

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020223\
 Data File : BM038676.D
 Acq On : 02 Feb 2023 23:01
 Operator : CG/JU
 Sample : 01348-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 N-H5(32-34)

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038676.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.063	144	149	157	rBV	61996	78546	2.40%	0.502%
2	5.022	306	312	321	rBV	539616	736100	22.47%	4.703%
3	5.404	373	377	382	rBV	24735	34014	1.04%	0.217%
4	5.493	386	392	397	rVV	394183	552813	16.88%	3.532%
5	5.540	397	400	410	rVB	46144	86889	2.65%	0.555%
6	5.916	454	464	469	rBV4	23584	48038	1.47%	0.307%
7	7.110	660	667	679	rVB	843403	1320711	40.32%	8.437%
8	7.563	740	744	751	rVB2	29184	43894	1.34%	0.280%
9	7.928	800	806	813	rBV	279130	420726	12.84%	2.688%
10	9.104	998	1006	1018	rBV	551327	873144	26.66%	5.578%
11	10.739	1277	1284	1289	rBV	287517	483495	14.76%	3.089%
12	10.786	1289	1292	1301	rVB	75545	110247	3.37%	0.704%
13	13.192	1694	1701	1712	rBV	1833483	2492149	76.08%	15.921%
14	14.568	1927	1935	1944	rBV	462072	665056	20.30%	4.249%
15	16.057	2182	2188	2197	rBV	76284	105169	3.21%	0.672%
16	17.309	2395	2401	2406	rBV	534905	737962	22.53%	4.714%
17	17.351	2406	2408	2415	rVB	45035	53881	1.64%	0.344%
18	18.192	2546	2551	2556	rBV2	91984	128845	3.93%	0.823%
19	19.362	2741	2750	2755	rBV	40934	81971	2.50%	0.524%
20	19.468	2764	2768	2775	rBV2	34821	59052	1.80%	0.377%
21	19.727	2808	2812	2820	rBV	31059	44648	1.36%	0.285%
22	19.927	2840	2846	2852	rBV	2948192	3275561	100.00%	20.926%
23	20.609	2956	2962	2969	rBV	310561	395375	12.07%	2.526%
24	21.180	3055	3059	3069	rBV	182816	256146	7.82%	1.636%
25	21.386	3091	3094	3098	rVB	88963	87907	2.68%	0.562%
26	21.486	3106	3111	3117	rBV	657278	869566	26.55%	5.555%
27	22.709	3314	3319	3324	rVB	456237	616478	18.82%	3.938%
28	23.885	3513	3519	3528	rVB2	518527	994653	30.37%	6.354%

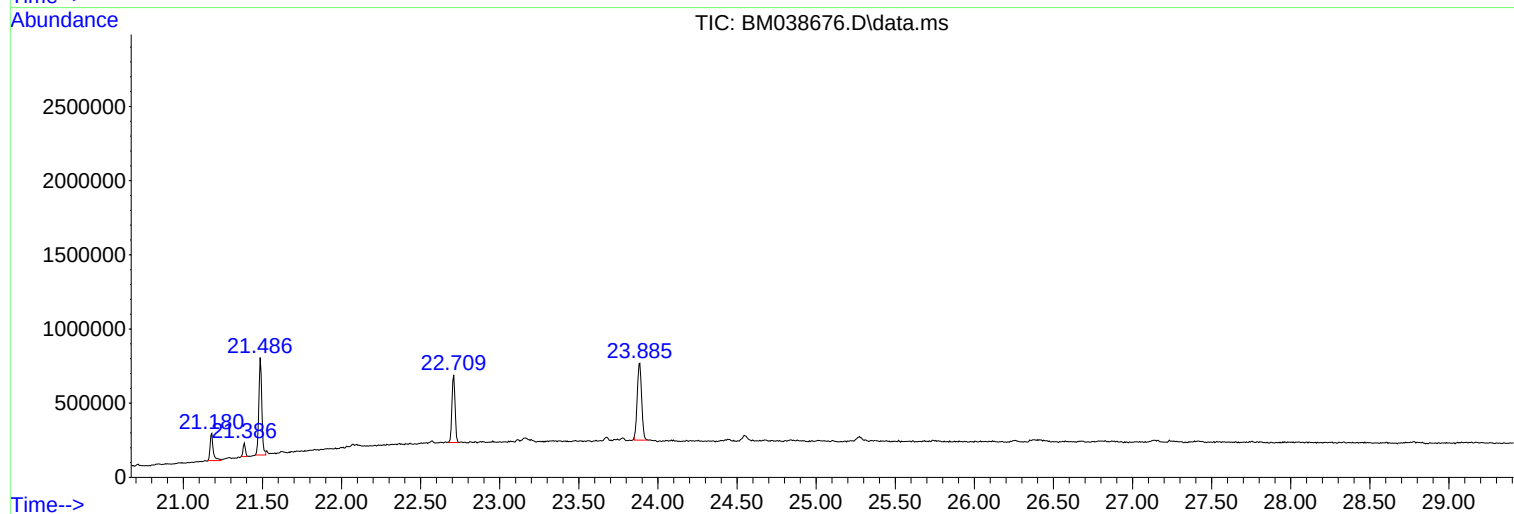
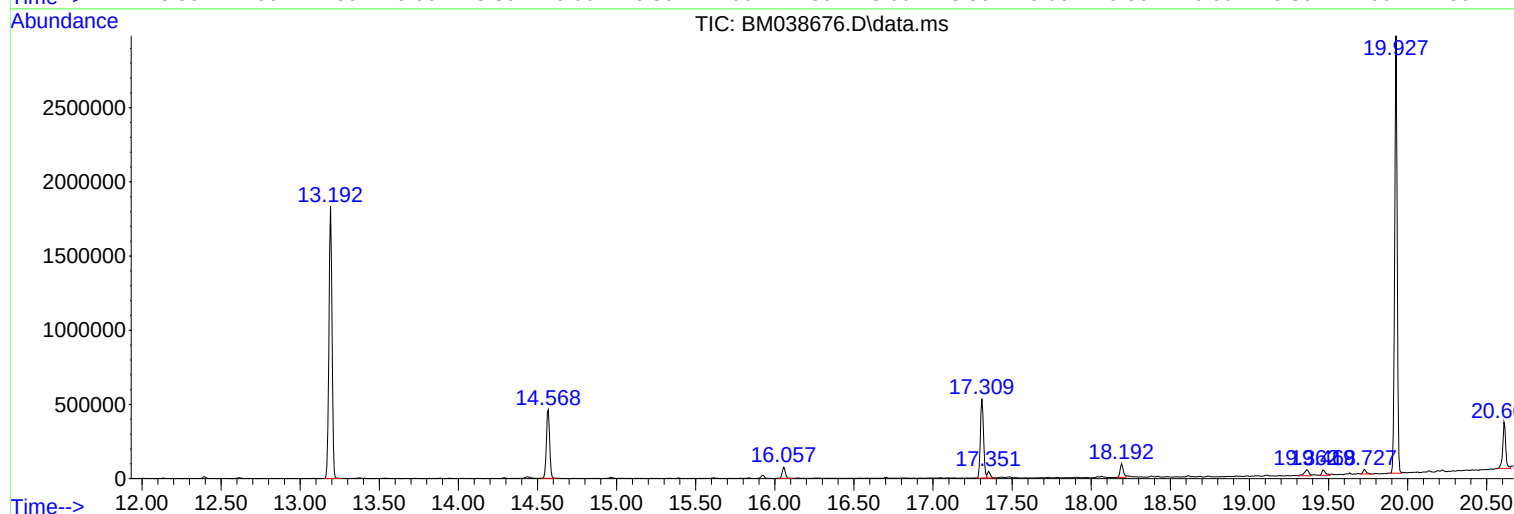
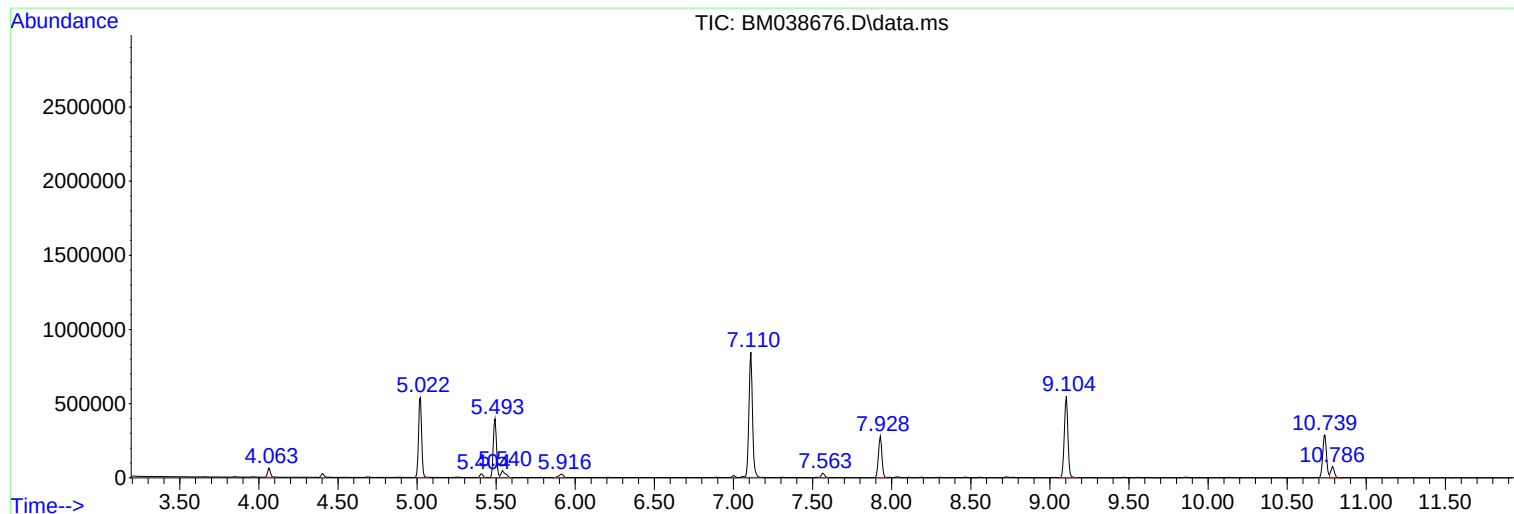
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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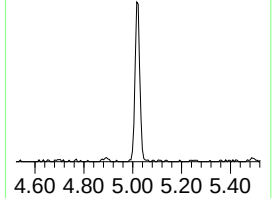
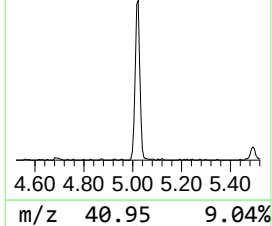
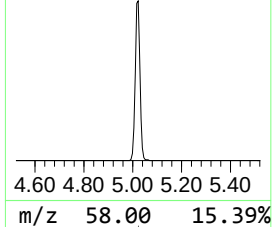
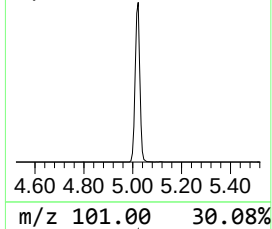
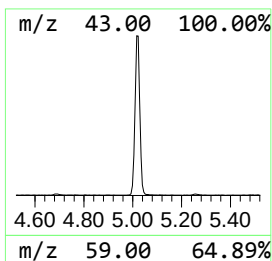
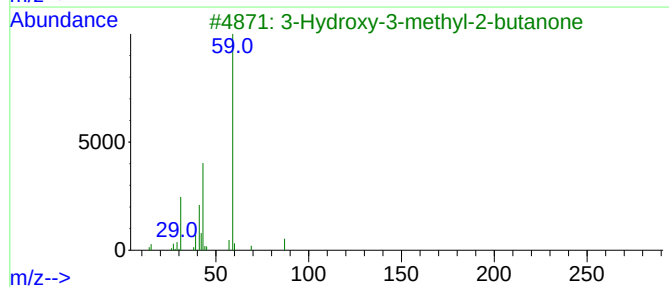
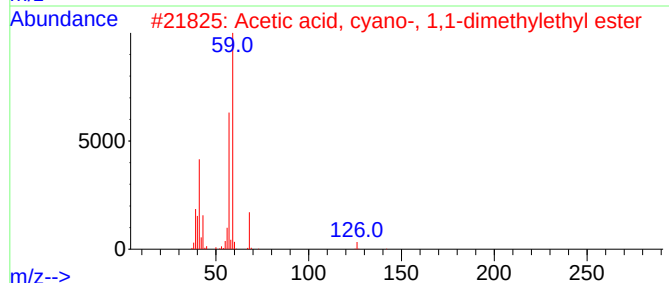
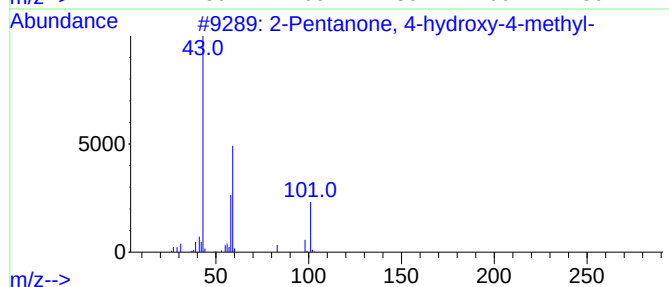
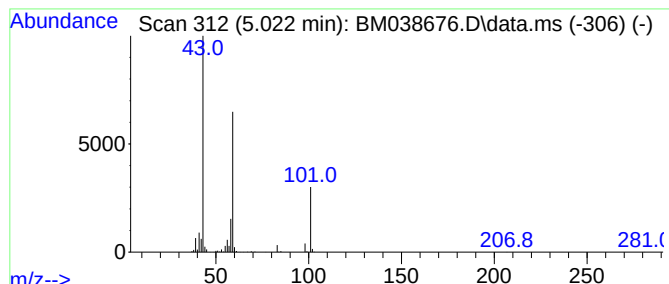
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	34.99 ng	736100	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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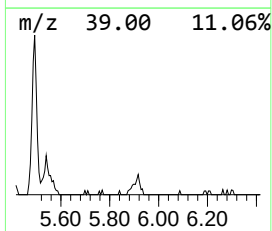
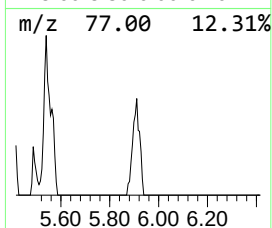
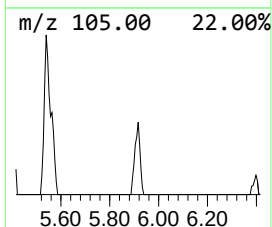
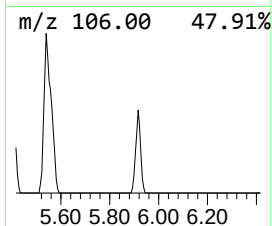
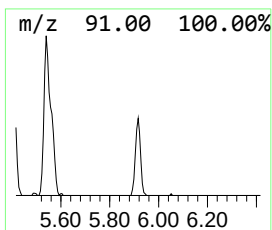
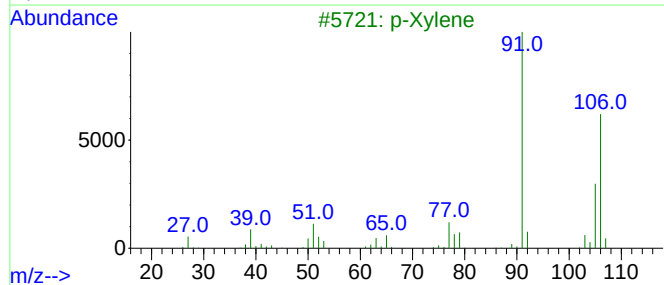
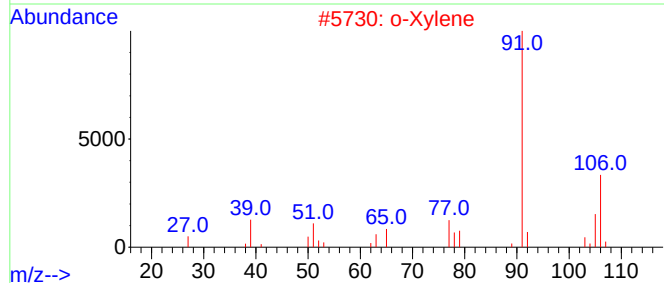
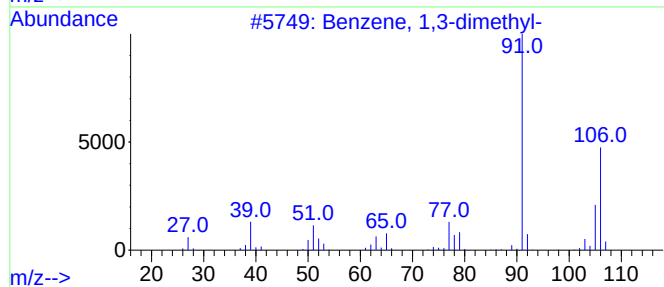
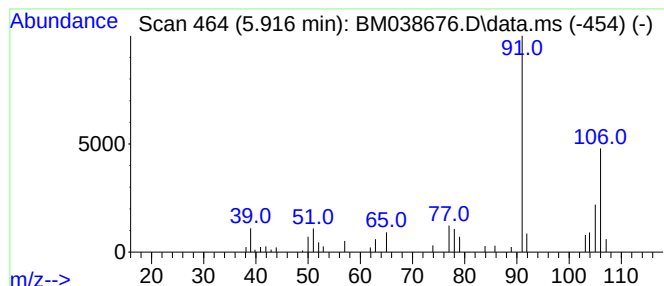
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Peak Number 3 Benzene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.916	2.28 ng	48038	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	94
2			o-Xylene	106	C8H10	000095-47-6	94
3			p-Xylene	106	C8H10	000106-42-3	93
4			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	90
5			Ethylbenzene	106	C8H10	000100-41-4	81



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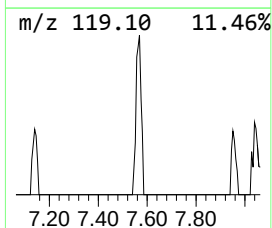
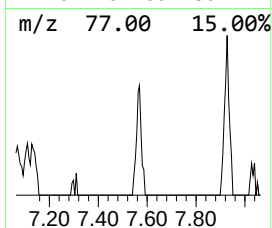
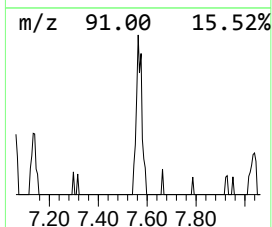
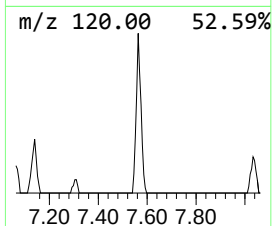
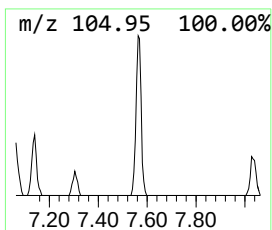
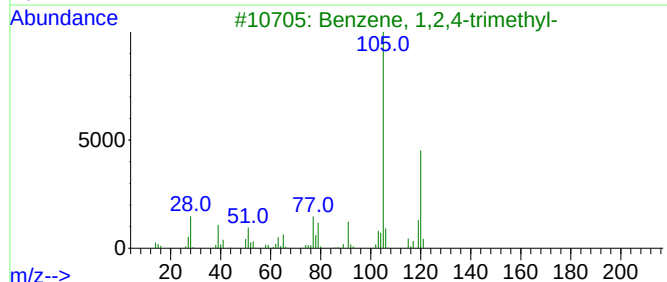
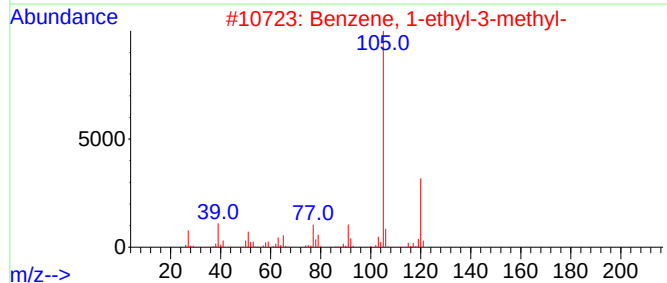
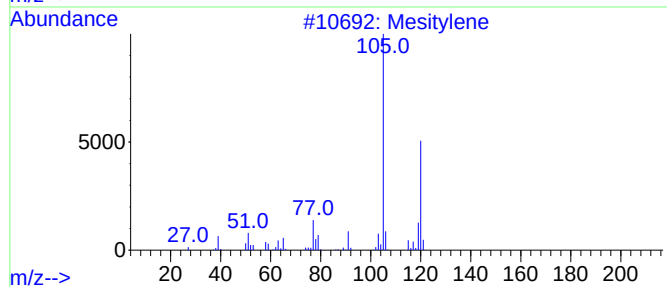
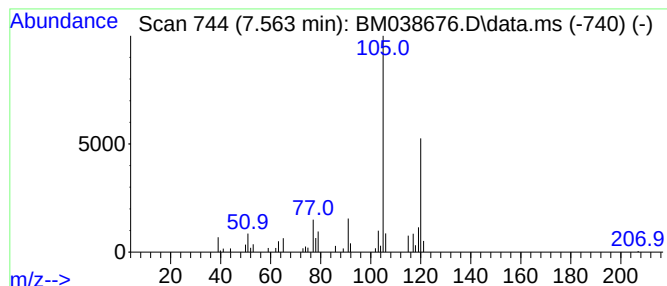
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Mesitylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	2.09 ng	43894	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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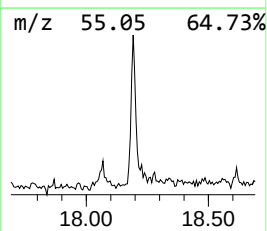
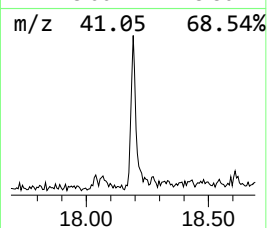
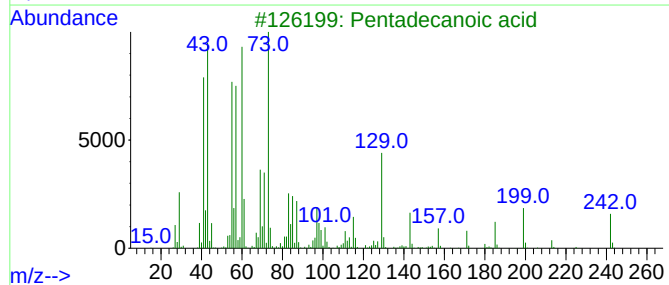
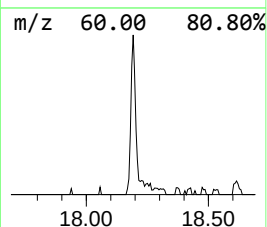
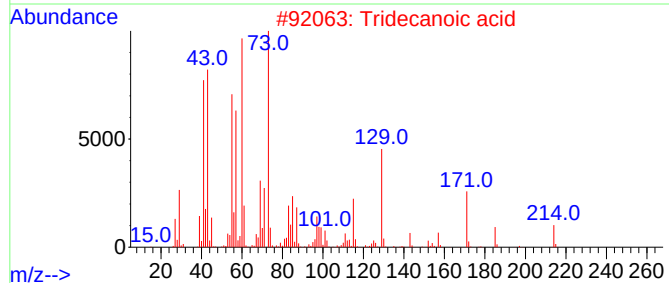
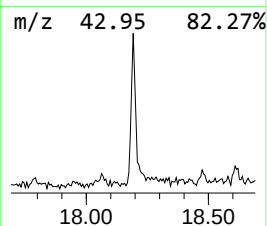
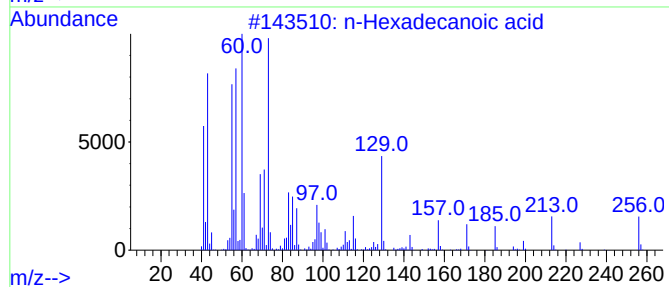
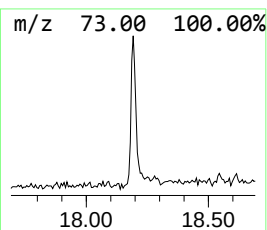
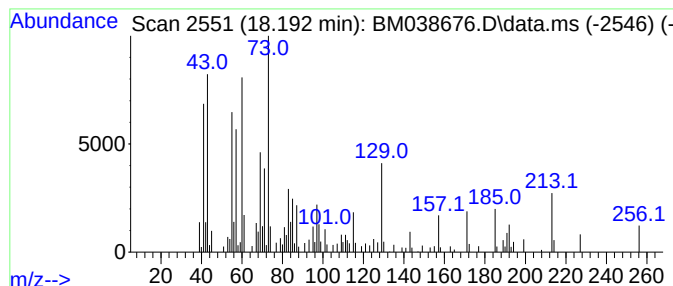
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	3.49 ng	128845	Phenanthrene-d10	17.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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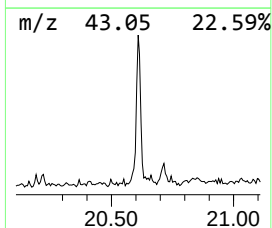
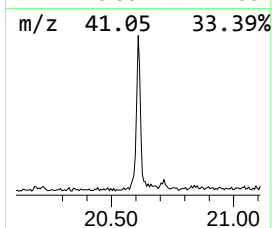
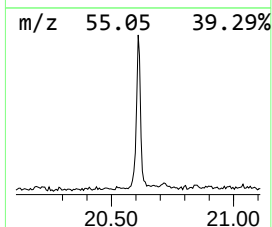
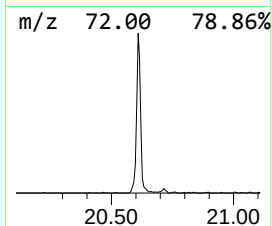
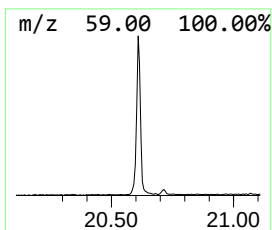
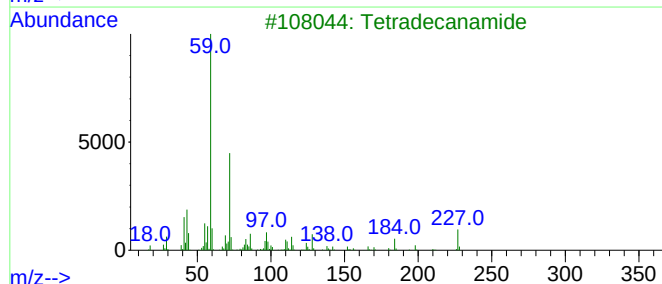
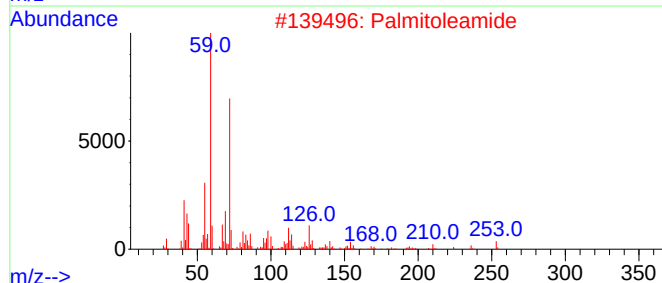
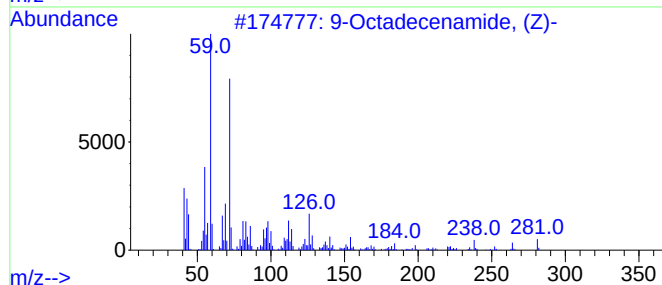
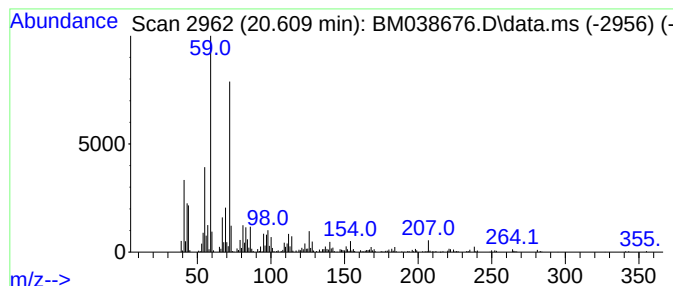
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Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.609	9.09 ng	395375	Chrysene-d12	21.486

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Palmitoleamide	253	C16H31NO	106010-22-4	72
3		Tetradecanamide	227	C14H29NO	000638-58-4	50
4		Octanamide	143	C8H17NO	000629-01-6	50
5		Dodecanamide	199	C12H25NO	001120-16-7	43



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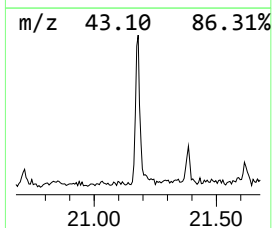
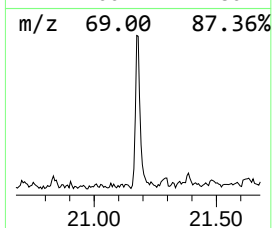
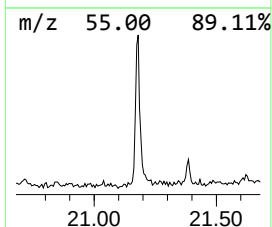
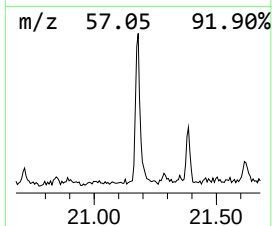
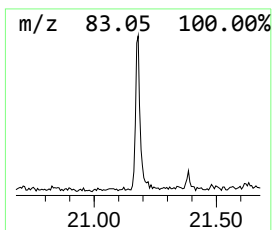
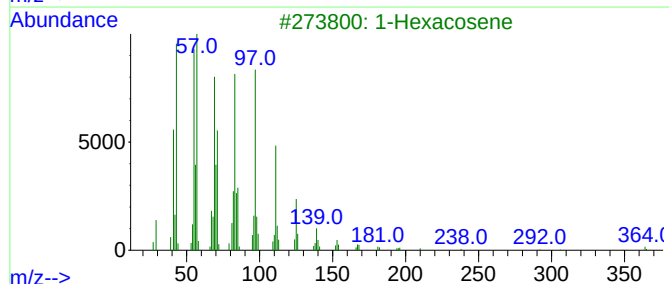
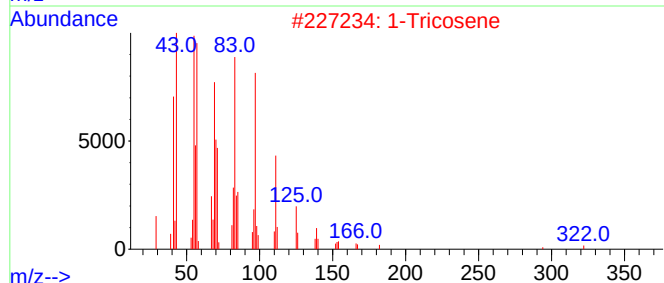
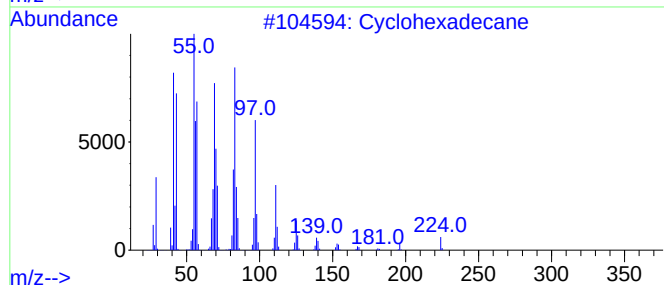
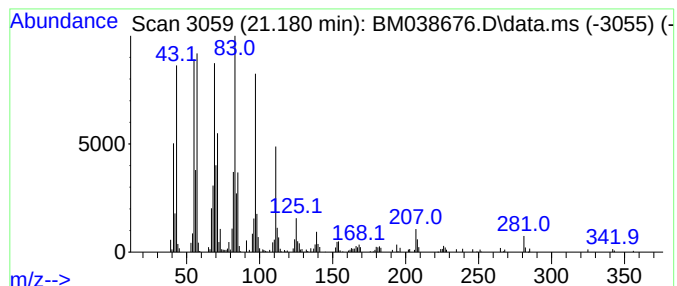
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	5.89 ng	256146	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	97
2			1-Tricosene	322	C23H46	018835-32-0	95
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Tetracosene	336	C24H48	010192-32-2	94
5			1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020223\
Data File : BM038676.D
Acq On : 02 Feb 2023 23:01
Operator : CG/JU
Sample : 01348-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
N-H5(32-34)

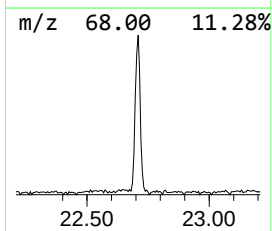
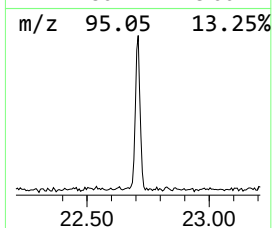
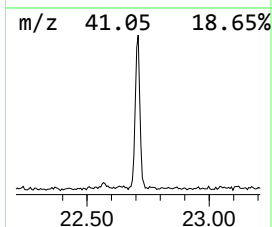
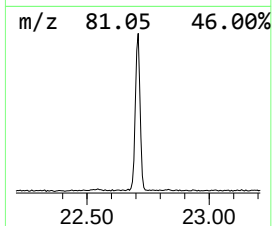
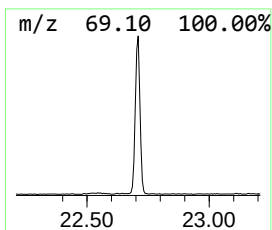
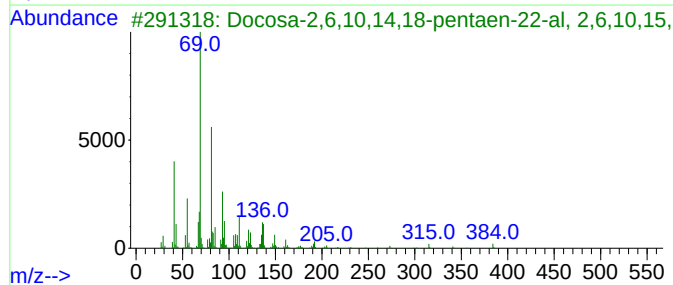
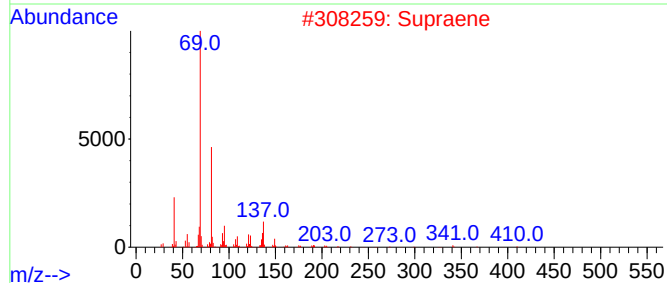
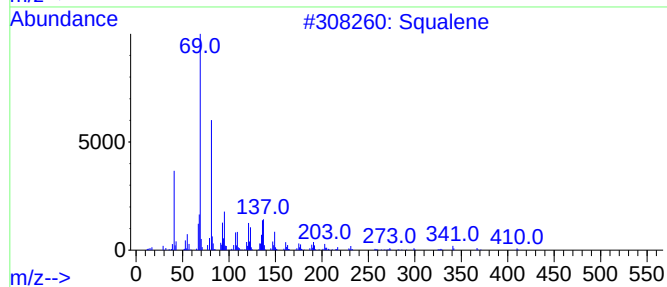
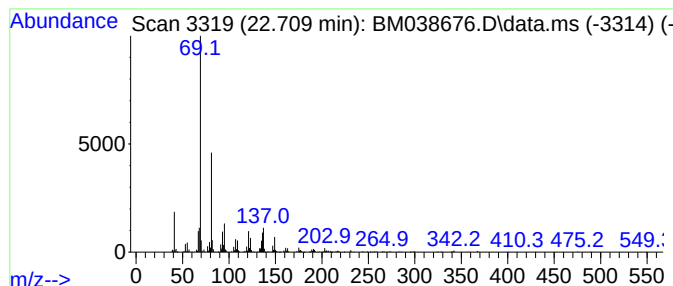
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.709	12.40 ng	616478	Perylene-d12	23.885

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	87
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	78
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020223\
Data File : BM038676.D
Acq On : 02 Feb 2023 23:01
Operator : CG/JU
Sample : 01348-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
N-H5(32-34)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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
2-Pentanone, 4-...	5.022	35.0	ng	736100	1	7.928	420726	20.0
Benzene, 1,3-di...	5.916	2.3	ng	48038	1	7.928	420726	20.0
Mesitylene	7.563	2.1	ng	43894	1	7.928	420726	20.0
n-Hexadecanoic ...	18.192	3.5	ng	128845	4	17.309	737962	20.0
9-Octadecenamid...	20.609	9.1	ng	395375	5	21.486	869566	20.0
Cyclohexadecane	21.180	5.9	ng	256146	5	21.486	869566	20.0
Squalene	22.709	12.4	ng	616478	6	23.885	994653	20.0