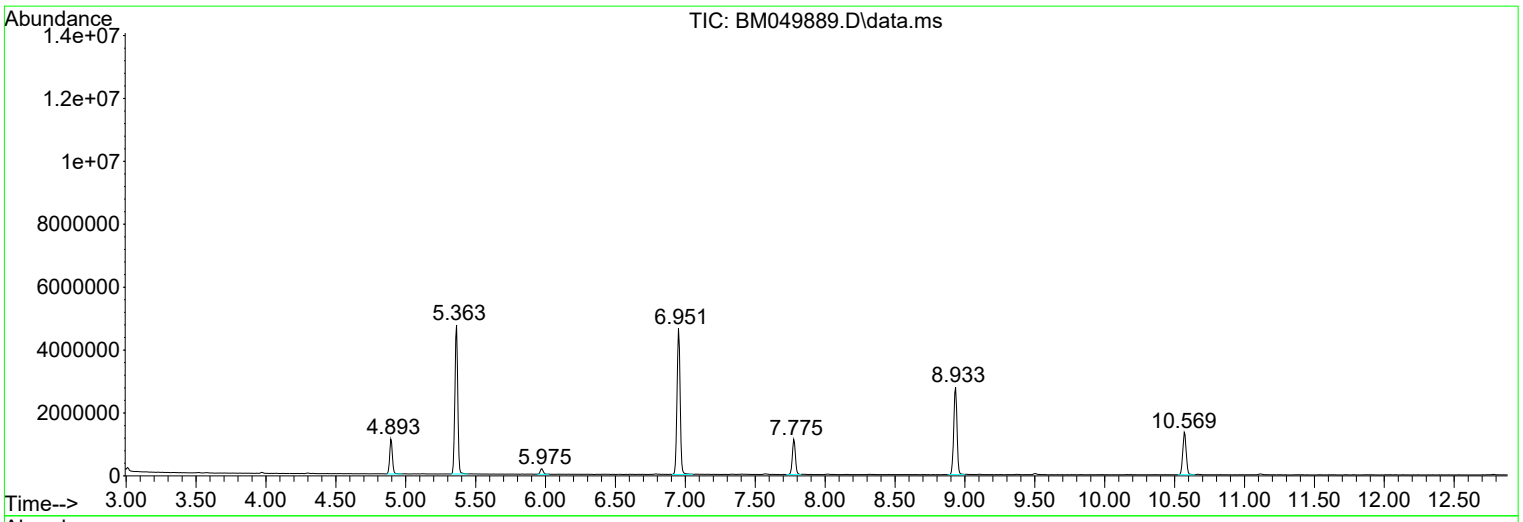
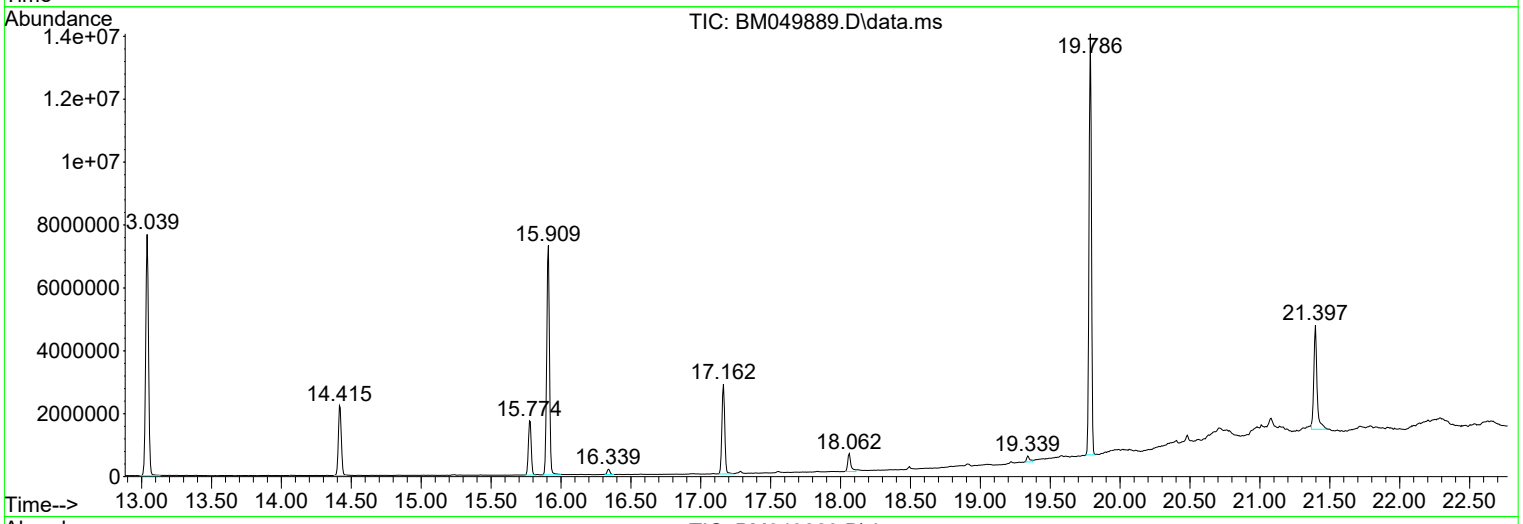
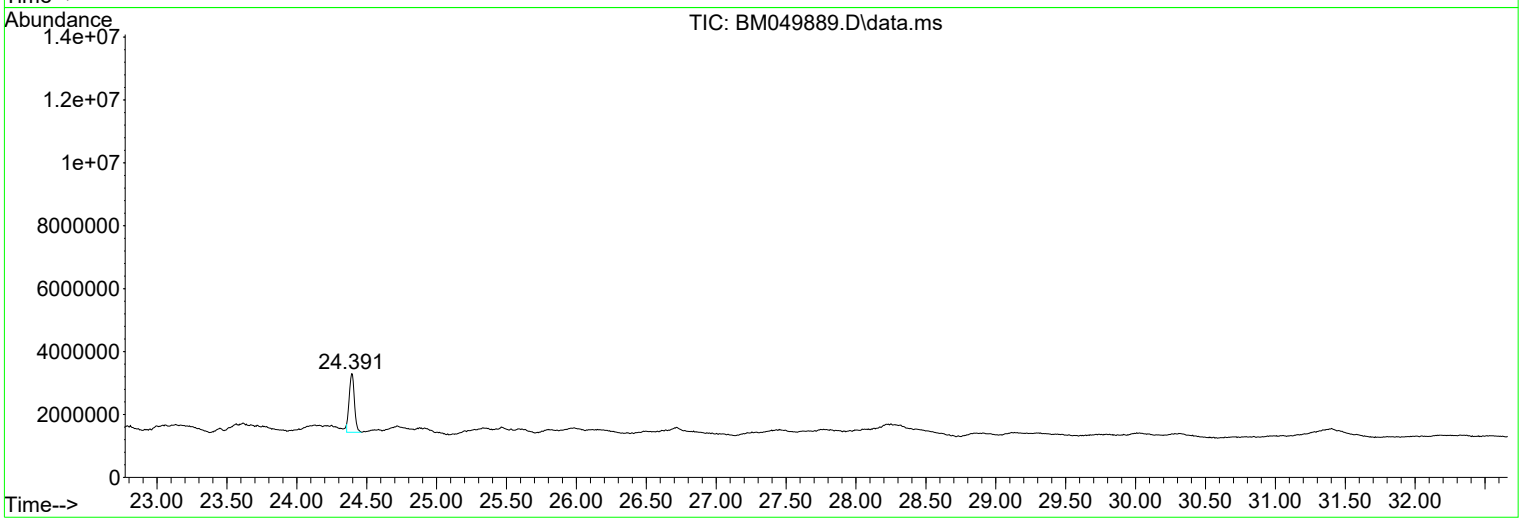
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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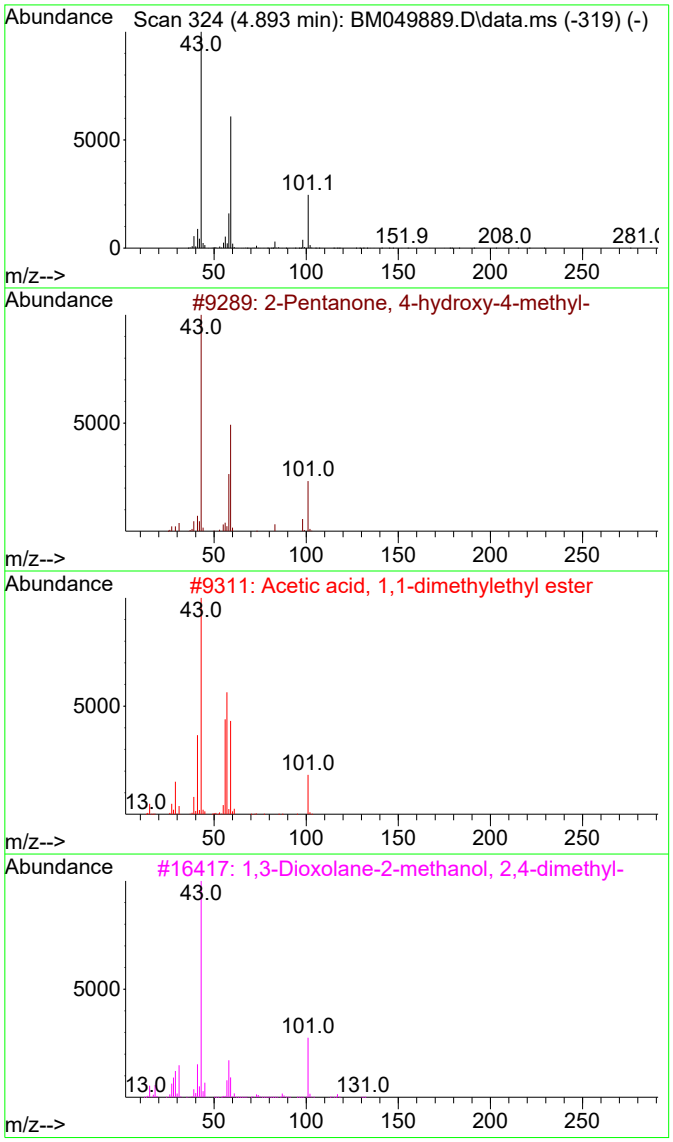
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

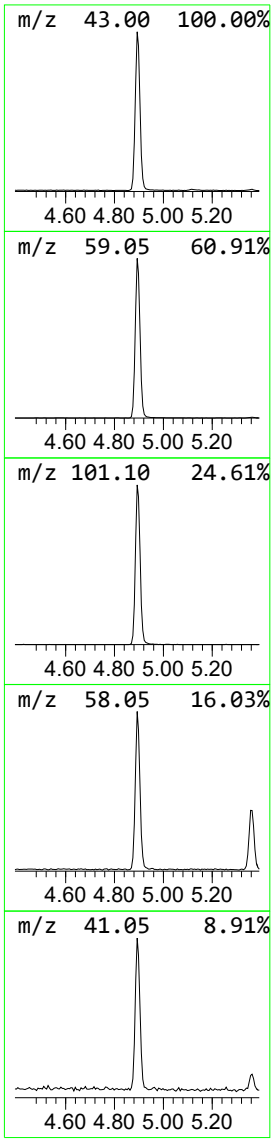
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	17.46 ng	1510110	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23





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Instrument :
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ClientSampleId :
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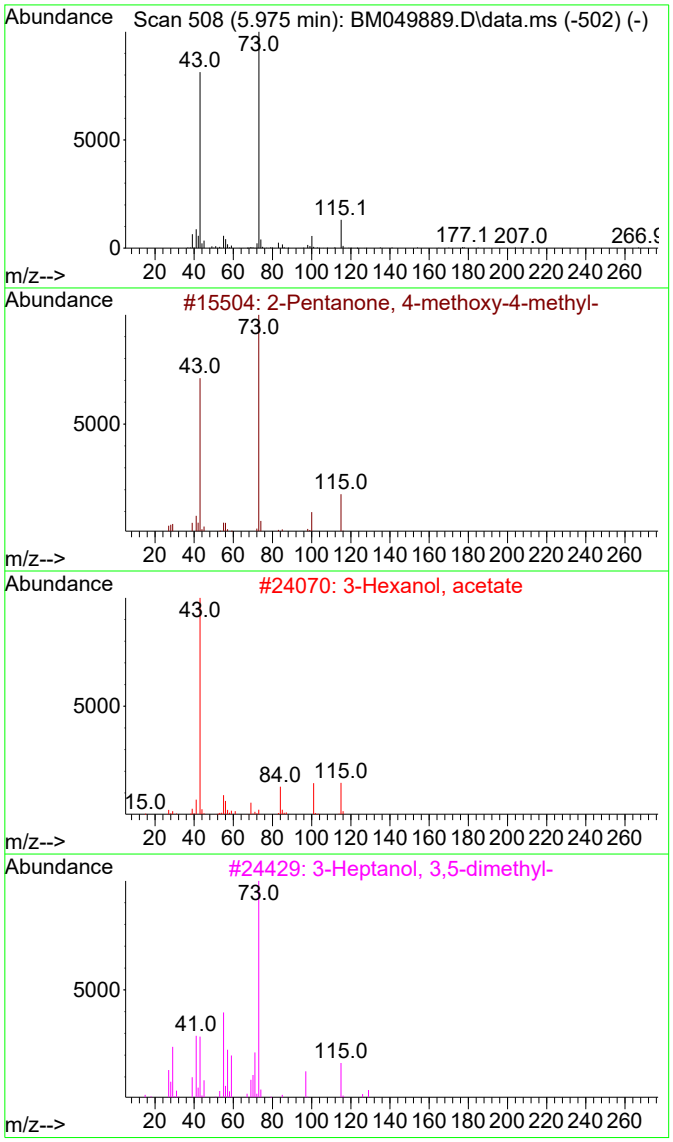
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

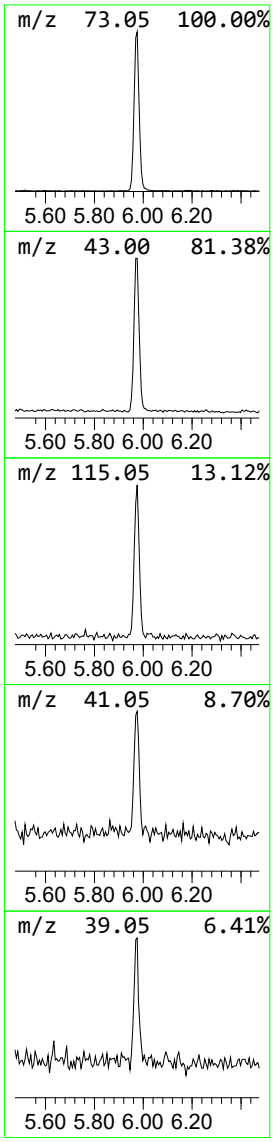
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.975	2.98 ng	257524	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3-Hexanol, acetate	144	C8H16O2	040780-64-1	37
3	3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	10





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Operator : RC/JU
Sample : Q1749-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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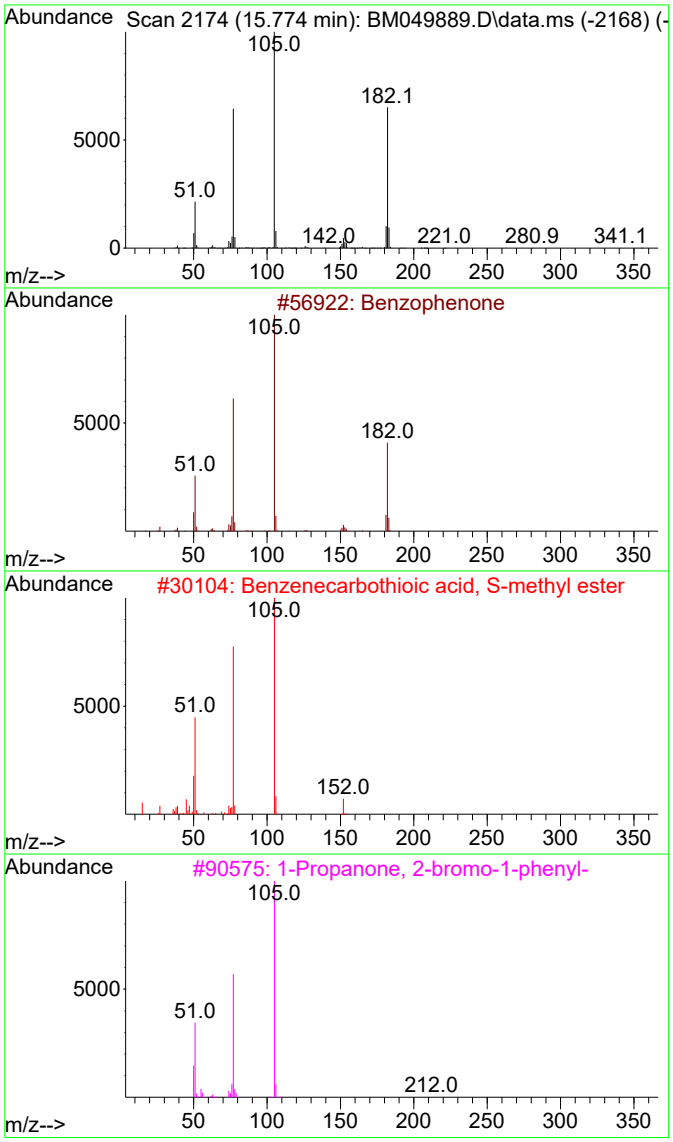
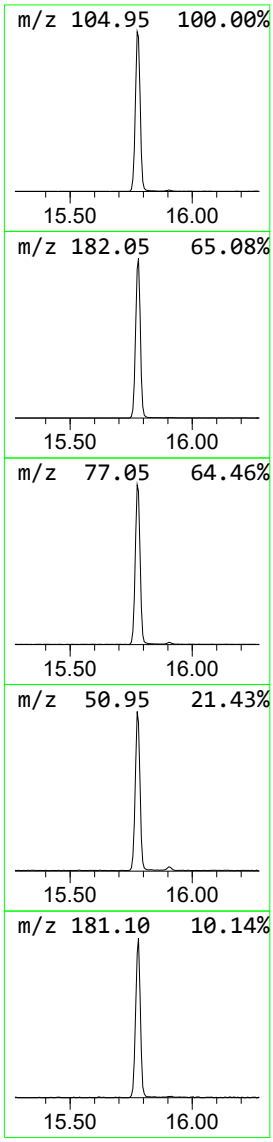
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	14.71 ng	2420370	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43





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Instrument :
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TIC Library : C:\Database\NIST20.L
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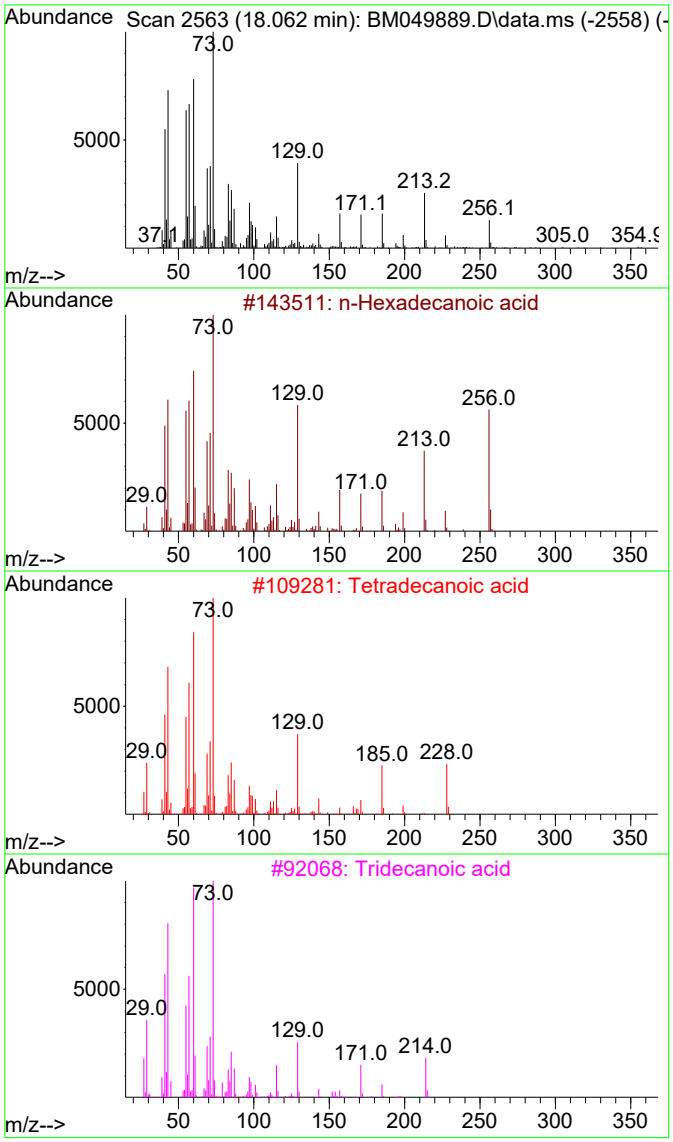
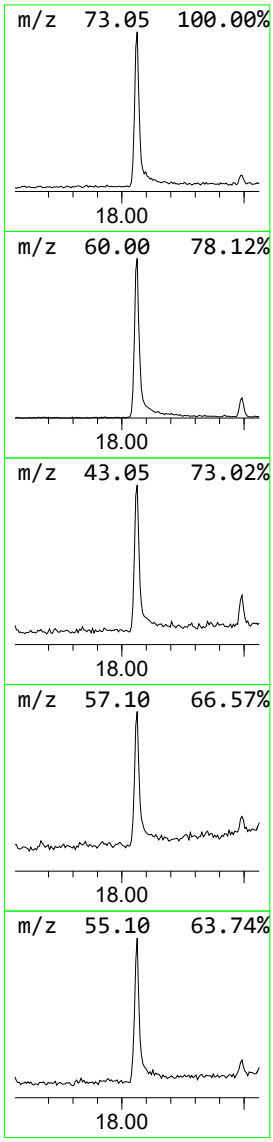
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	4.47 ng	888568	Phenanthrene-d10	17.162

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Tentatively Identified Compound (LSC) summary

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Sample : Q1749-01
Misc :
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Instrument :
BNA_M
ClientSampleId :
TP-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-...	4.893	17.5	ng	1510110	1	7.775	1729330	20.0
2-Pentanone, 4-...	5.975	3.0	ng	257524	1	7.775	1729330	20.0
Benzophenone	15.774	14.7	ng	2420370	3	14.416	3289830	20.0
n-Hexadecanoic ...	18.062	4.5	ng	888568	4	17.162	3972470	20.0