

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
 Data File : BM042592.D
 Acq On : 04 Nov 2023 15:29
 Operator : MA/JU
 Sample : 05234-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-B

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: BM042592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.446	378	384	398	rBV	952453	1381524	37.10%	7.417%
2	7.081	655	662	677	rBV	931643	1476016	39.64%	7.924%
3	7.510	729	735	747	rBV	19809	42024	1.13%	0.226%
4	7.910	795	803	815	rVB	200378	308170	8.28%	1.654%
5	9.116	1000	1008	1023	rBV	558842	951932	25.56%	5.111%
6	10.733	1275	1283	1291	rBV	229834	394917	10.61%	2.120%
7	13.186	1693	1700	1709	rBV	1450292	2055399	55.20%	11.035%
8	13.410	1730	1738	1746	rBV	572705	894893	24.03%	4.804%
9	13.927	1821	1826	1830	rBV	41509	60667	1.63%	0.326%
10	14.245	1875	1880	1884	rBV3	69224	111764	3.00%	0.600%
11	14.339	1891	1896	1901	rVB2	87091	128415	3.45%	0.689%
12	14.416	1902	1909	1912	rBV8	37037	72935	1.96%	0.392%
13	14.480	1918	1920	1929	rVB8	29129	56755	1.52%	0.305%
14	14.563	1929	1934	1940	rBV	377152	586528	15.75%	3.149%
15	15.163	2033	2036	2040	rVB3	56631	67887	1.82%	0.364%
16	15.298	2055	2059	2066	rBV	189251	271548	7.29%	1.458%
17	15.398	2070	2076	2080	rVV3	134086	242187	6.50%	1.300%
18	16.062	2184	2189	2197	rVB	1466411	2040371	54.80%	10.954%
19	17.321	2399	2403	2407	rVB	568277	782959	21.03%	4.203%
20	18.174	2545	2548	2553	rVB	831381	1065017	28.60%	5.718%
21	19.450	2762	2765	2769	rBV	327730	360883	9.69%	1.937%
22	19.939	2843	2848	2852	rVB	3036865	3723643	100.00%	19.991%
23	21.497	3110	3113	3121	rVB	577744	789541	21.20%	4.239%
24	23.921	3520	3525	3533	rVB	395055	760941	20.44%	4.085%

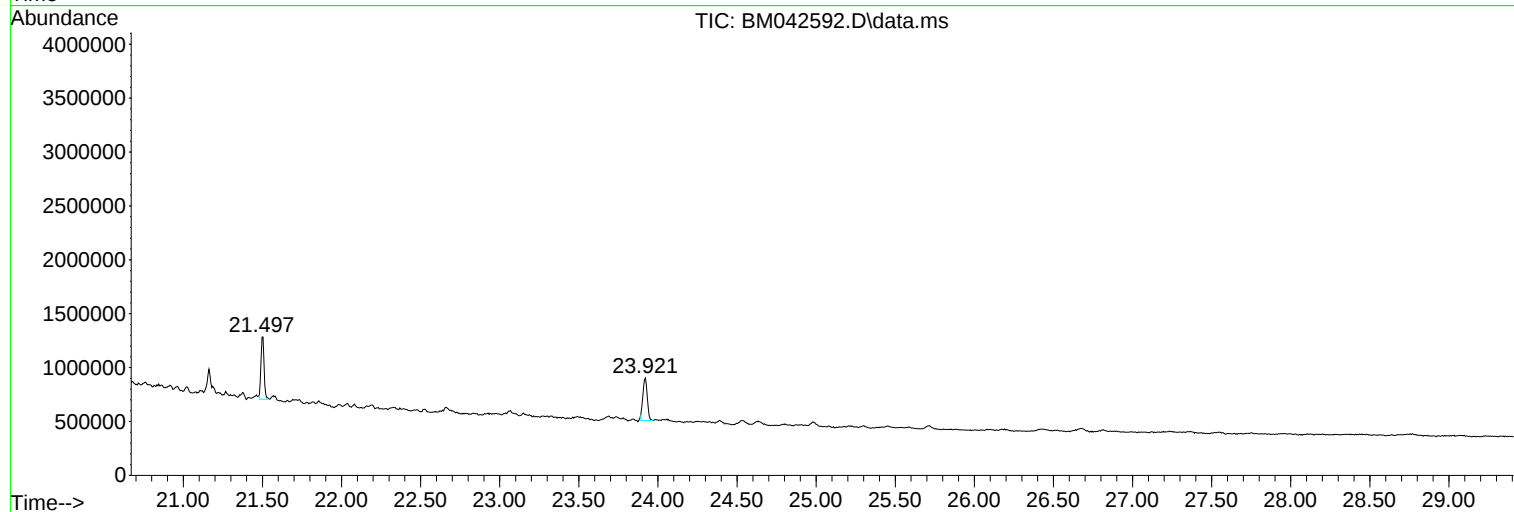
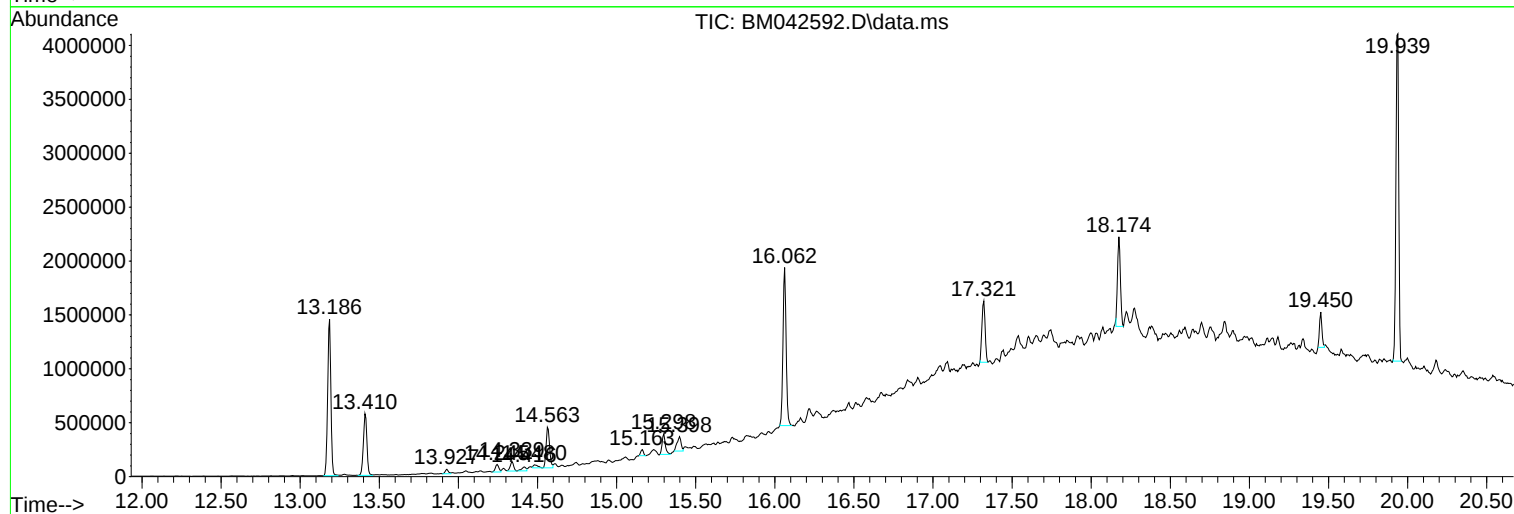
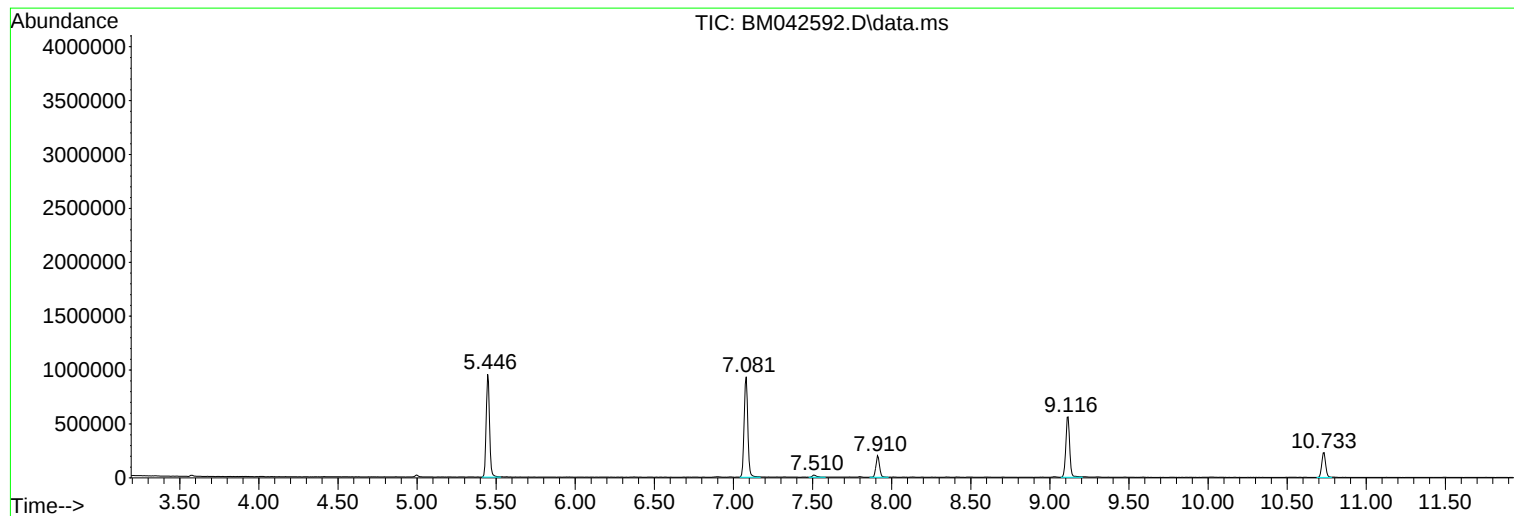
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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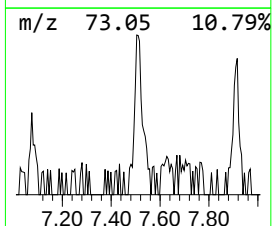
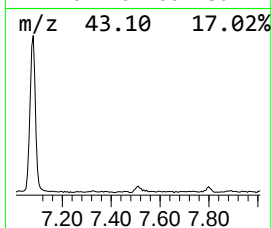
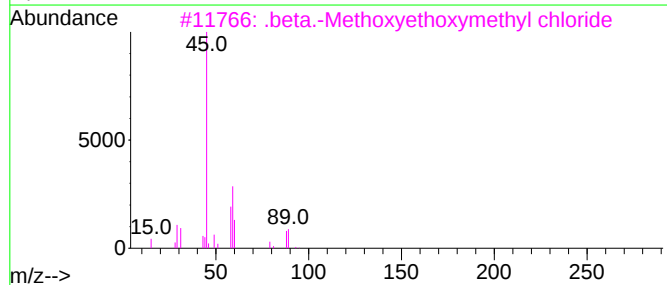
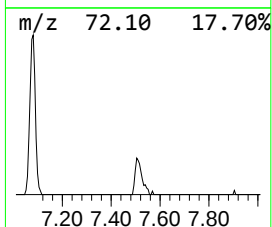
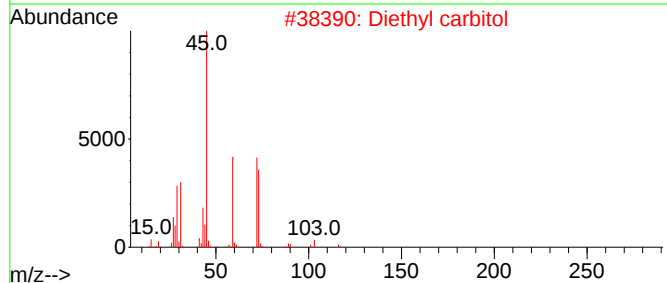
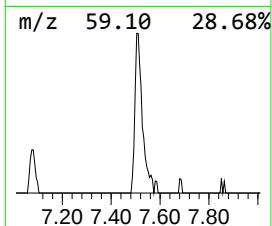
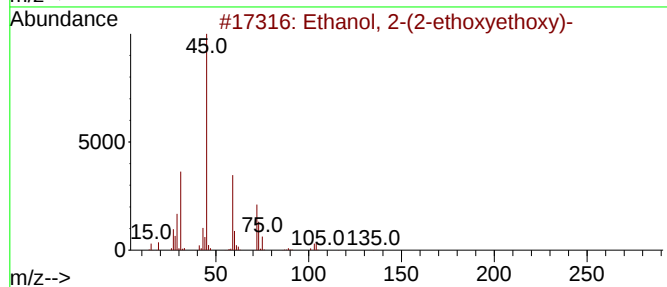
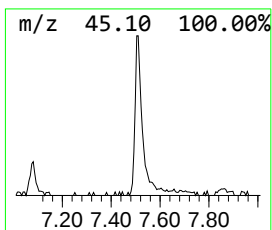
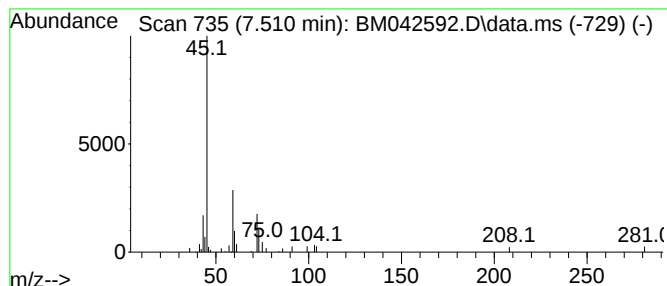
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.510	2.73 ng	42024	1,4-Dichlorobenzene-d4	7.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	38
4			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	33
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	32



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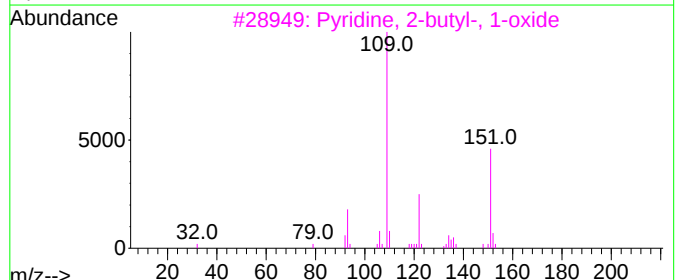
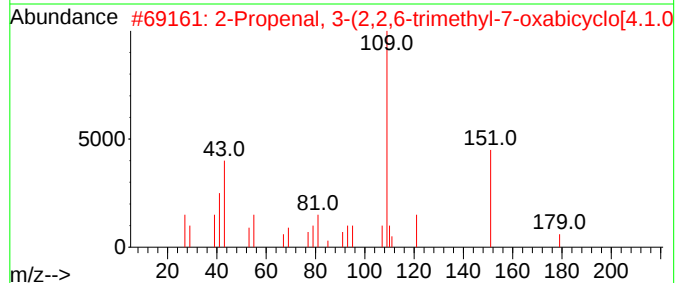
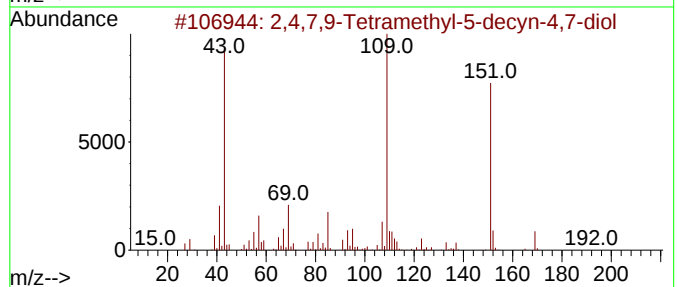
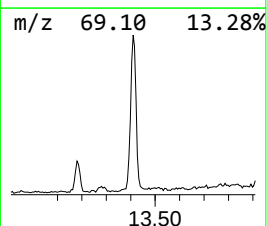
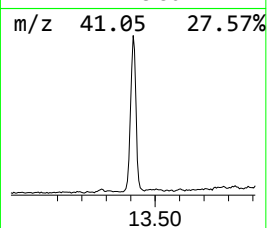
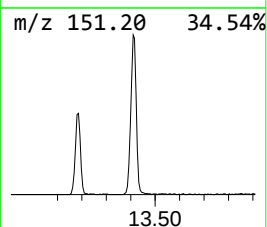
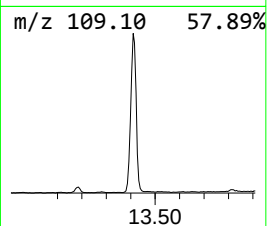
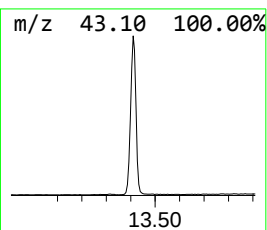
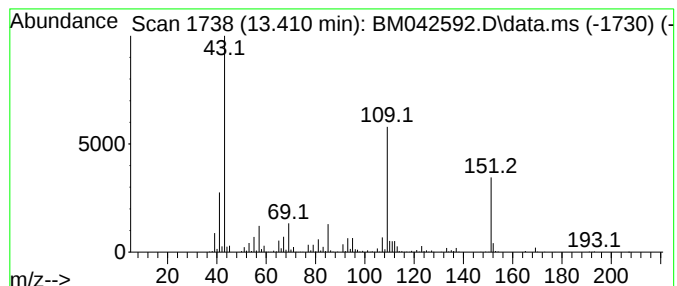
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.410	30.51 ng	894893	Acenaphthene-d10		14.563	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	2-Propenal, 3-(2,2,6-trimethyl-7...		194	C12H18O2	055759-91-6	59
3	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	53
4	7-Oxa-bicyclo[2.2.1]heptan-2-ol,...		254	C14H22O4	329362-13-2	50
5	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	47



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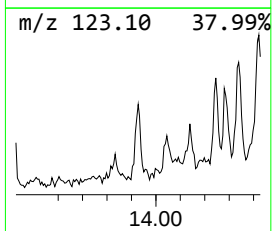
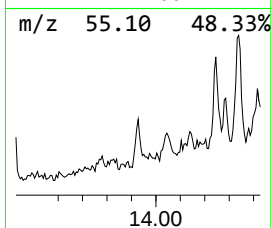
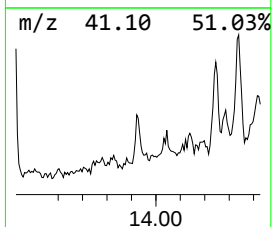
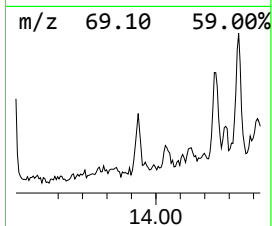
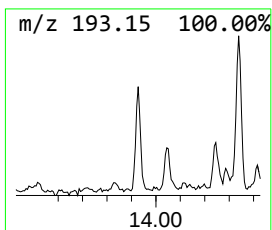
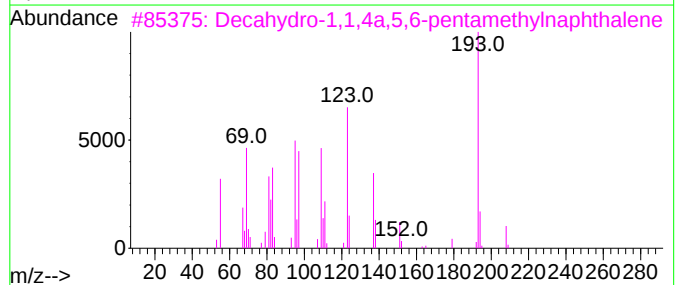
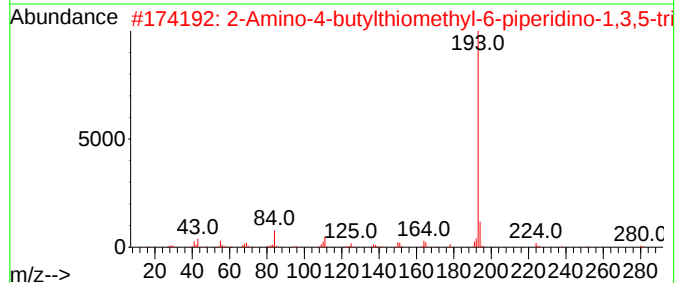
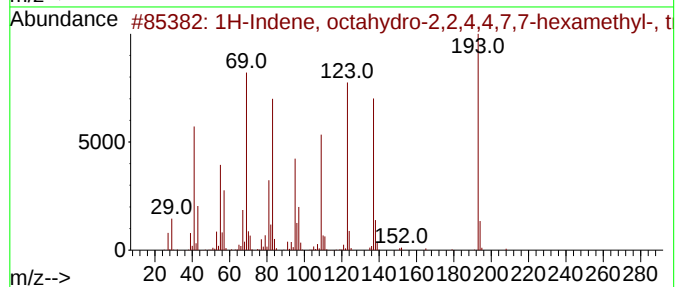
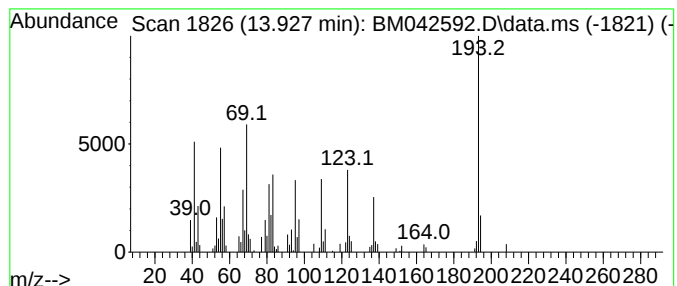
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Peak Number 3 1H-Indene, octahydro-2,2,4,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.927	2.07 ng	60667	Acenaphthene-d10		14.563	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...		208	C15H28	054832-83-6	50
2	2-Amino-4-butylthiomethyl-6-pipe...		281	C13H23N5S	022362-21-6	43
3	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	43
4	2-Anthracenamine		193	C14H11N	000613-13-8	38
5	3-pyridinamine, 2-(1H-1,2,4-tria...		193	C7H7N5S	1000400-27-7	38



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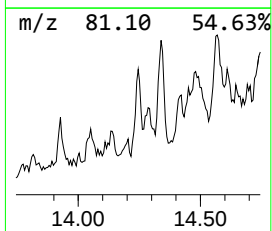
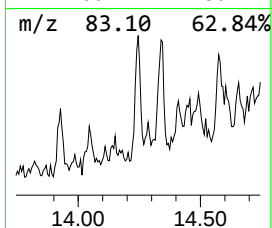
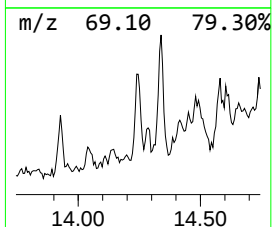
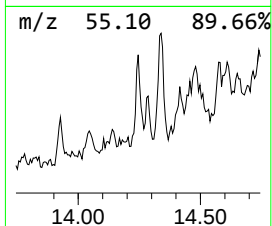
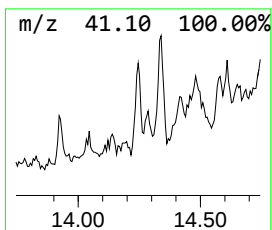
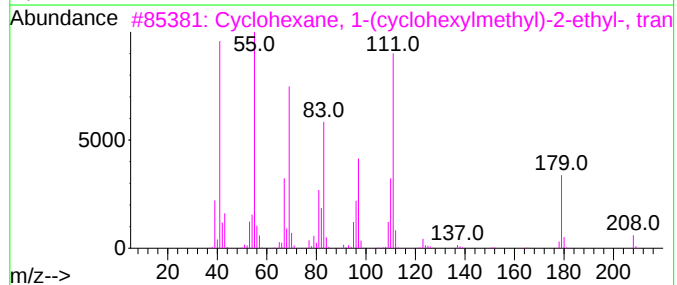
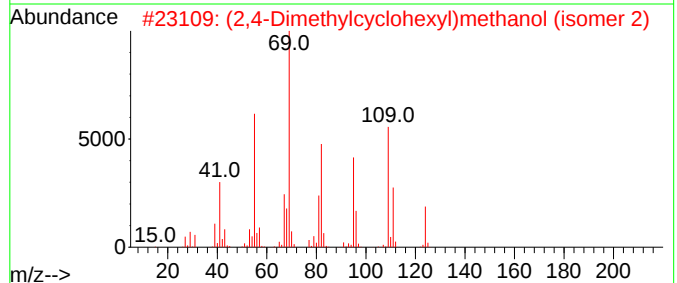
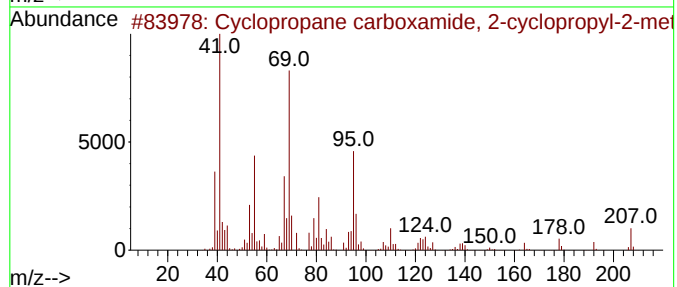
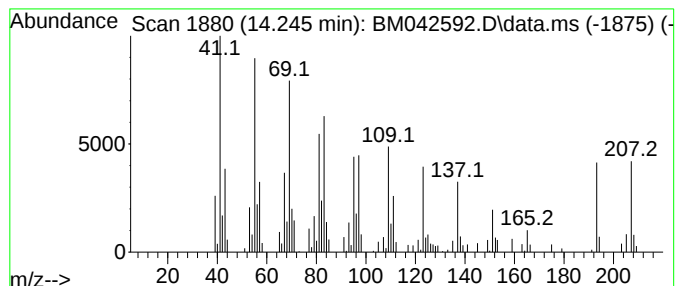
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Peak Number 4 unknown14.245 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.245	3.81 ng	111764	Acenaphthene-d10	14.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	42
2	(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-7	27
3	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-92-8	25
4	1,4-Heptadiene, 3,3,6-trimethyl-	138	C10H18	074498-89-8	22
5	Cetene	224	C16H32	000629-73-2	22



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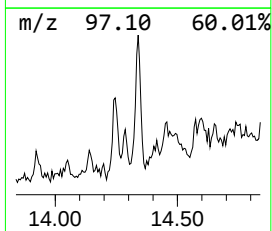
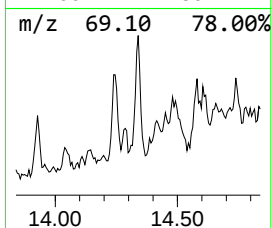
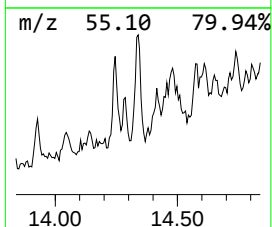
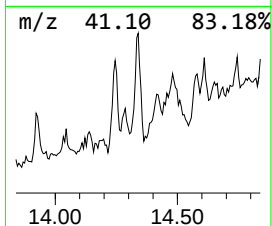
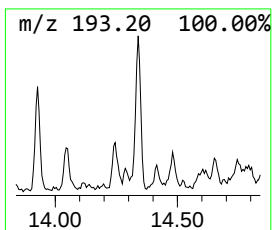
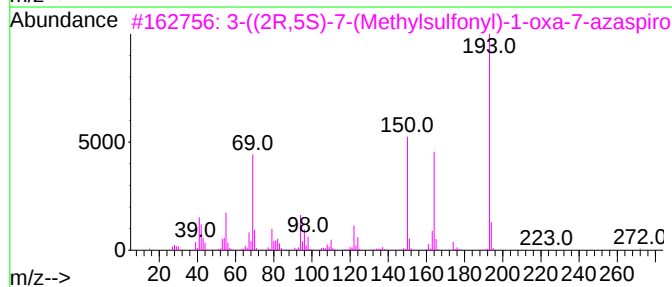
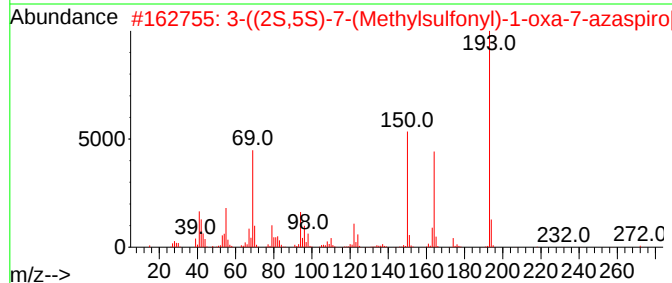
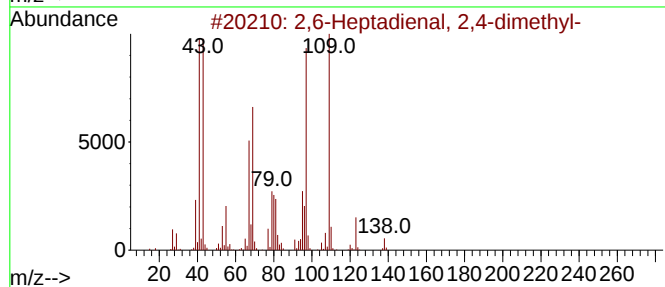
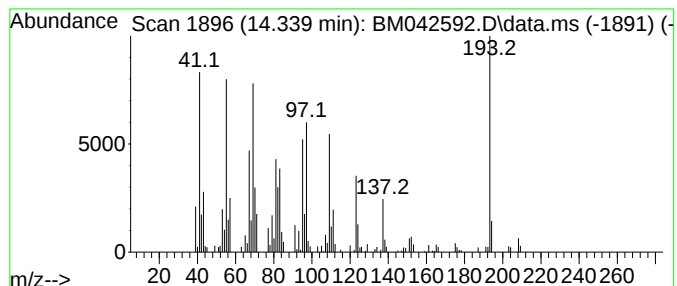
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Peak Number 5 unknown14.339 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.339	4.38 ng	128415	Acenaphthene-d10	14.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	41		
2	3-((2S,5S)-7-(Methylsulfonyl)-1-...	272	C12H20N2O3S	1465868-22-7	35		
3	3-((2R,5S)-7-(Methylsulfonyl)-1-...	272	C12H20N2O3S	1465866-05-0	35		
4	1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	35		
5	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30		



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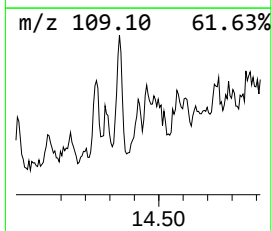
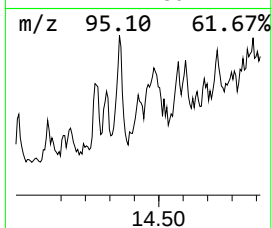
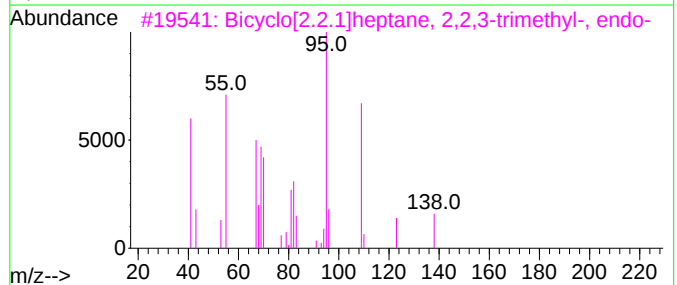
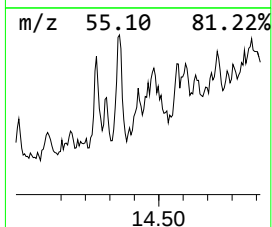
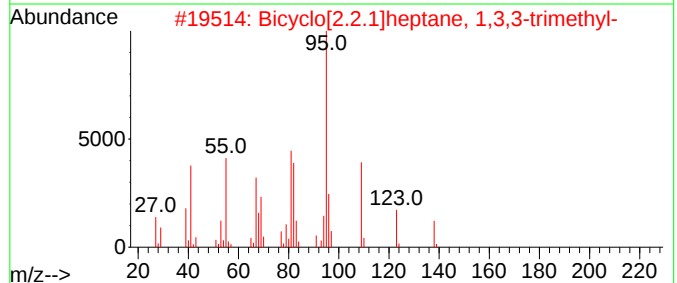
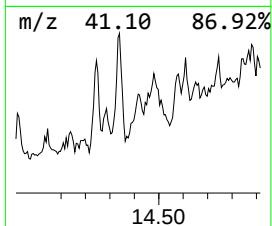
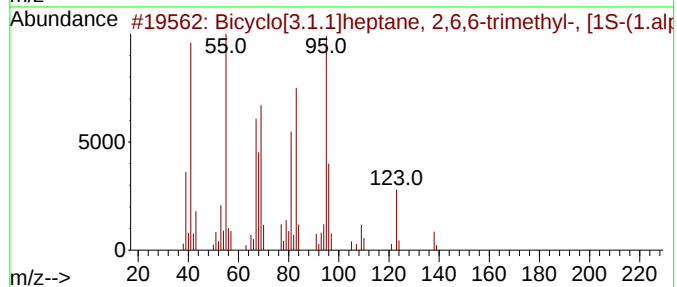
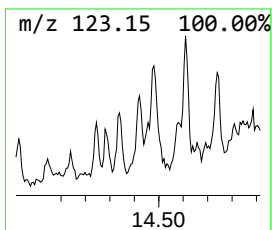
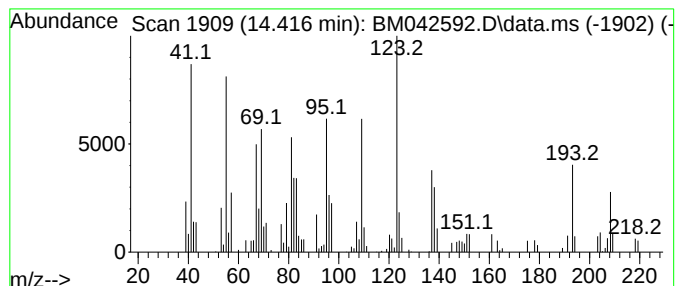
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ClientSampleId :
SP-B

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 6 unknown14.416 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.416	2.49 ng	72935	Acenaphthene-d10	14.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	41
2	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	38
3	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
4	5-(3,3-Dimethylbicyclo[2.2.1]hep...	206	C14H22O	1000497-97-7	38
5	Diallyldivinylsilane	164	C10H16Si	119901-88-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042592.D
Acq On : 04 Nov 2023 15:29
Operator : MA/JU
Sample : 05234-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-B

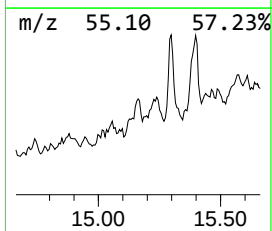
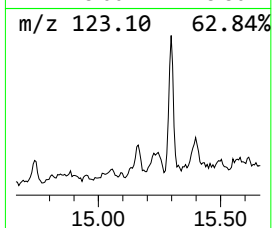
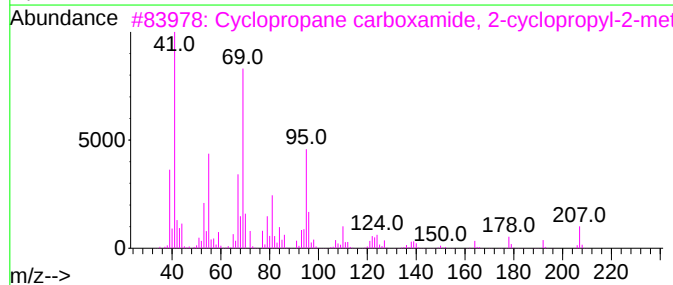
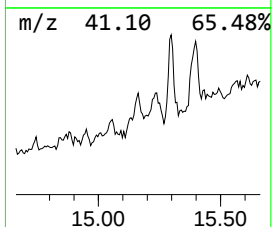
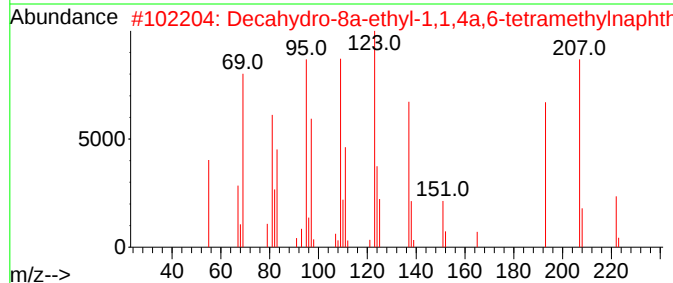
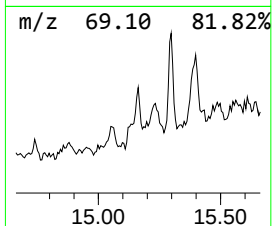
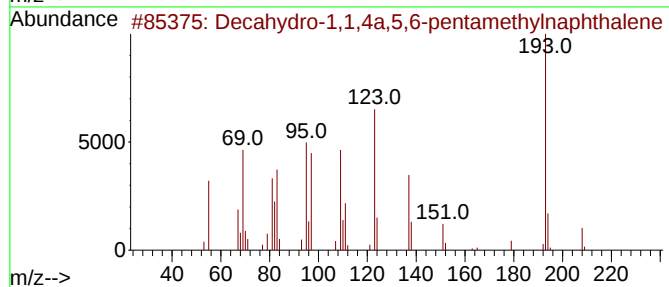
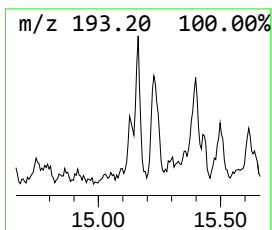
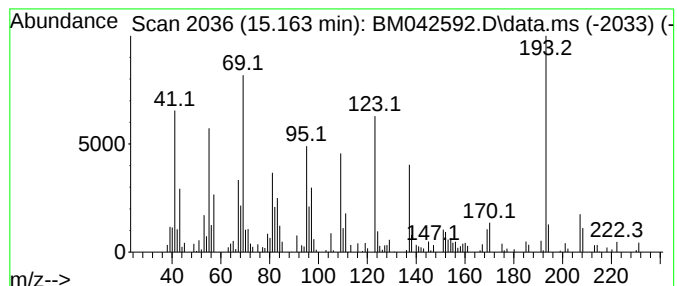
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.163 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.31 ng	67887	Acenaphthene-d10	14.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	46
3			Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	38
4			Desoxy-minoxidyl	193	C9H15N5	024867-26-3	30
5			Cyclohexanone, 2-(1-mercapto-1-m...	186	C10H18OS	033281-91-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042592.D
Acq On : 04 Nov 2023 15:29
Operator : MA/JU
Sample : 05234-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

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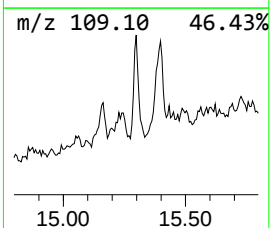
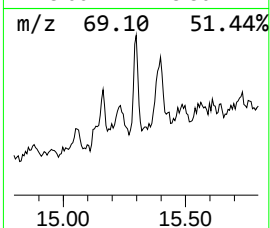
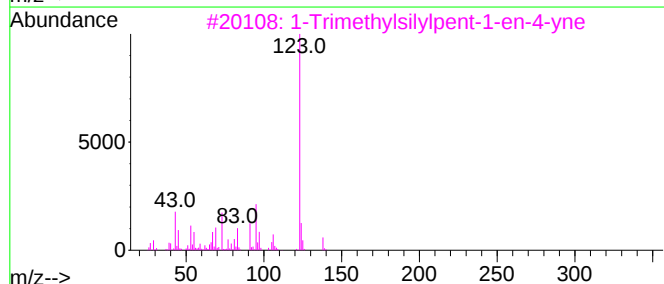
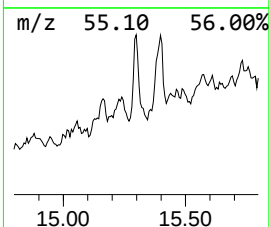
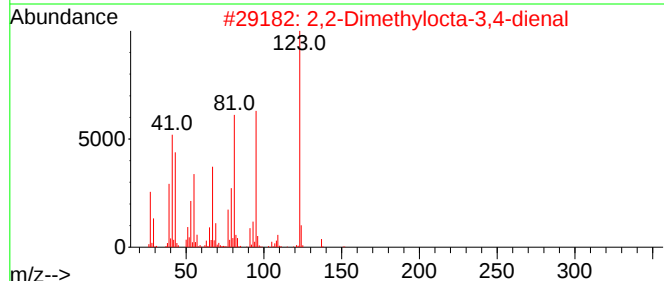
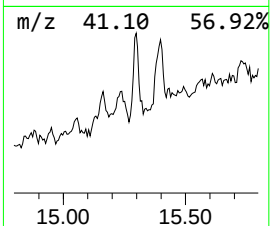
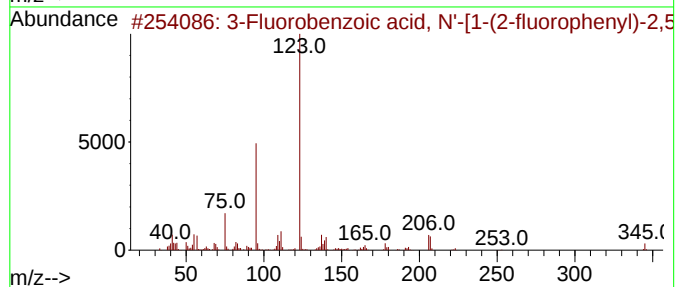
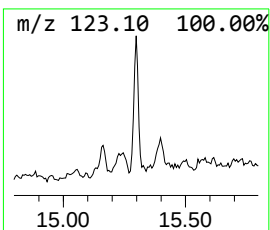
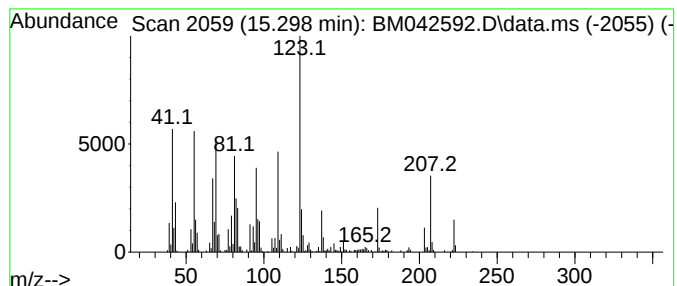
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.298 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	9.26 ng	271548	Acenaphthene-d10	14.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Fluorobenzoic acid, N'-[1-(2-f...	345	C17H13F2N3O3	1000304-52-3	38
2		2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	38
3		1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	38
4		Diallyldivinylsilane	164	C10H16Si	119901-88-1	38
5		4-Fluorobenzoic acid, 2-methylph...	230	C14H11FO2	1000299-05-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042592.D
Acq On : 04 Nov 2023 15:29
Operator : MA/JU
Sample : 05234-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-B

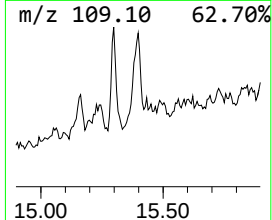
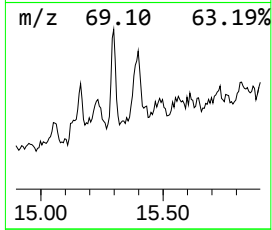
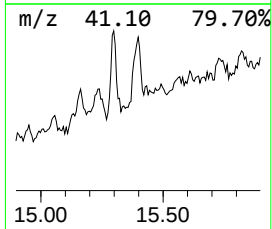
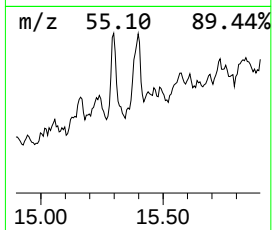
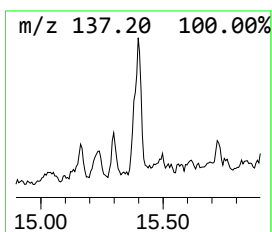
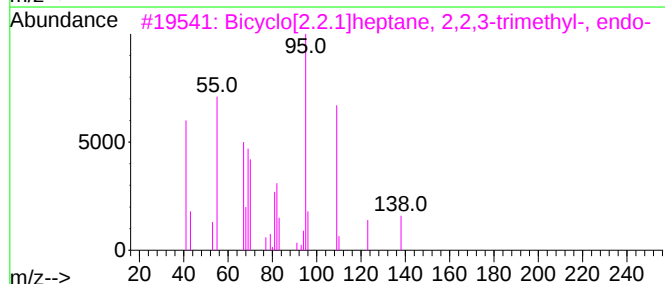
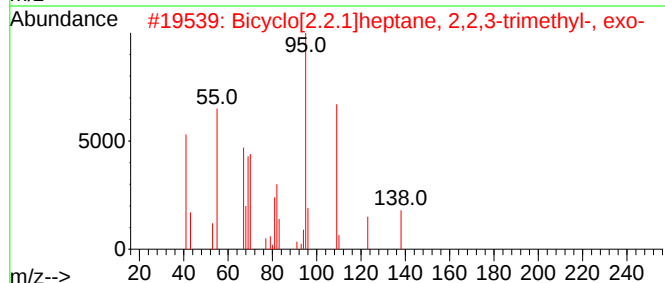
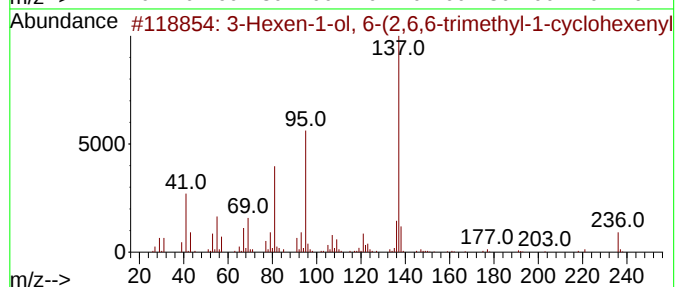
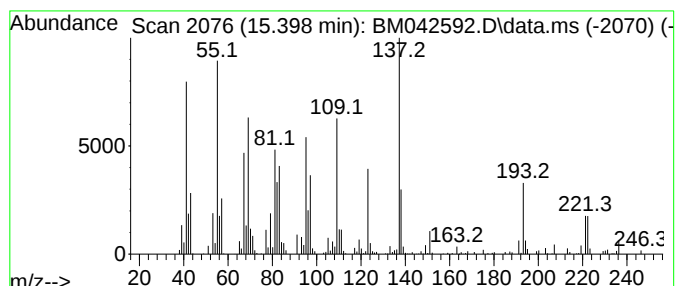
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.398 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	8.26 ng	242187	Acenaphthene-d10	14.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Hexen-1-ol, 6-(2,6,6-trimethyl...	236	C16H28O	110202-07-8	30
2		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	30
3		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	30
4		2-Pentenoic acid, 3-methyl-5-(2,...	236	C15H24O2	1000196-81-2	27
5		2-Dodecyne	166	C12H22	000629-49-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042592.D
Acq On : 04 Nov 2023 15:29
Operator : MA/JU
Sample : 05234-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-B

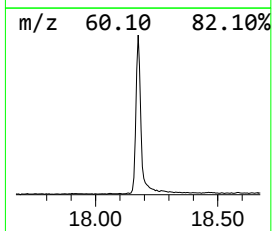
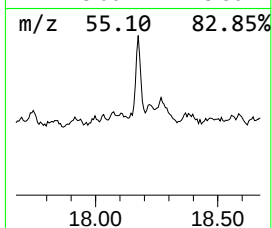
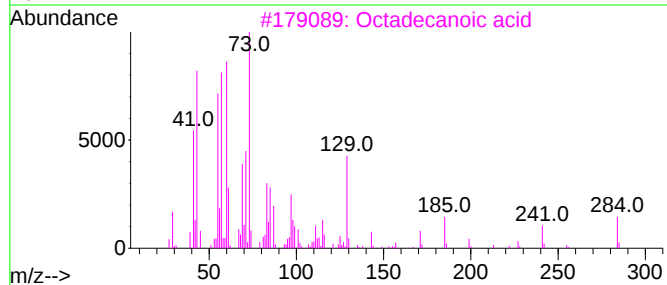
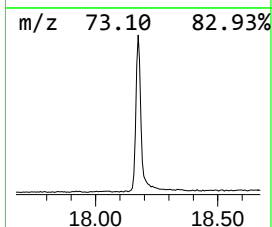
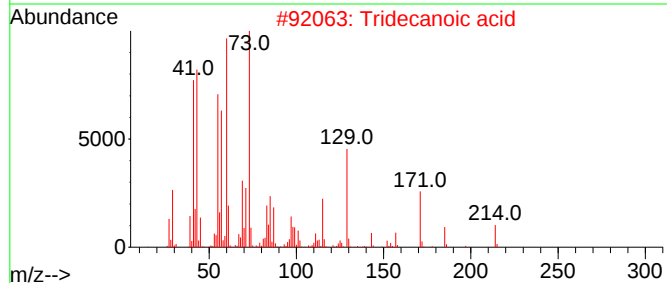
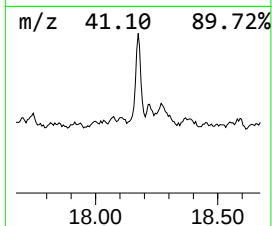
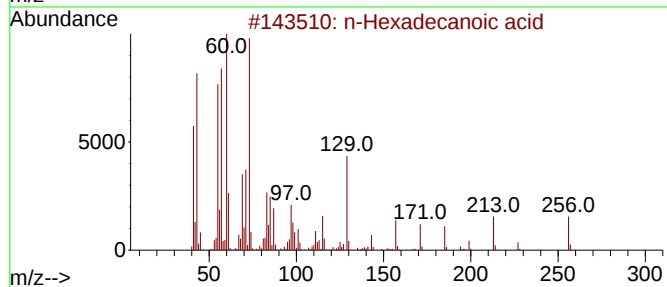
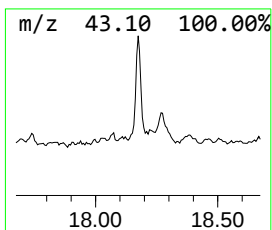
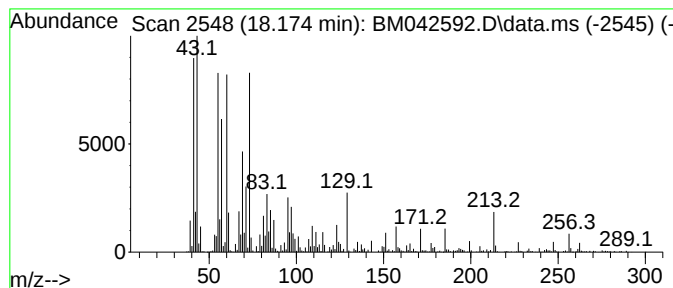
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	27.20 ng	1065020	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	86
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042592.D
Acq On : 04 Nov 2023 15:29
Operator : MA/JU
Sample : 05234-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-B

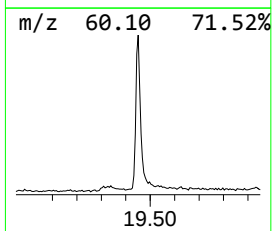
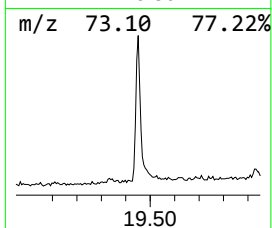
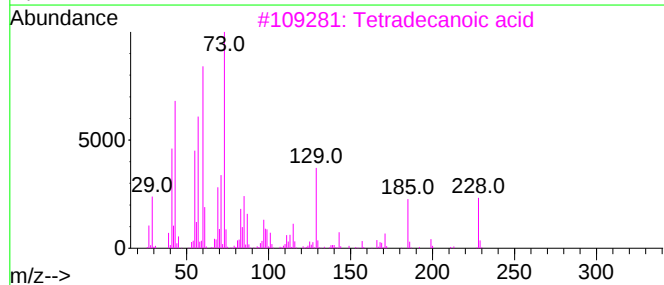
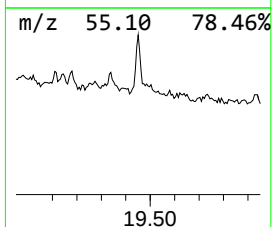
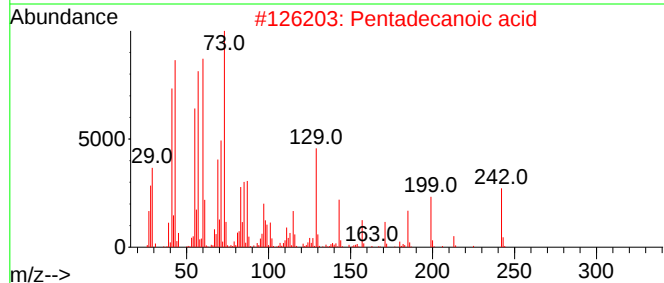
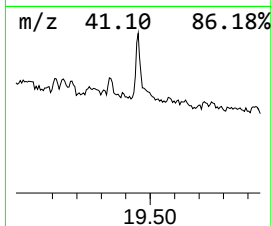
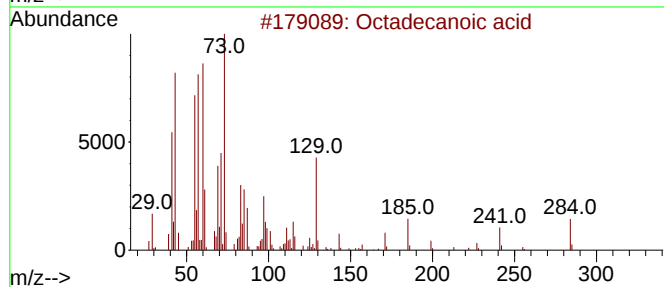
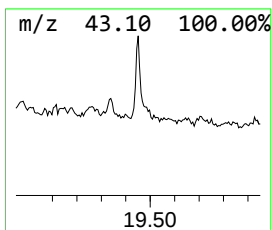
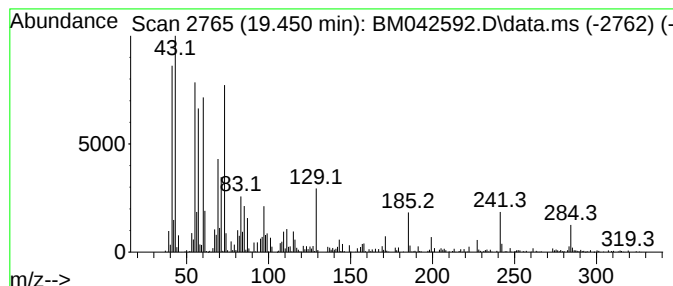
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	9.14 ng	360883	Chrysene-d12	21.503

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	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042592.D
Acq On : 04 Nov 2023 15:29
Operator : MA/JU
Sample : 05234-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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
Ethanol, 2-(2-e...	7.510	2.7	ng	42024	1	7.910	308170	20.0
2,4,7,9-Tetrame...	13.410	30.5	ng	894893	3	14.563	586528	20.0
1H-Indene, octa...	13.927	2.1	ng	60667	3	14.563	586528	20.0
unknown14.245	14.245	3.8	ng	111764	3	14.563	586528	20.0
unknown14.339	14.339	4.4	ng	128415	3	14.563	586528	20.0
unknown14.416	14.416	2.5	ng	72935	3	14.563	586528	20.0
unknown15.163	15.163	2.3	ng	67887	3	14.563	586528	20.0
unknown15.298	15.298	9.3	ng	271548	3	14.563	586528	20.0
unknown15.398	15.398	8.3	ng	242187	3	14.563	586528	20.0
n-Hexadecanoic ...	18.174	27.2	ng	1065020	4	17.321	782959	20.0
Octadecanoic acid	19.451	9.1	ng	360883	5	21.503	789541	20.0