

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
 Data File : BM042426.D
 Acq On : 24 Oct 2023 19:06
 Operator : MA/JU
 Sample : 04977-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 NB-406-COMP-02

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042426.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.504	49	54	63	rVB	58672	76021	1.17%	0.177%
2	4.446	209	214	227	rVB	1653833	2088587	32.22%	4.858%
3	5.075	315	321	330	rVB	2792565	3767439	58.11%	8.764%
4	5.522	391	397	407	rBV	2835958	3980152	61.39%	9.258%
5	6.157	498	505	512	rBV	103078	151885	2.34%	0.353%
6	7.145	665	673	686	rBV	2695148	4173826	64.38%	9.709%
7	7.992	809	817	829	rBV	588883	909291	14.03%	2.115%
8	9.192	1013	1021	1030	rBV	1593278	2568937	39.63%	5.976%
9	10.816	1289	1297	1312	rBV	743439	1225098	18.90%	2.850%
10	13.263	1706	1713	1731	rVB	3065111	4535216	69.96%	10.549%
11	14.639	1940	1947	1955	rVB	998949	1446926	22.32%	3.366%
12	16.133	2192	2201	2211	rBV	2513533	3640964	56.16%	8.469%
13	17.392	2408	2415	2420	rBV	1244266	1700558	26.23%	3.956%
14	18.239	2553	2559	2569	rBV	480462	783247	12.08%	1.822%
15	19.445	2760	2764	2769	rVB	157465	199798	3.08%	0.465%
16	19.515	2771	2776	2787	rBV	244528	427619	6.60%	0.995%
17	19.809	2822	2826	2832	rVB	133589	182018	2.81%	0.423%
18	20.003	2853	2859	2867	rBV	5625125	6482864	100.00%	15.080%
19	21.233	3063	3068	3075	rBV3	258201	469201	7.24%	1.091%
20	21.574	3120	3126	3130	rBV	1544167	2060804	31.79%	4.794%
21	24.038	3538	3545	3558	rVB	993404	2119599	32.70%	4.930%

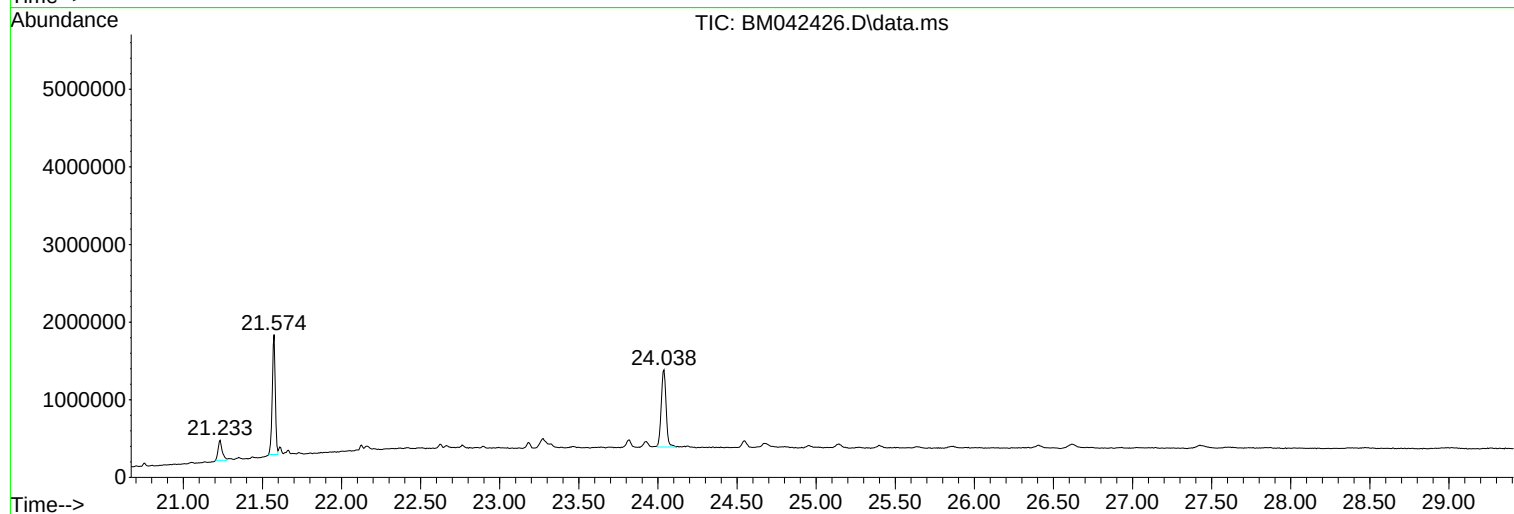
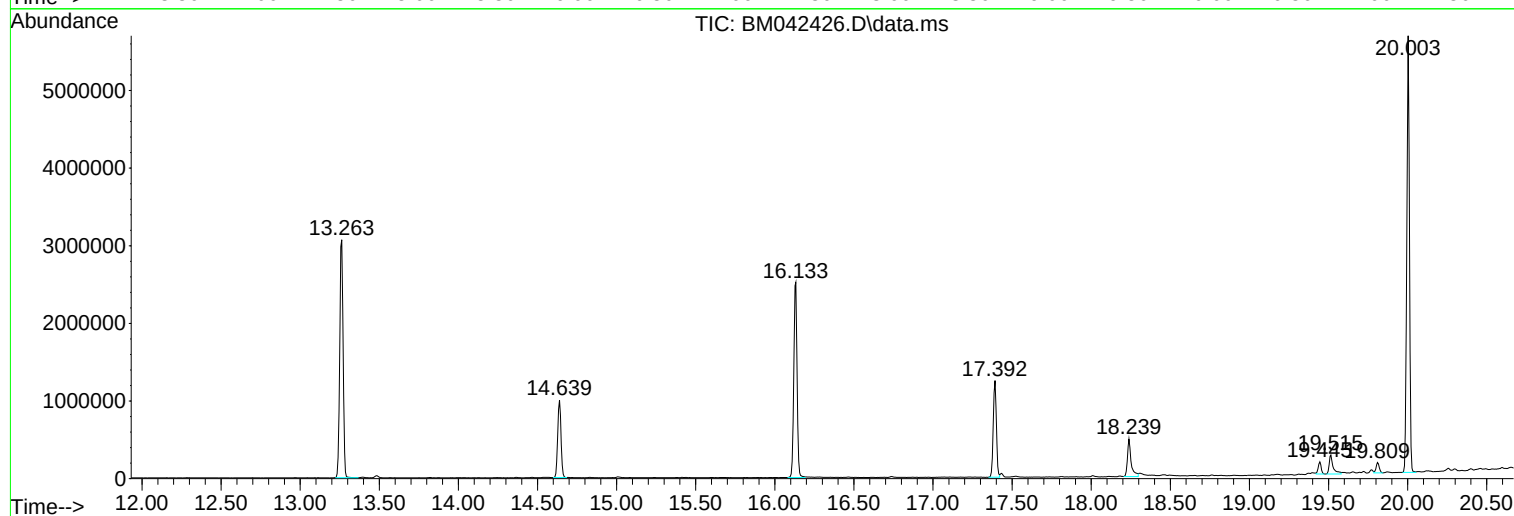
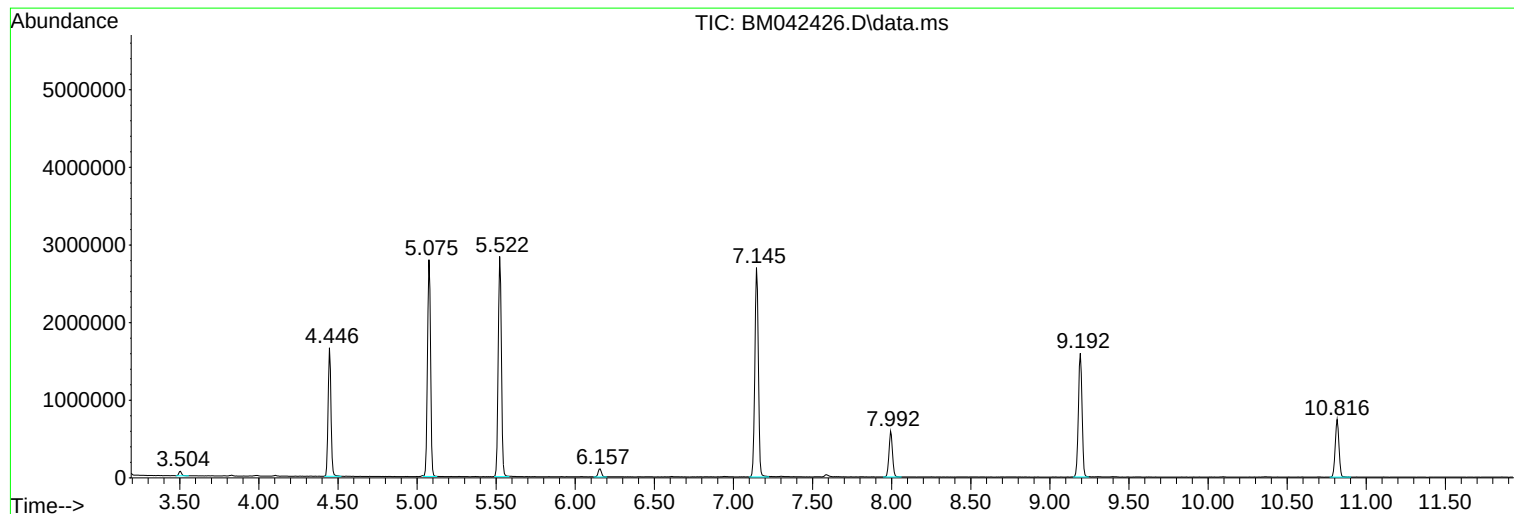
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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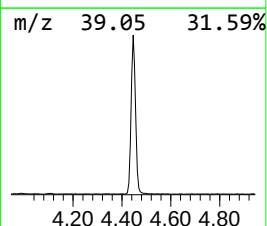
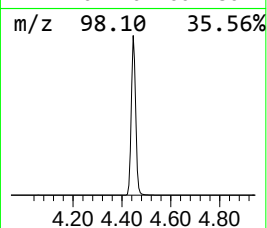
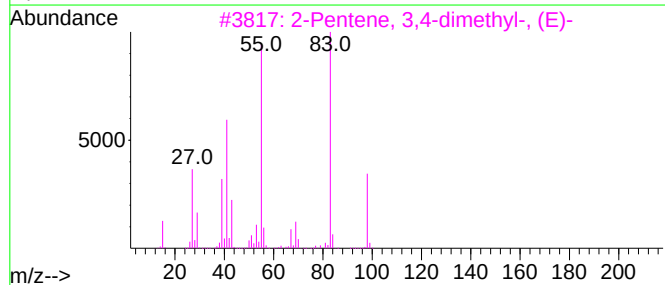
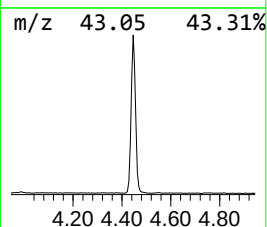
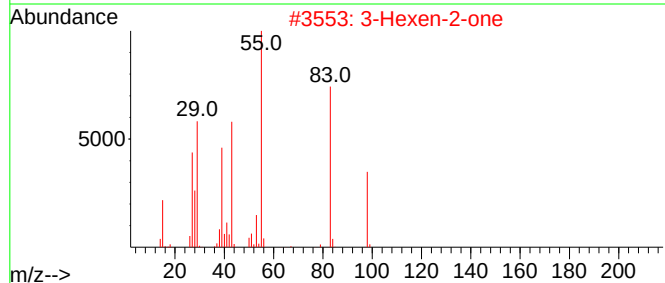
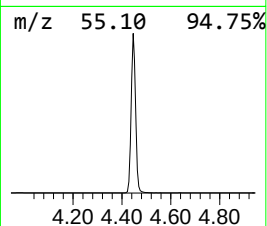
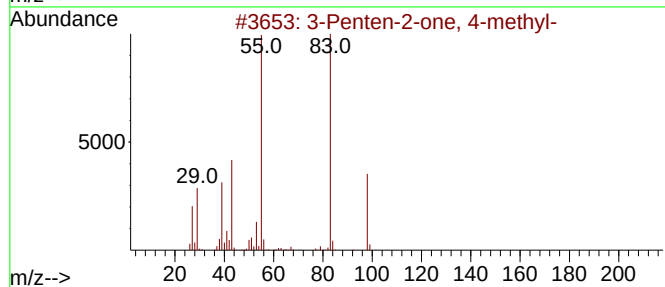
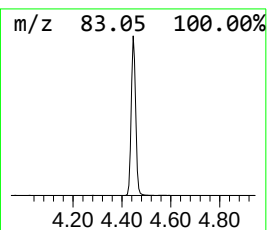
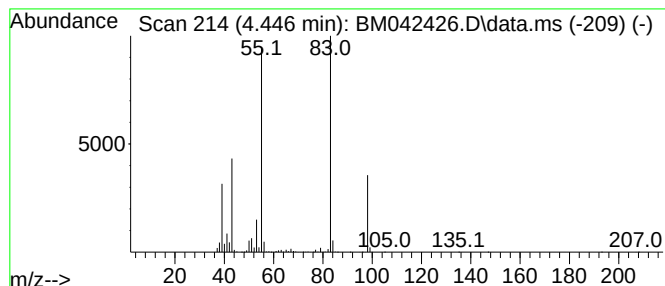
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	45.94 ng	2088590	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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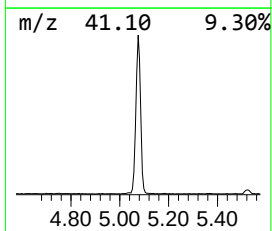
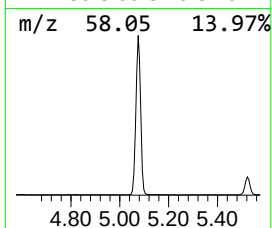
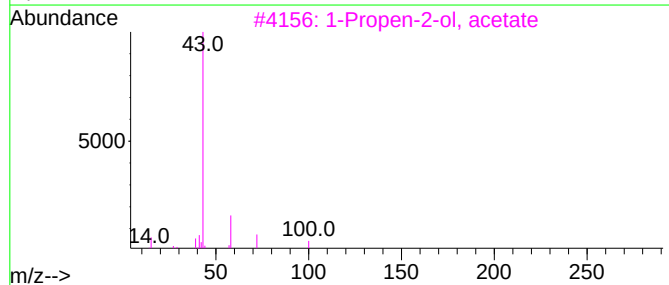
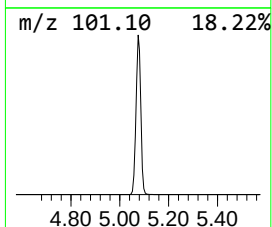
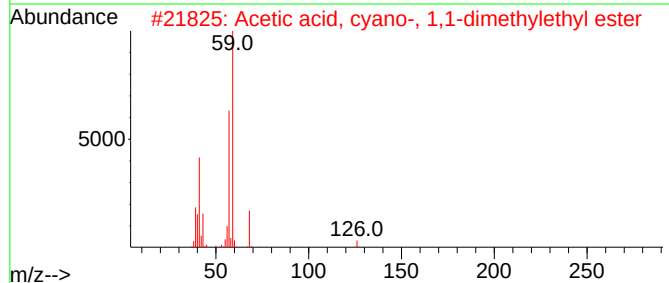
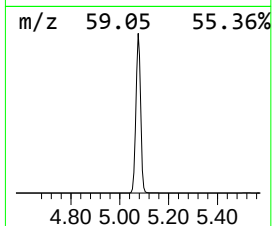
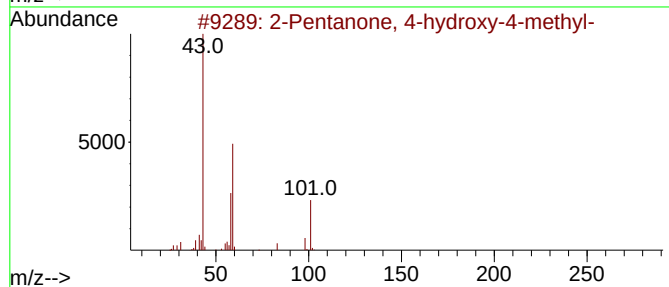
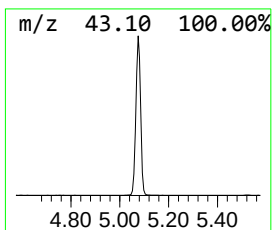
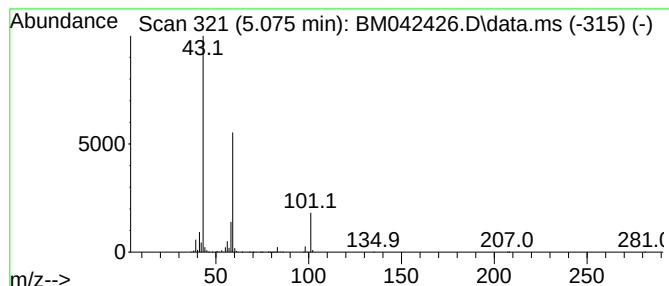
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.075	82.87 ng	3767440	1,4-Dichlorobenzene-d4	7.992	
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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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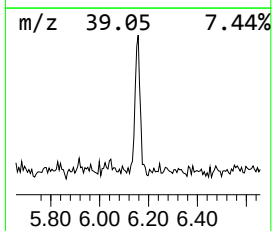
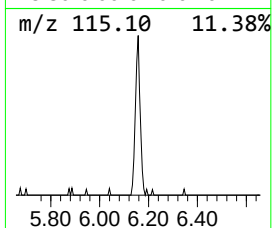
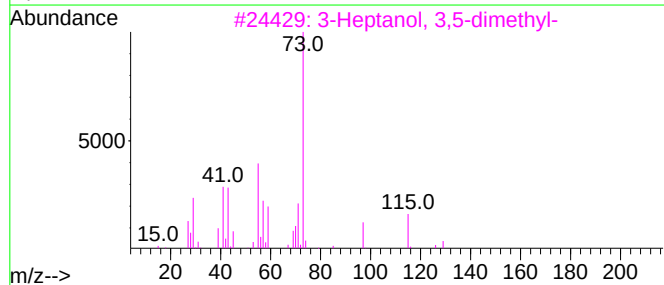
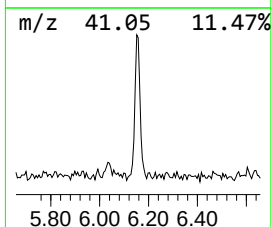
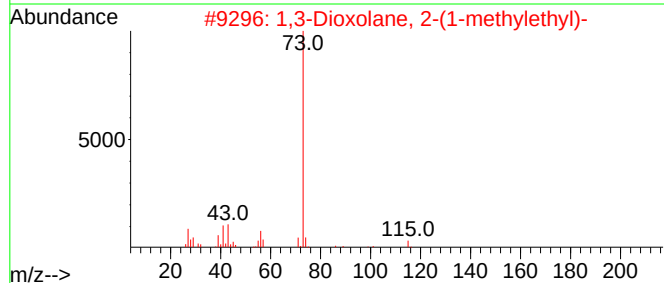
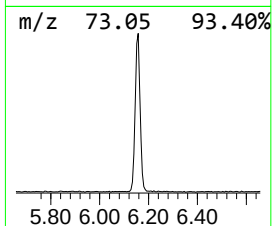
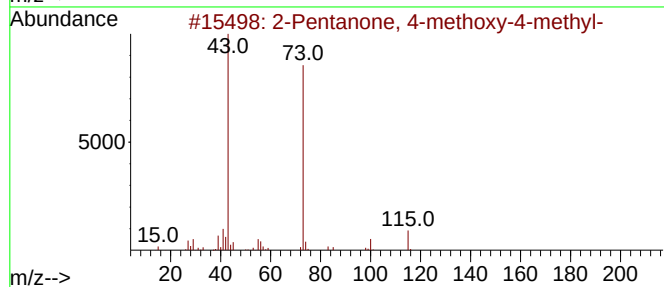
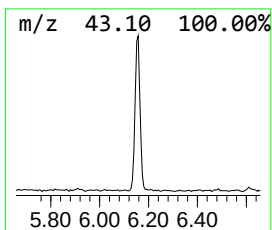
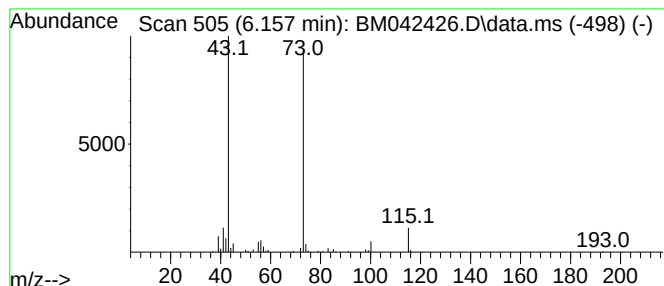
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.157	3.34 ng	151885	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32
3			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
4			Isobutyl acetate	116	C6H12O2	000110-19-0	23
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10



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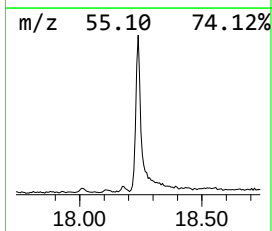
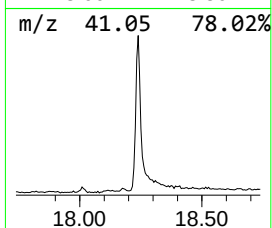
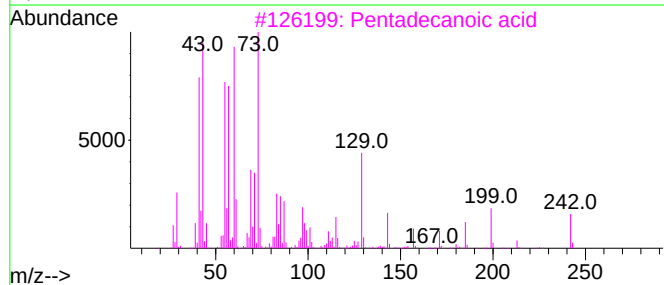
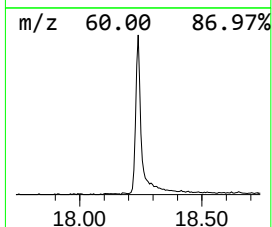
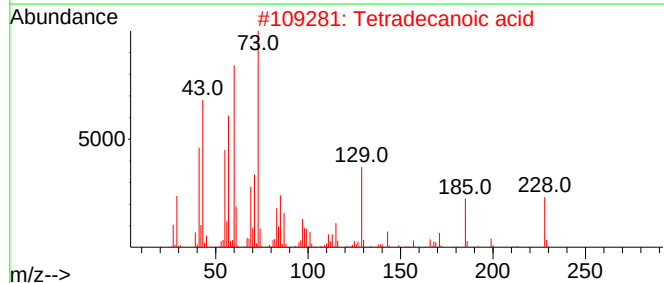
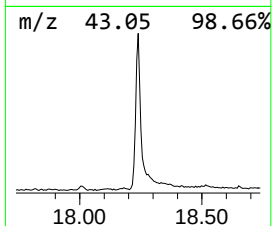
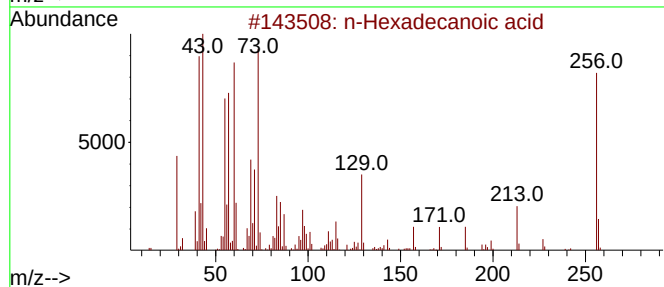
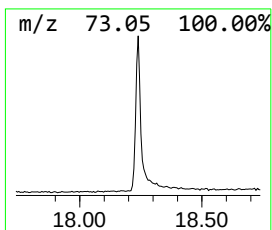
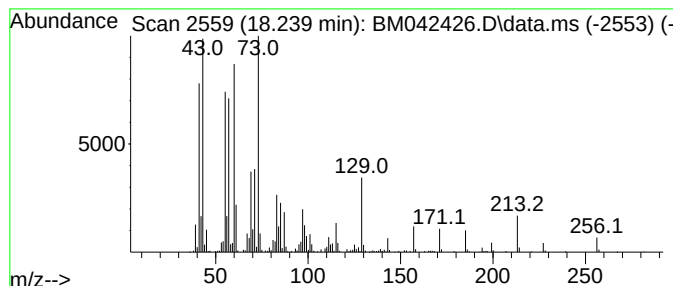
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.239	9.21 ng	783247	Phenanthrene-d10	17.392	
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	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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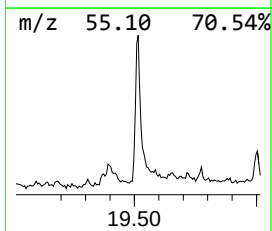
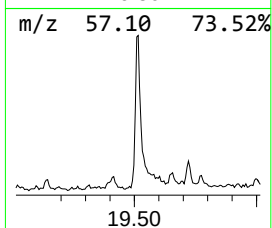
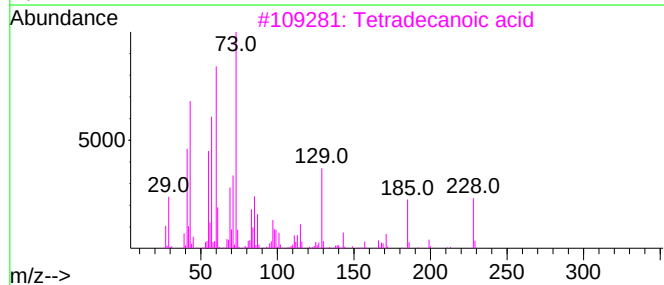
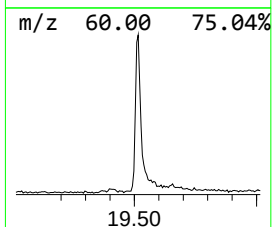
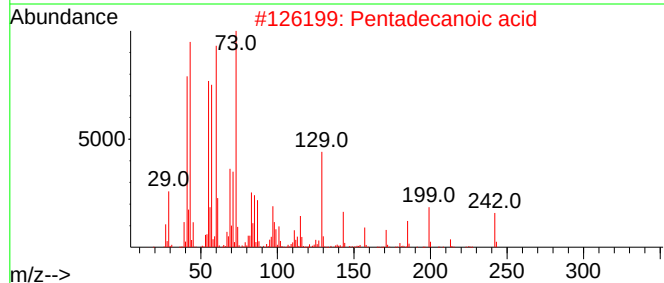
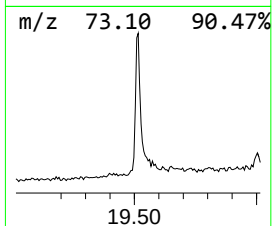
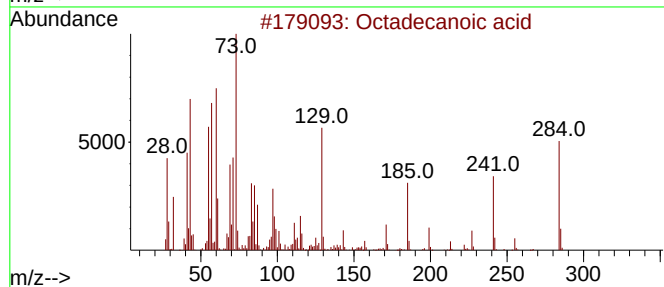
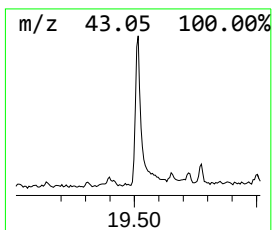
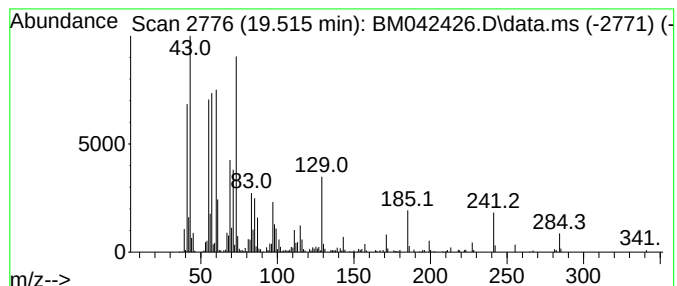
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	4.15 ng	427619	Chrysene-d12	21.574

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	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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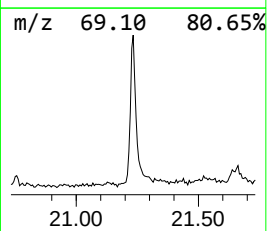
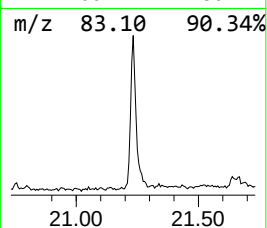
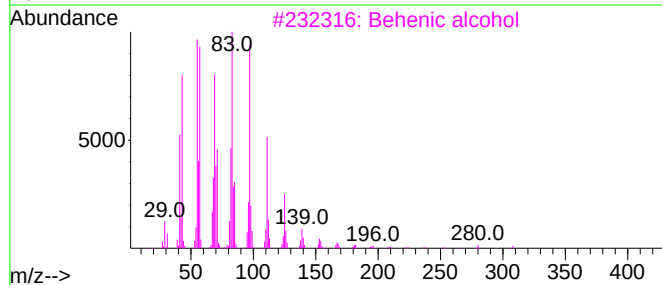
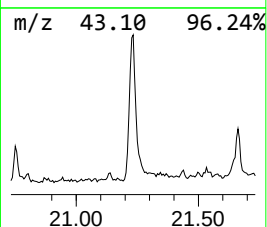
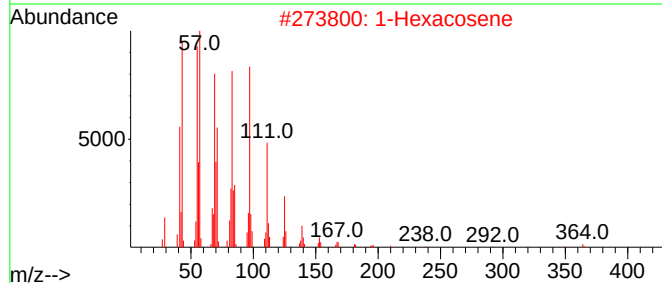
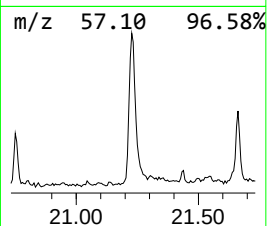
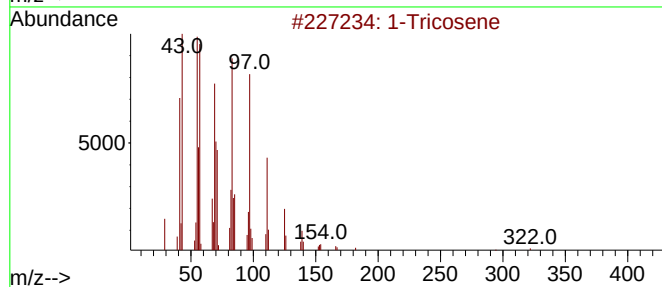
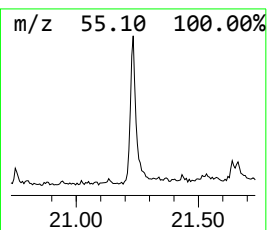
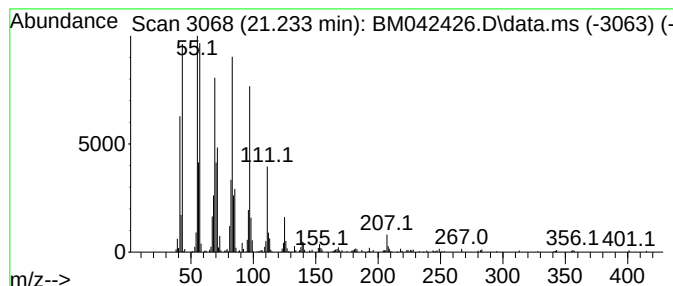
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	4.55 ng	469201	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	94
2	1-Hexacosene			364	C26H52	018835-33-1	91
3	Behenic alcohol			326	C22H46O	000661-19-8	91
4	1-Nonadecene			266	C19H38	018435-45-5	91
5	Pentacos-1-ene			350	C25H50	016980-85-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042426.D
Acq On : 24 Oct 2023 19:06
Operator : MA/JU
Sample : 04977-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-406-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.446	45.9	ng	2088590	1	7.992	909291	20.0
2-Pentanone, 4-...	5.075	82.9	ng	3767440	1	7.992	909291	20.0
2-Pentanone, 4-...	6.157	3.3	ng	151885	1	7.992	909291	20.0
n-Hexadecanoic ...	18.239	9.2	ng	783247	4	17.392	1700560	20.0
Octadecanoic acid	19.515	4.2	ng	427619	5	21.574	2060800	20.0
1-Tricosene	21.233	4.5	ng	469201	5	21.574	2060800	20.0