LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042534.D
Acq On : 01 Nov 2023 11:43
Operator : MA/JU
Sample : PB156350BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156350BL

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-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042534.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.752	91	96	102	rBV	108065	125789	2.47%	0.432%
2	4.375	197	202	220	rBV	1559351	1966597	38.65%	6.748%
3	5.010	304	310	329	rVB	1471486	2056628	40.42%	7.057%
4	5.463	380	387	400	rBV	2128135	2946024	57.89%	10.109%
5	6.087	488	493	501	rVB	46702	66380	1.30%	0.228%
6	7.093	657	664	675	rBV	1965501	3015256	59.25%	10.347%
7	7.922	798	805	816	rVB	358830	539659	10.60%	1.852%
8	9.128	1001	1010	1019	rBV	1138095	1890775	37.16%	6.488%
9	10.739	1277	1284	1293	rBV	402318	670578	13.18%	2.301%
10	13.192	1694	1701	1715	rBV	2789640	3974475	78.10%	13.638%
11	14.574	1929	1936	1946	rVB	581691	841547	16.54%	2.888%
12	16.068	2183	2190	2202	rBV	2370394	3219572	63.27%	11.048%
13	17.321	2397	2403	2417	rBV	650682	933008	18.33%	3.202%
14	18.174	2543	2548	2561	rBV	106437	212259	4.17%	0.728%
15	19.451	2761	2765	2771	rBV2	60201	96958	1.91%	0.333%
16	19.939	2842	2848	2859	rBV	4314803	5088748	100.00%	17.462%
17	21.503	3110	3114	3121	rBV	608749	811360	15.94%	2.784%
18	23.921	3520	3525	3533	rVB2	343745	687019	13.50%	2.357%

Sum of corrected areas: 29142632

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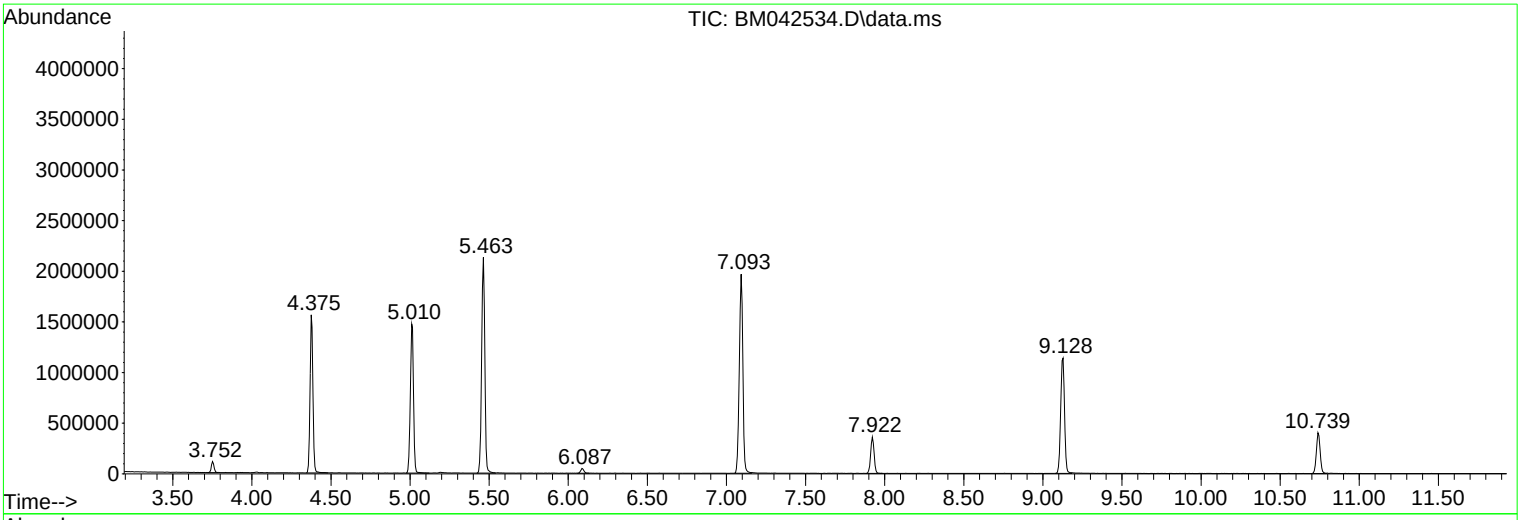
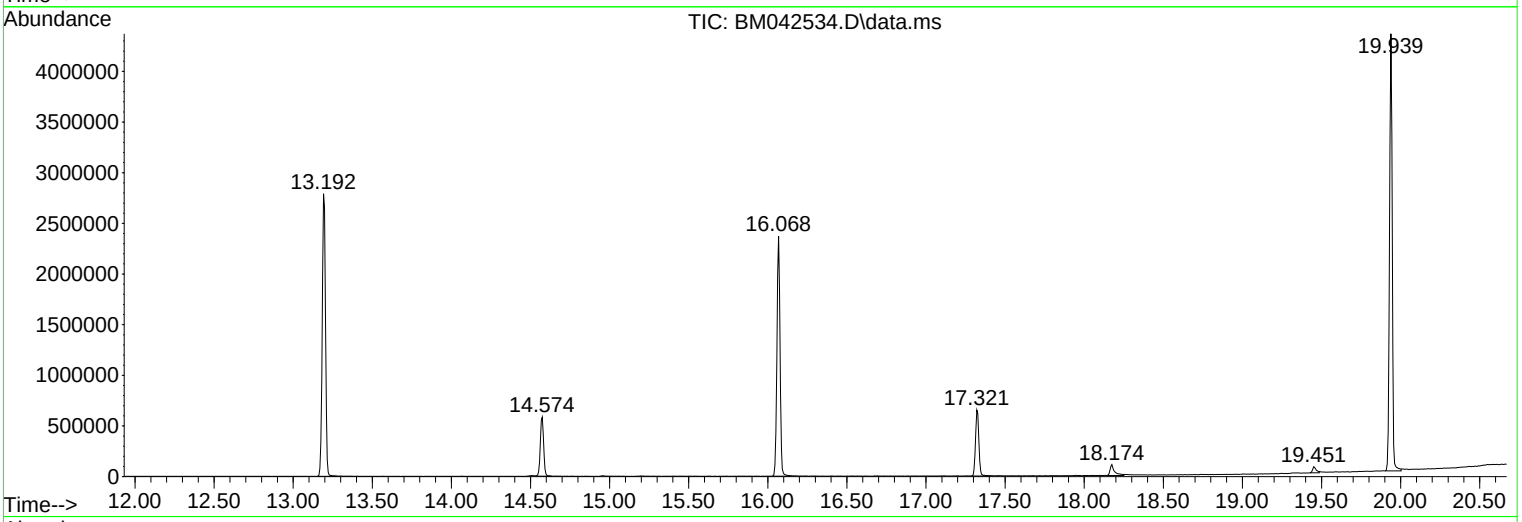
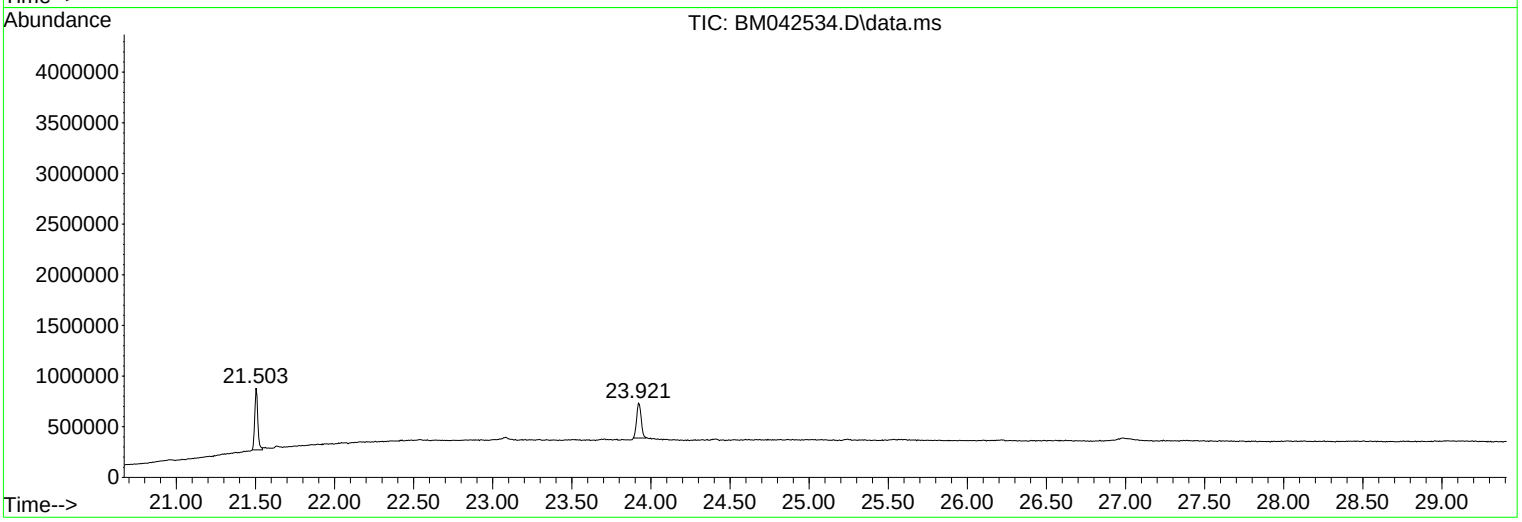
ClientSampleId :
PB156350BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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 : BM042534.D
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Operator : MA/JU
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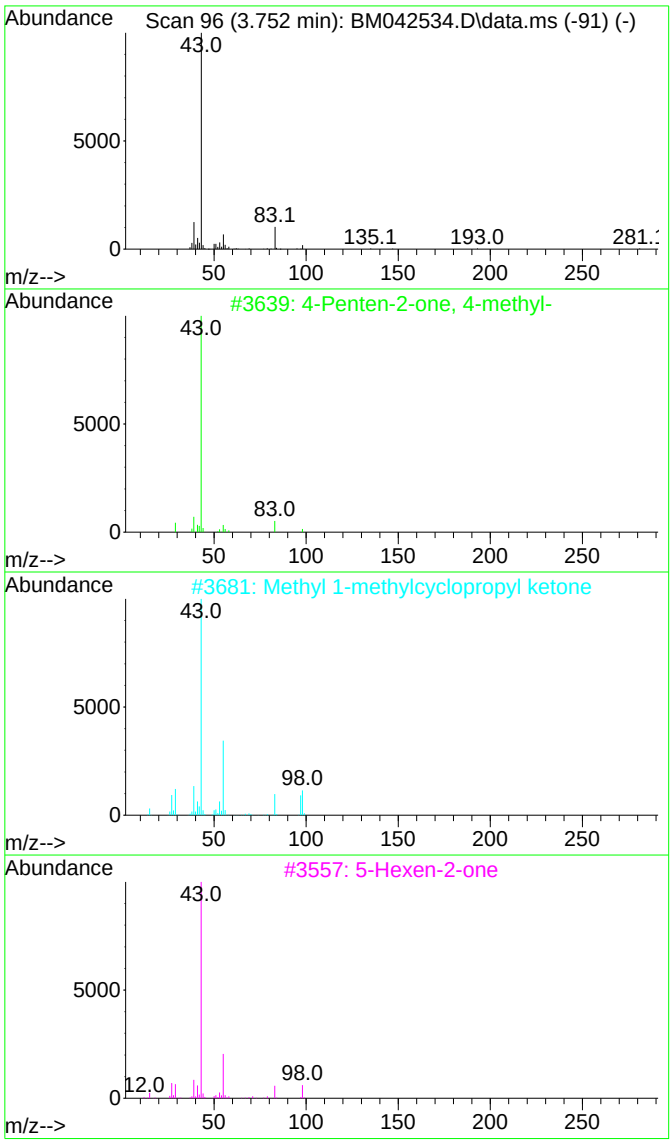
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

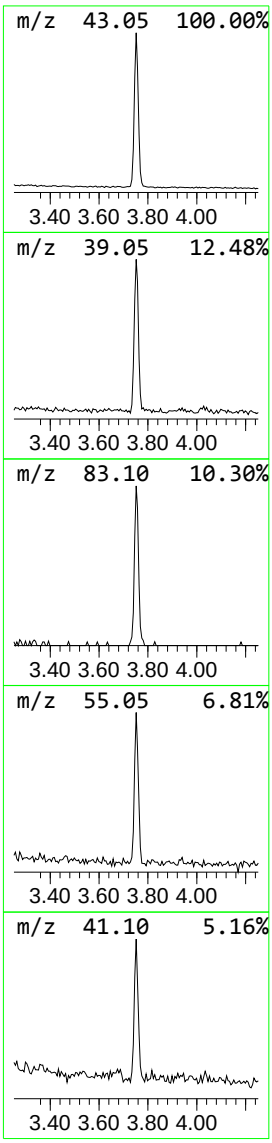
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.752	4.66 ng	125789	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	58
2	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	27
3	5-Hexen-2-one	98	C6H10O	000109-49-9	25
4	3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	9
5	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9





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Instrument :
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ClientSampleId :
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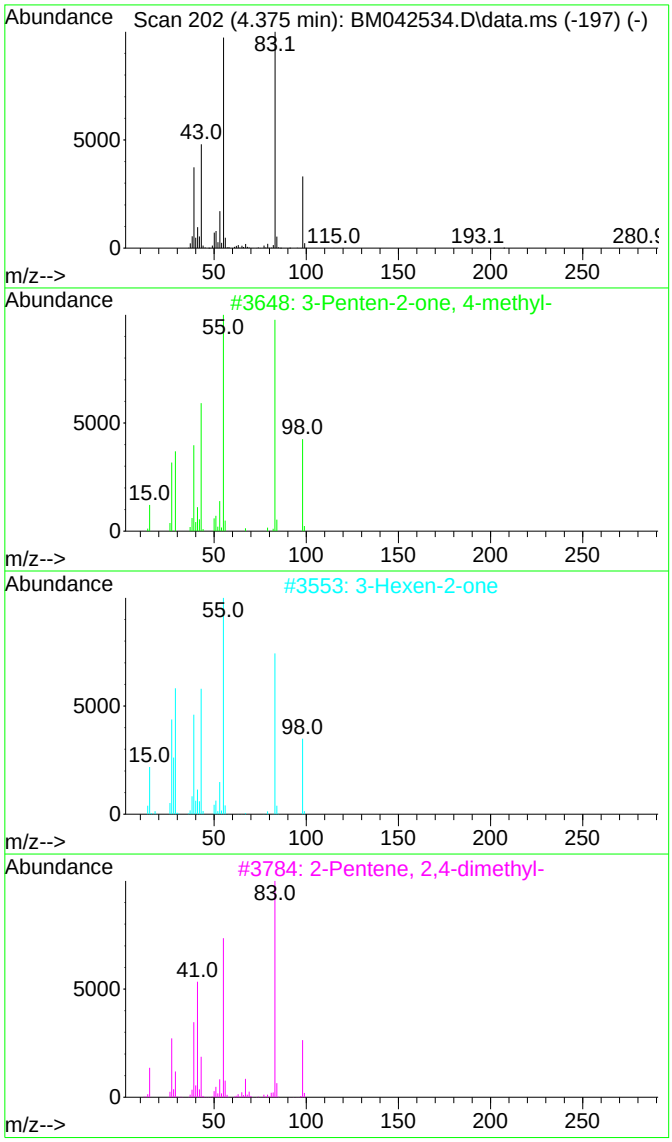
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

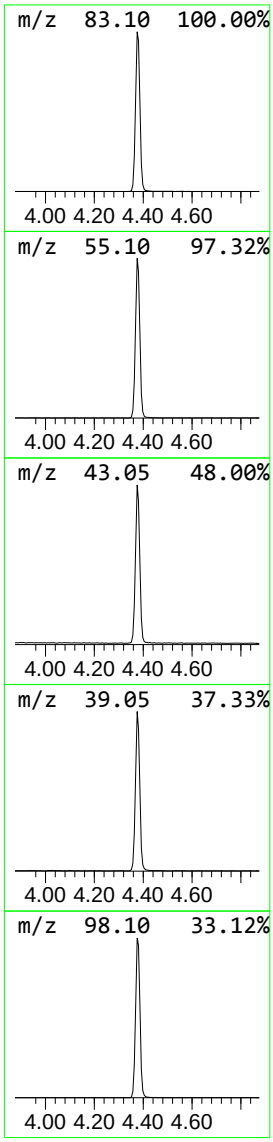
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.375	72.88 ng	1966600	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Operator : MA/JU
Sample : PB156350BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156350BL

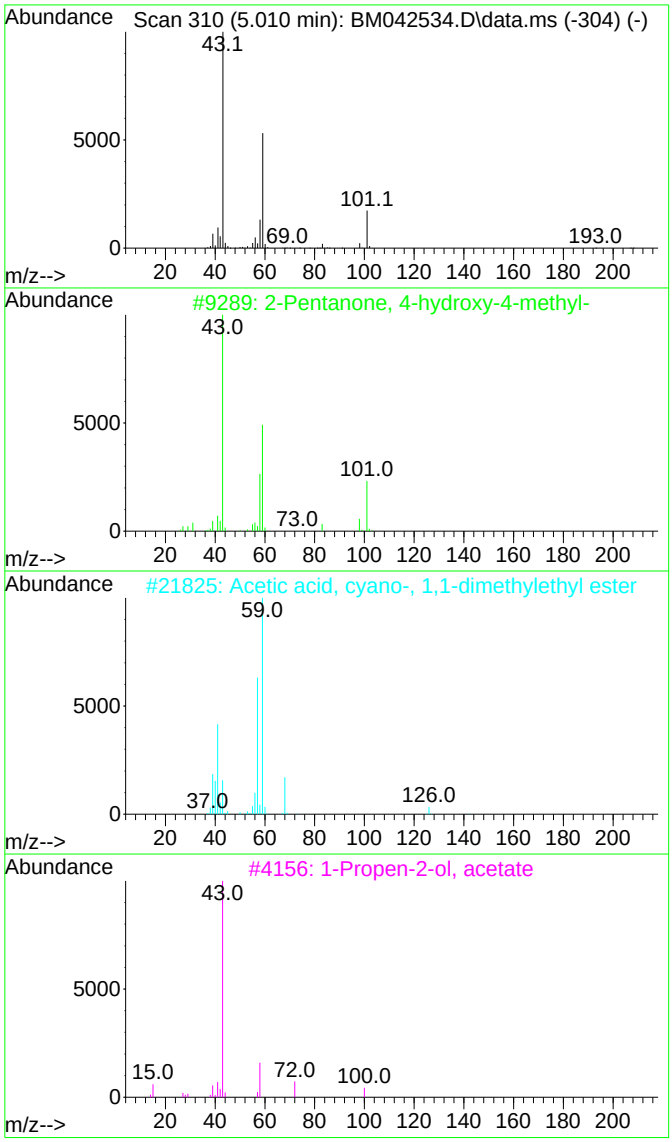
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

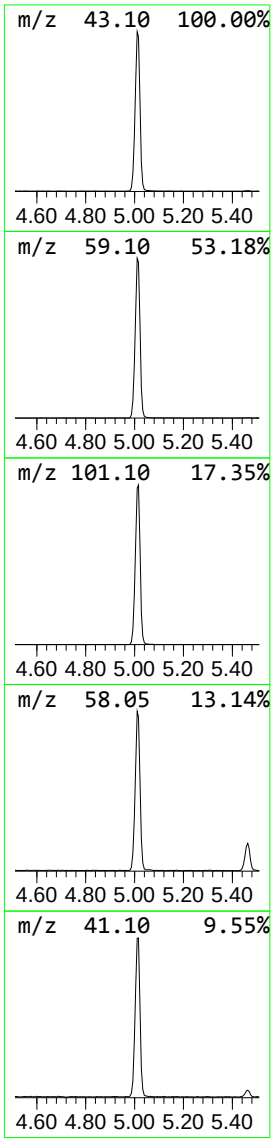
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	76.22 ng	2056630	1,4-Dichlorobenzene-d4	7.922

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	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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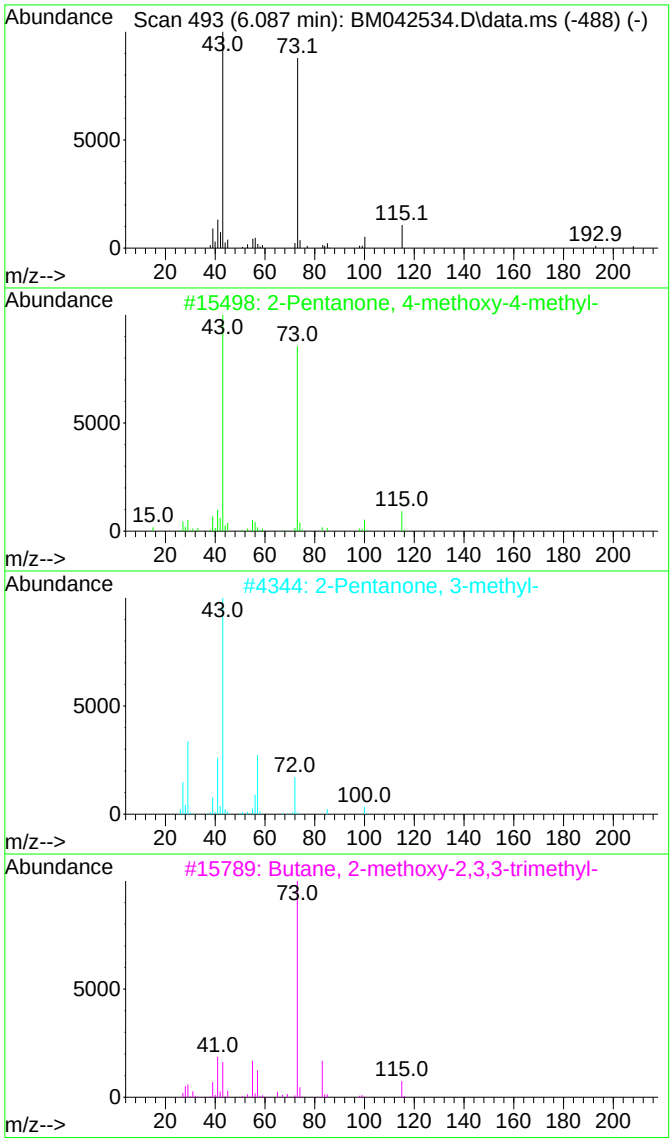
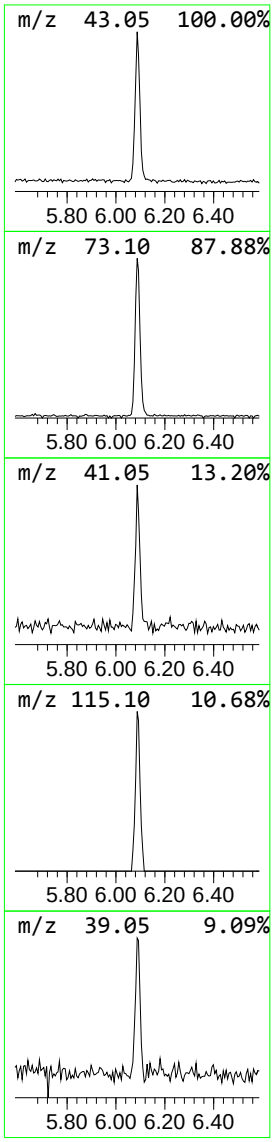
****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.087	2.46 ng	66380	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	27
3	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4	Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	1000223-34-1	12
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
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TIC Library : C:\Database\NIST20.L
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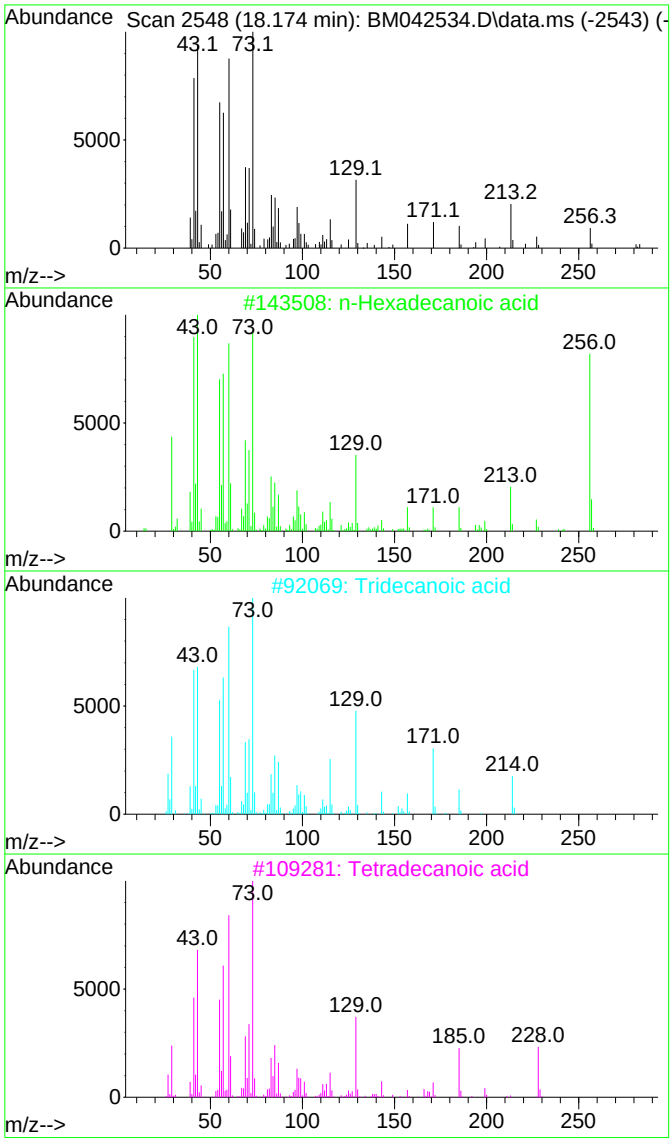
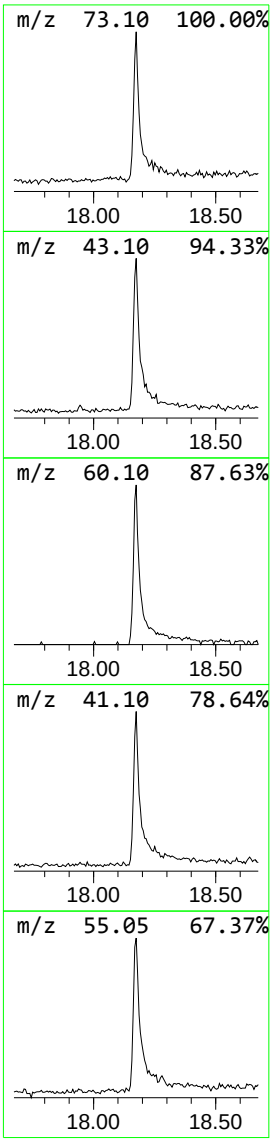
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	4.55 ng	212259	Phenanthrene-d10	17.321

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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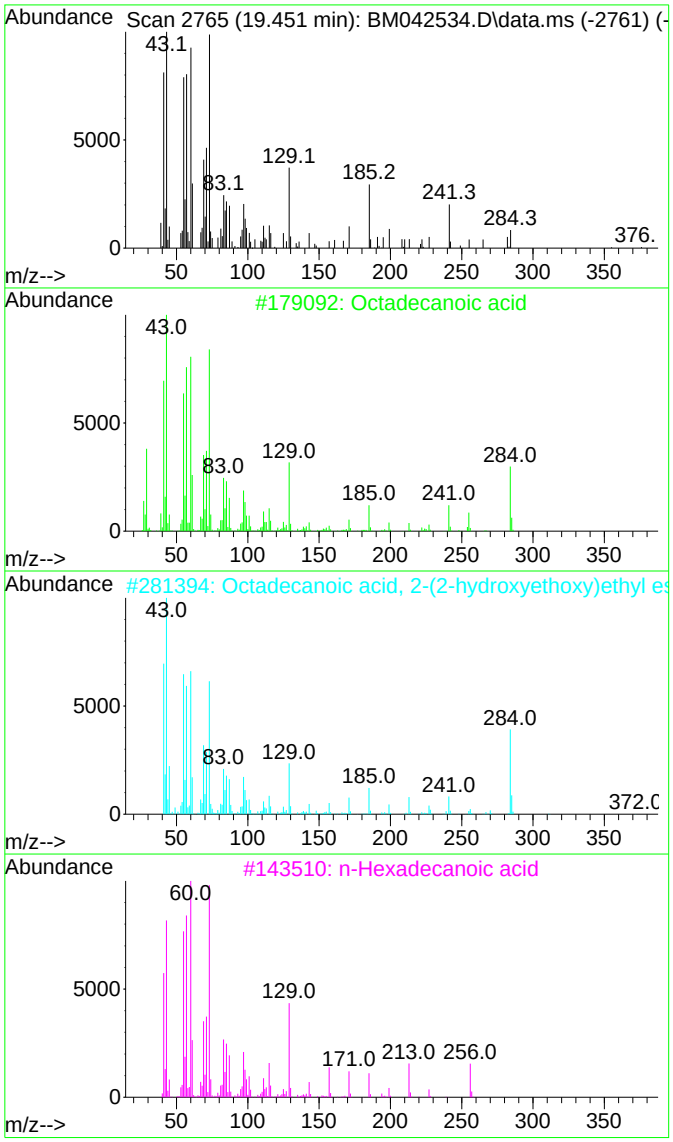
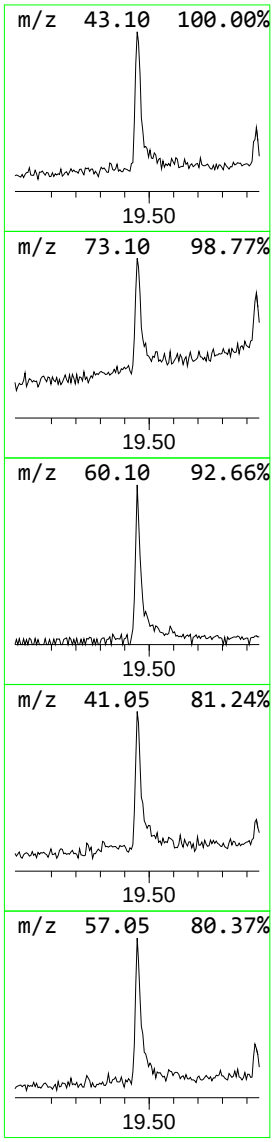
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.39 ng	96958	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25





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
4-Penten-2-one,...	3.752	4.7	ng	125789	1	7.922	539659	20.0
3-Penten-2-one,...	4.375	72.9	ng	1966600	1	7.922	539659	20.0
2-Pentanone, 4-...	5.010	76.2	ng	2056630	1	7.922	539659	20.0
2-Pentanone, 4-...	6.087	2.5	ng	66380	1	7.922	539659	20.0
n-Hexadecanoic ...	18.174	4.5	ng	212259	4	17.321	933008	20.0
Octadecanoic acid	19.451	2.4	ng	96958	5	21.503	811360	20.0