

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
 Data File : BG051096.D
 Acq On : 17 Nov 2021 17:41
 Operator : CG/JU
 Sample : M4673-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RO-72-11933

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_G\Methods\8270-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051096.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.762	380	387	397	rBV	492213	844840	5.33%	1.993%
2	7.377	653	662	679	rBV	505155	938756	5.93%	2.215%
3	8.223	800	806	818	rVB	146095	258212	1.63%	0.609%
4	9.399	998	1006	1015	rBV	329203	624933	3.95%	1.474%
5	11.050	1281	1287	1294	rBV	200378	367227	2.32%	0.866%
6	13.300	1666	1670	1674	rVB4	131478	202825	1.28%	0.479%
7	13.359	1676	1680	1688	rVB	309245	494632	3.12%	1.167%
8	13.476	1694	1700	1708	rVB	773018	1315603	8.31%	3.104%
9	13.635	1722	1727	1734	rBV6	327830	803851	5.08%	1.896%
10	14.275	1831	1836	1839	rBV	1406107	2314871	14.62%	5.461%
11	14.310	1839	1842	1845	rVB2	805476	1054404	6.66%	2.488%
12	14.592	1884	1890	1895	rBV5	1151825	2570113	16.23%	6.064%
13	14.681	1900	1905	1911	rVB	2133394	3723658	23.51%	8.785%
14	14.822	1923	1929	1941	rBV8	1095605	3257550	20.57%	7.685%
15	15.356	2016	2020	2026	rBV5	767924	1585288	10.01%	3.740%
16	15.656	2066	2071	2078	rVB	2310871	3691646	23.31%	8.710%
17	16.608	2225	2233	2237	rBV2	6886309	15838273	100.00%	37.366%
18	22.783	3279	3284	3291	rVB	890138	1590583	10.04%	3.753%
19	25.327	3713	3717	3726	rVB2	130695	309054	1.95%	0.729%
20	25.826	3798	3802	3812	rVB4	75644	195038	1.23%	0.460%
21	26.467	3904	3911	3922	rVB2	132865	404965	2.56%	0.955%

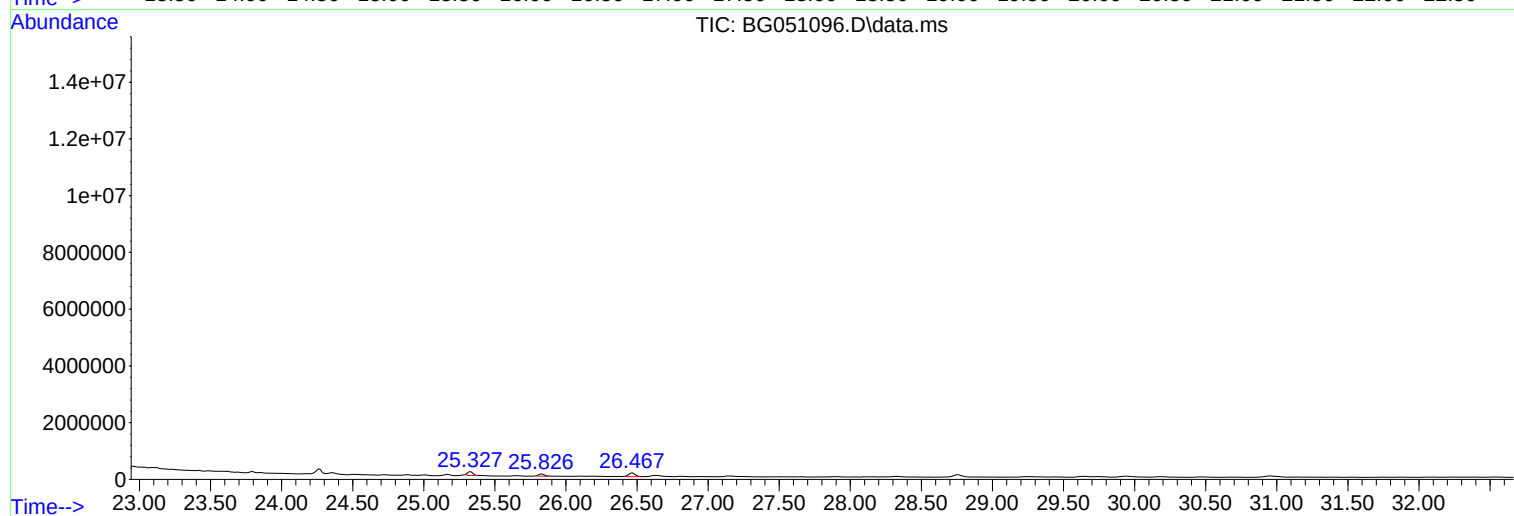
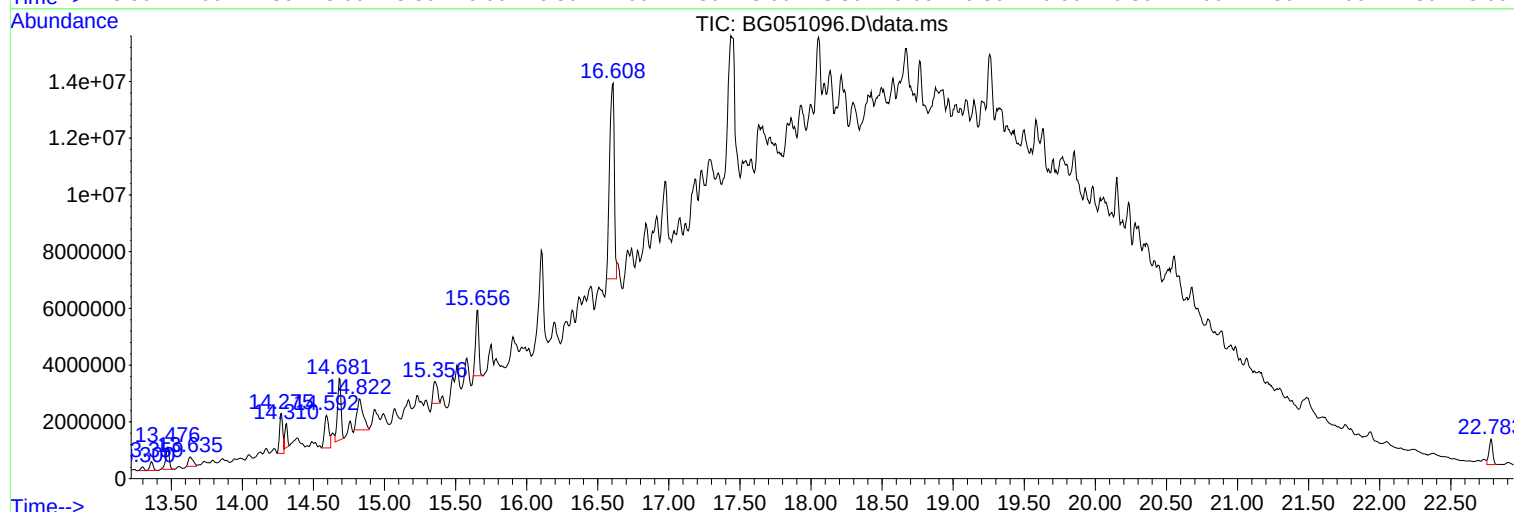
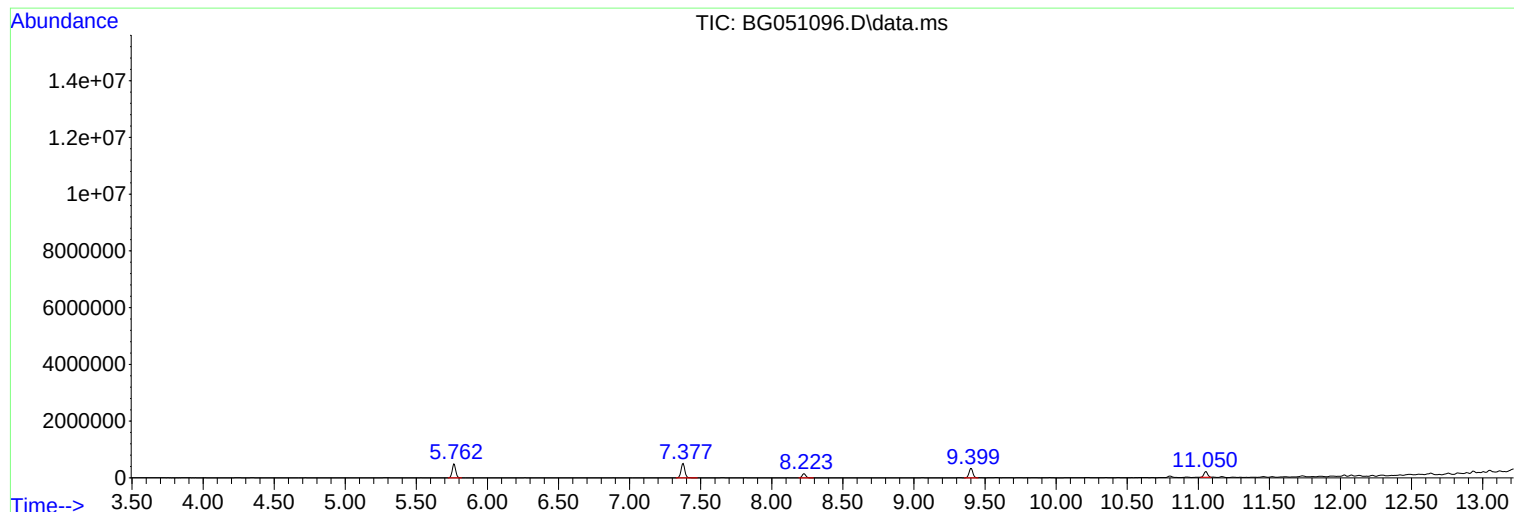
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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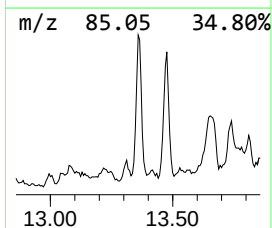
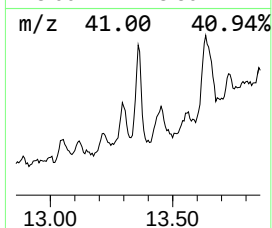
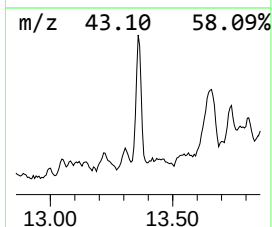
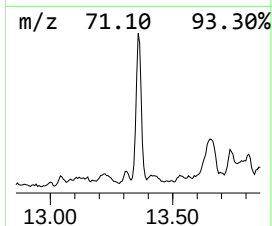
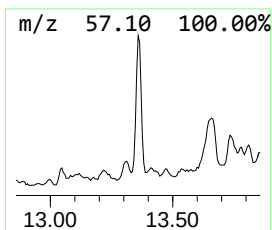
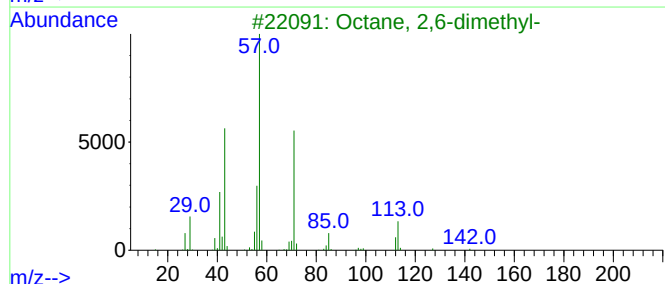
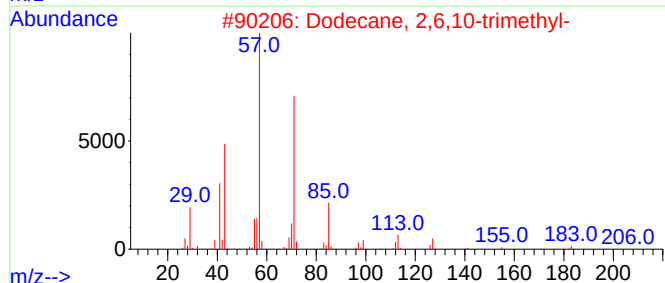
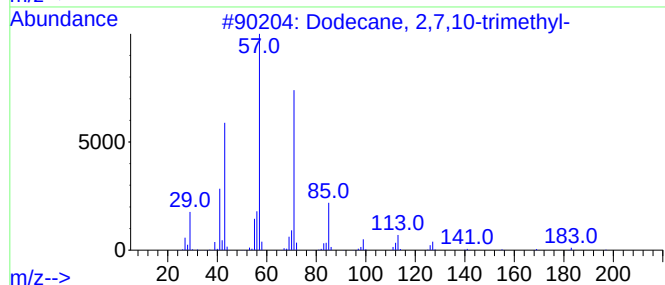
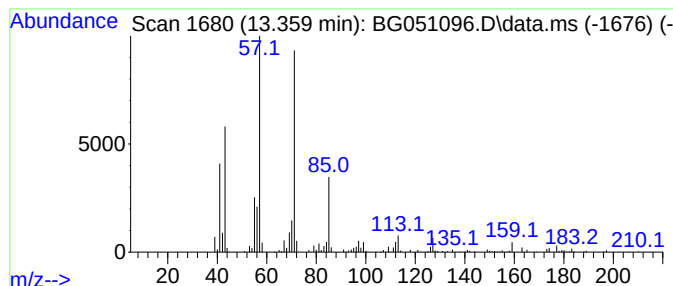
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Dodecane, 2,7,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.359	3.04 ng	494632	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	91
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	90
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4			Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	58
5			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	53



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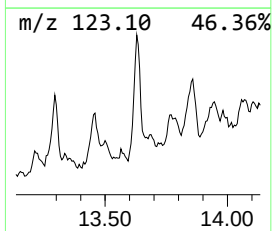
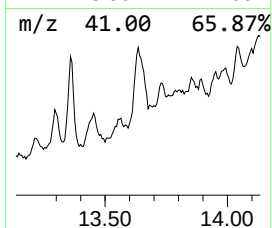
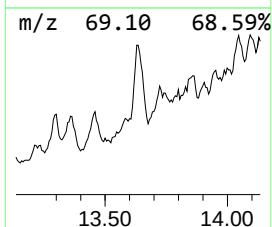
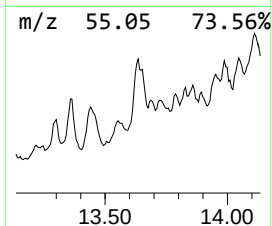
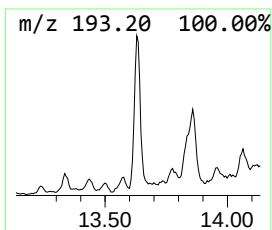
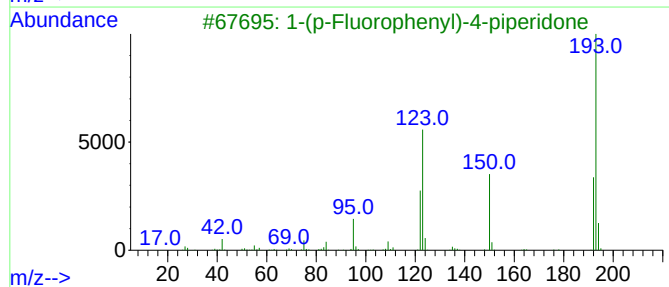
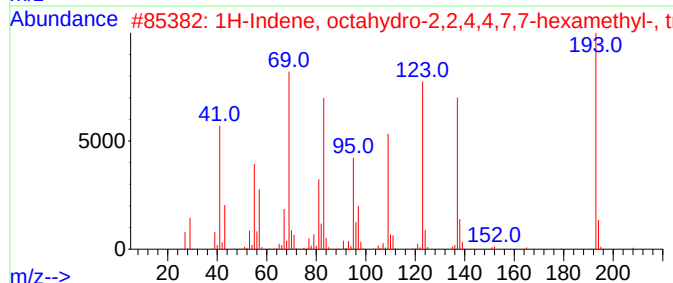
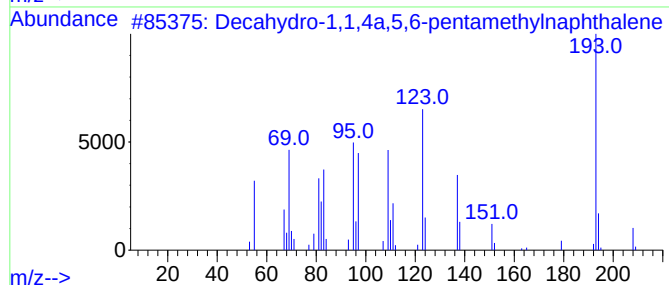
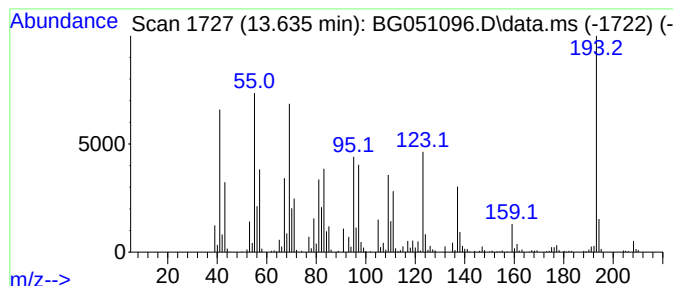
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown13.635 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.635	4.94 ng	803851	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	30
5			3-((2R,5S)-7-(Cyclohexylsulfonyl)...	340	C17H28N2O3S	1000483-82-6	27



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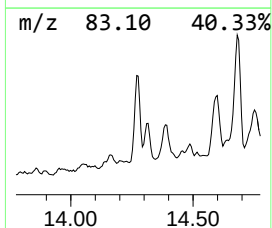
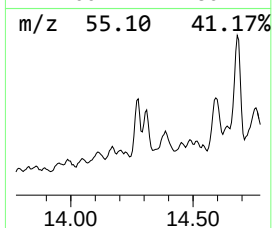
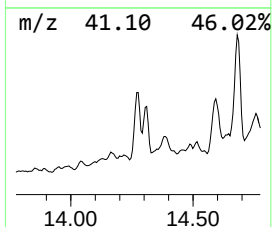
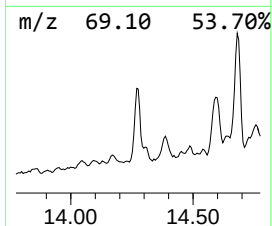
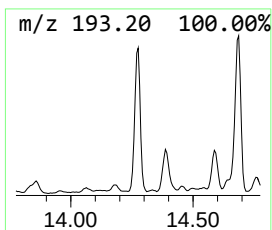
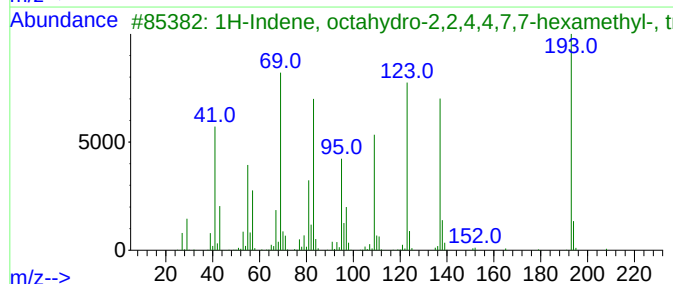
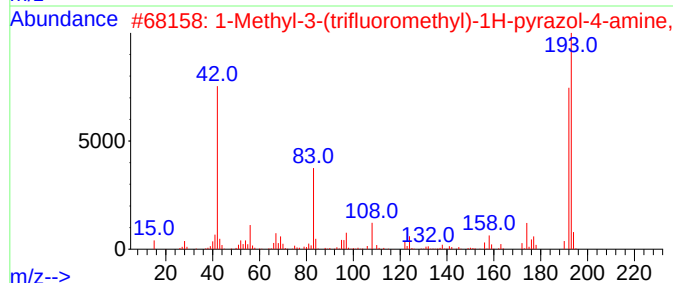
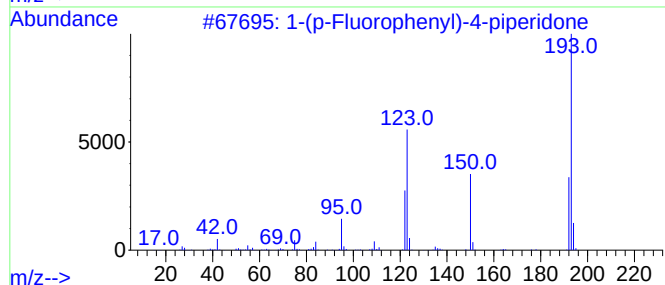
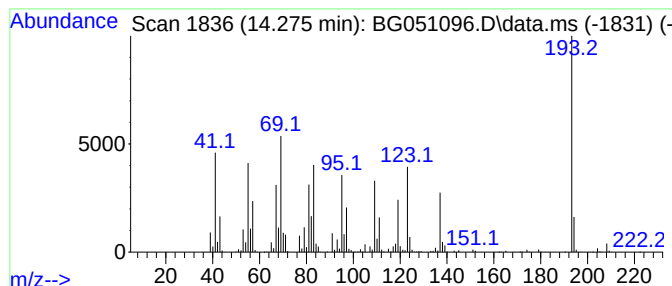
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.275 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.275	14.21 ng	2314870	Acenaphthene-d10		14.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
2		1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38
3		1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4		2-Anthracenamine	193	C14H11N	000613-13-8	30
5		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30



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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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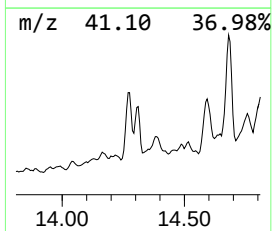
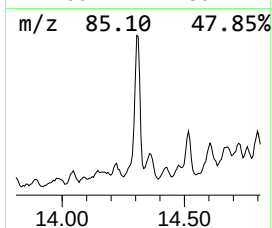
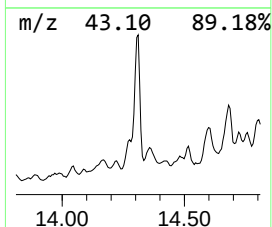
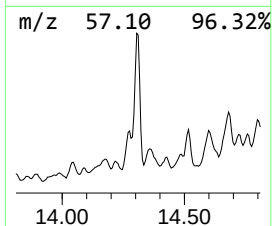
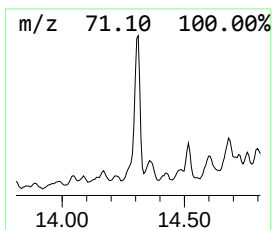
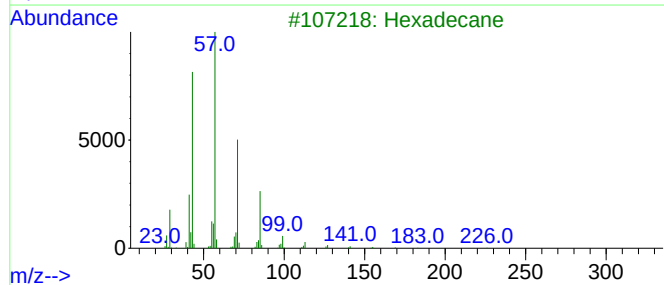
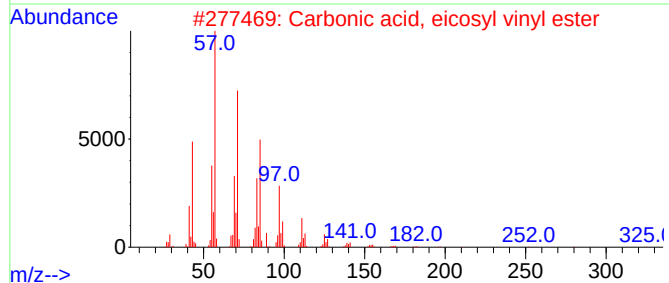
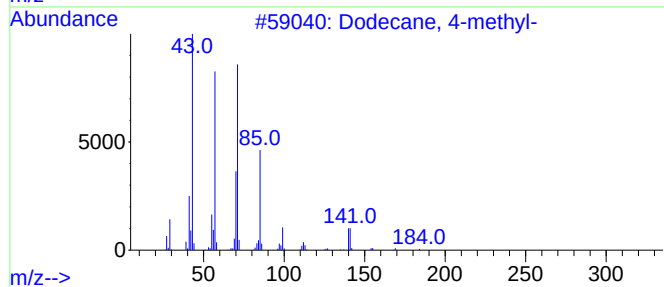
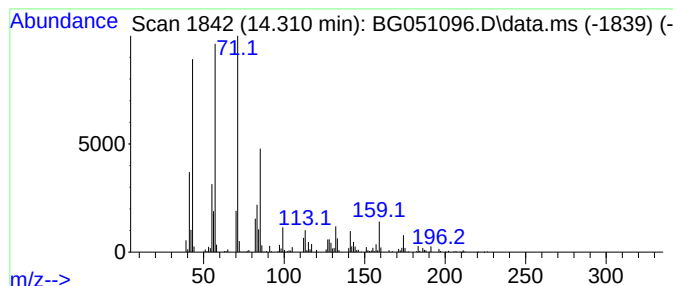
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Peak Number 4 Dodecane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	6.47 ng	1054400	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4-methyl-	184	C13H28	006117-97-1	64
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	64
3			Hexadecane	226	C16H34	000544-76-3	62
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58
5			Tridecane, 6-propyl-	226	C16H34	055045-10-8	58



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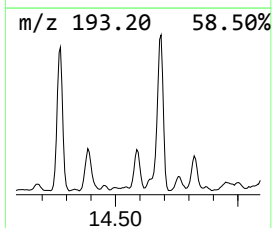
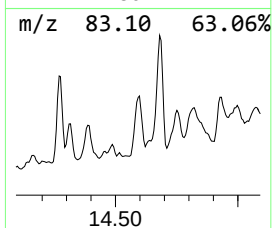
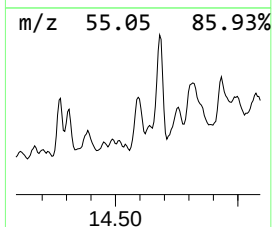
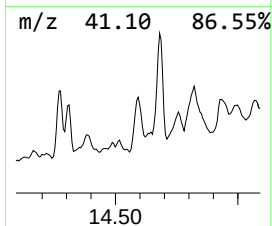
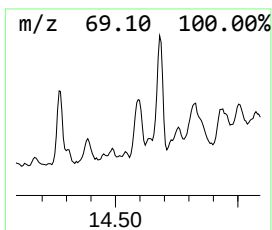
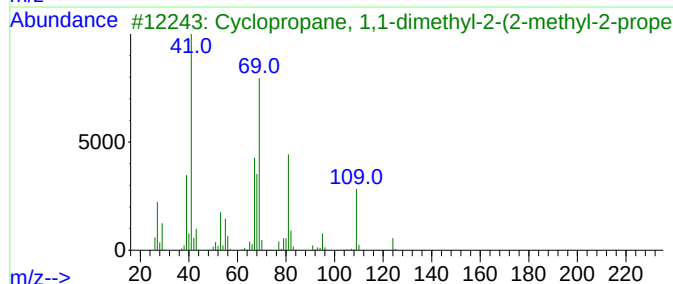
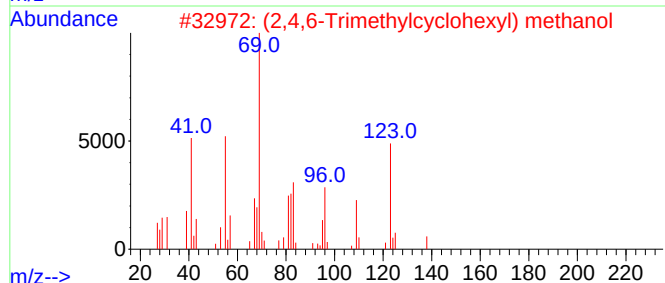
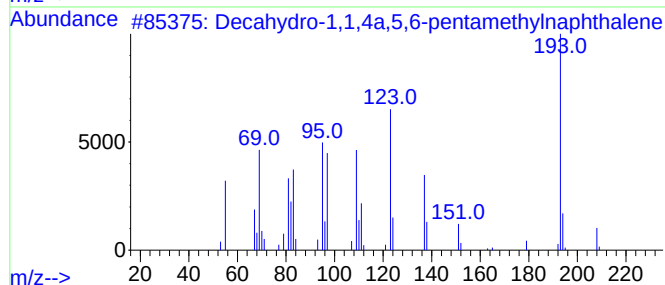
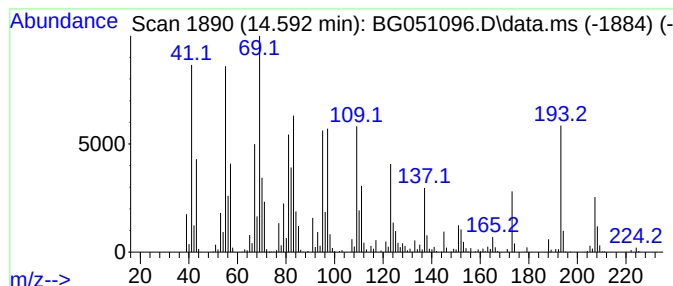
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.592	15.78 ng	2570110	Acenaphthene-d10		14.863	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	91
2	(2,4,6-Trimethylcyclohexyl) meth...		156	C10H20O	013702-56-2	27
3	Cyclopropane, 1,1-dimethyl-2-(2-...		124	C9H16	069147-03-1	25
4	1-Dodecanol		186	C12H26O	000112-53-8	25
5	Oxiranecarboxaldehyde, 3-methyl-...		168	C10H16O2	016996-12-6	22



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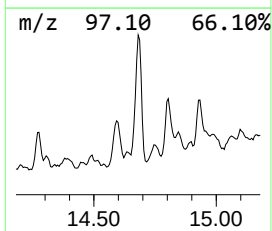
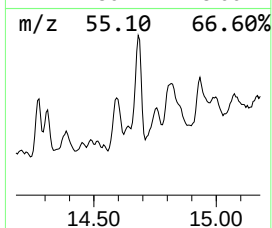
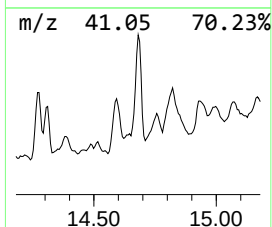
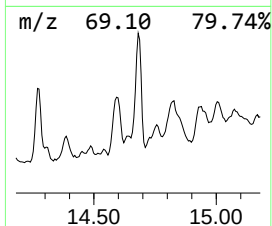
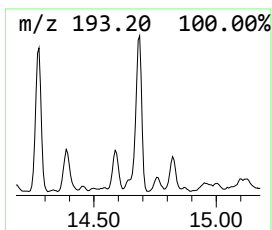
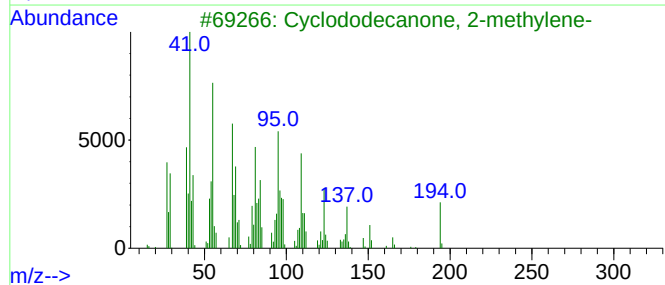
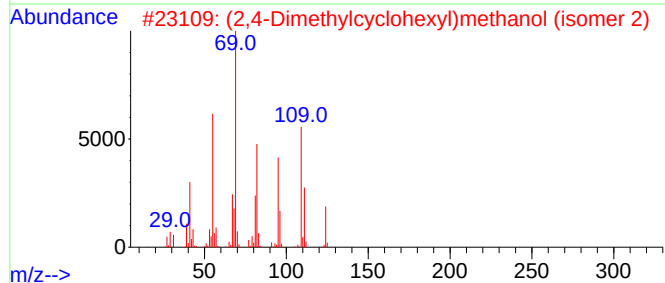
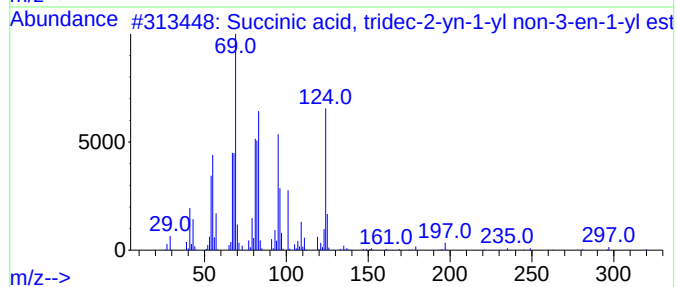
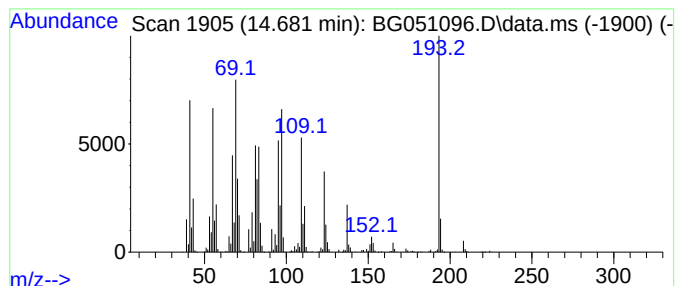
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.681 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.681	22.86 ng	3723660	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, tridec-2-yn-1-yl ...	420	C26H44O4	1010391-10-5	30
2			(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-7	27
3			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	25
4			3-Propylglutaric acid, monomethy...	188	C9H16O4	1000254-25-9	22
5			(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
Operator : CG/JU
Sample : M4673-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

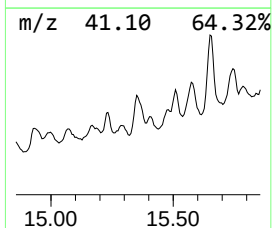
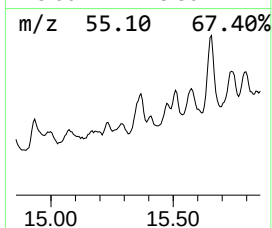
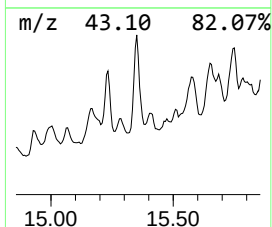
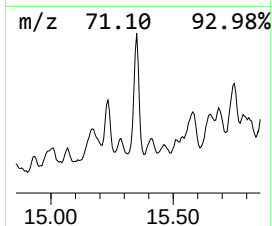
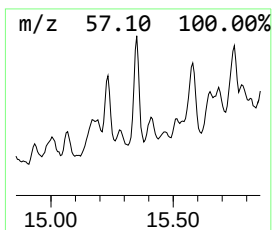
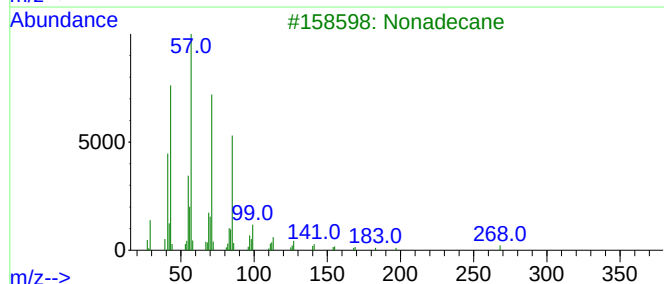
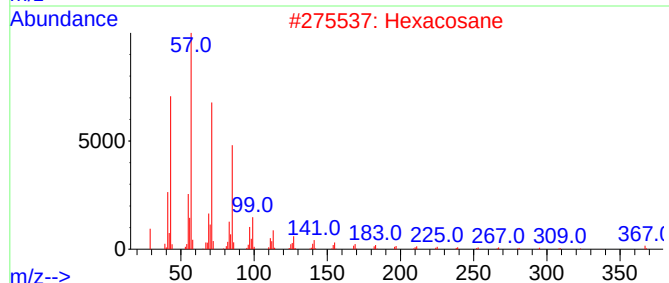
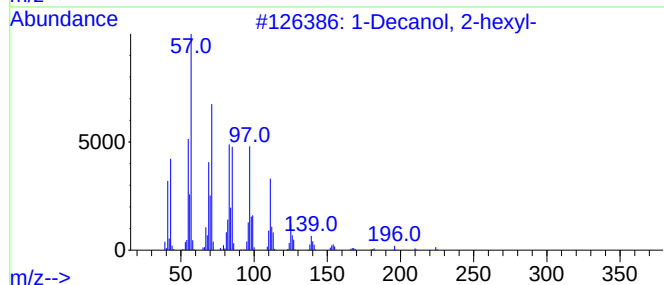
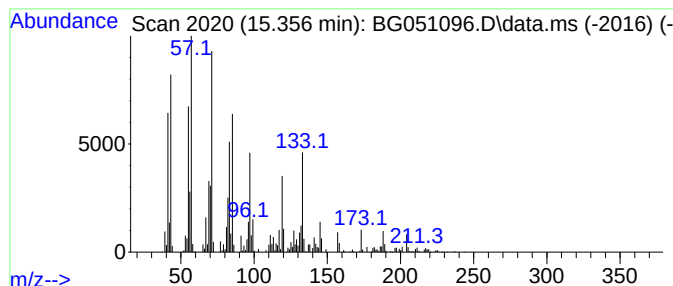
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.356	9.73 ng	1585290	Acenaphthene-d10		14.863	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	52
2	Hexacosane		366	C26H54	000630-01-3	38
3	Nonadecane		268	C19H40	000629-92-5	38
4	Tridecane, 6-propyl-		226	C16H34	055045-10-8	38
5	1,3-Dimethylcyclopentanol		114	C7H14O	019550-46-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
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Sample : M4673-01
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ClientSampleId :
RO-72-11933

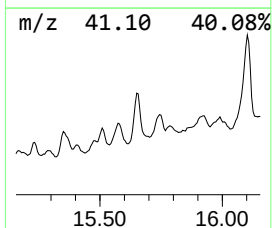
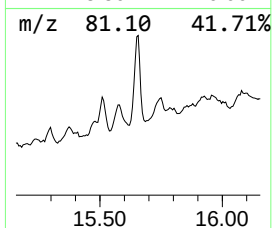
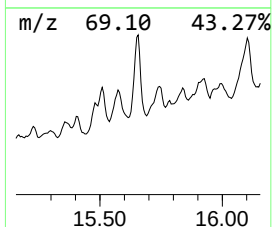
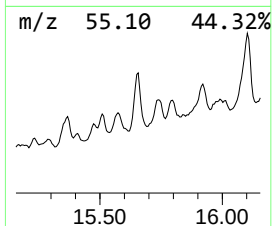
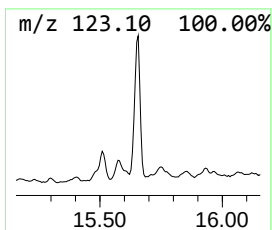
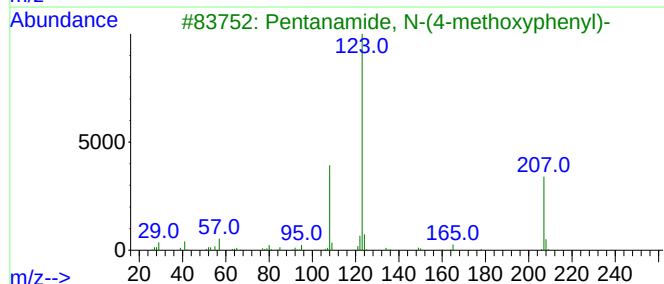
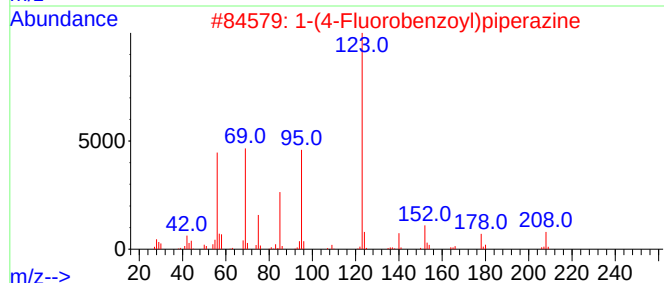
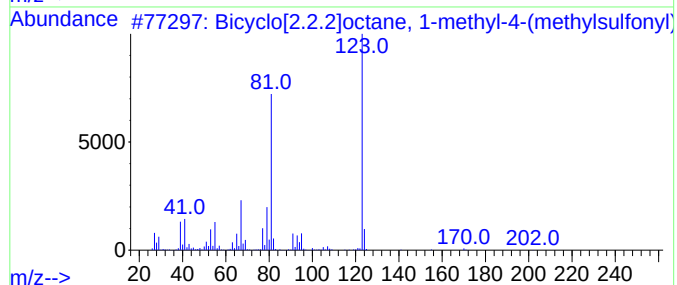
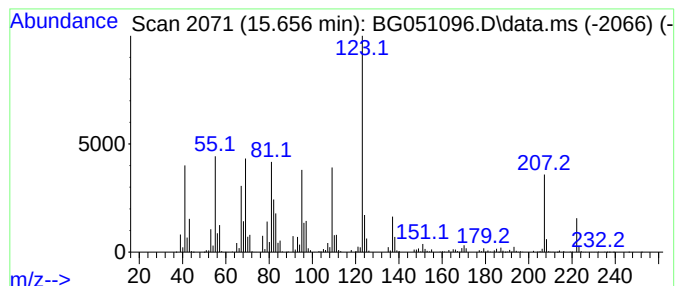
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.656 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	22.67 ng	3691650	Acenaphthene-d10	14.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[2.2.2]octane, 1-methyl-4...	202	C10H18O2S	069855-48-7	46
2		1-(4-Fluorobenzoyl)piperazine	208	C11H13FN2O	102391-98-0	43
3		Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
4		2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	43
5		Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
Operator : CG/JU
Sample : M4673-01
Misc :
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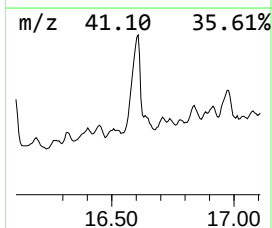
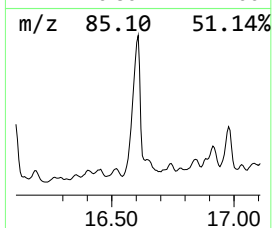
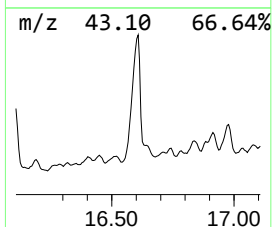
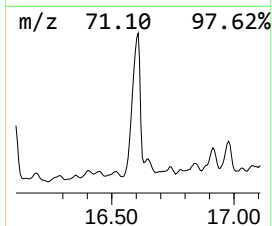
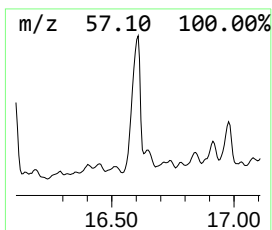
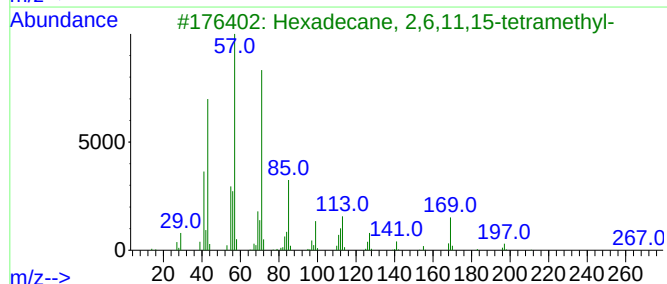
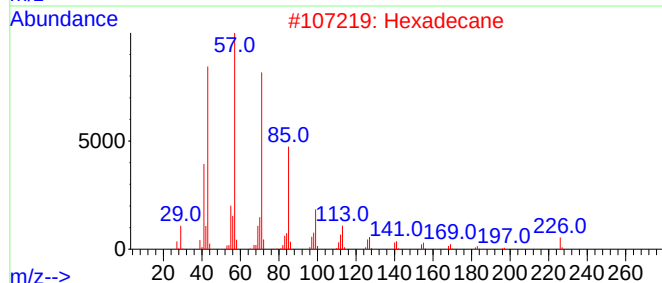
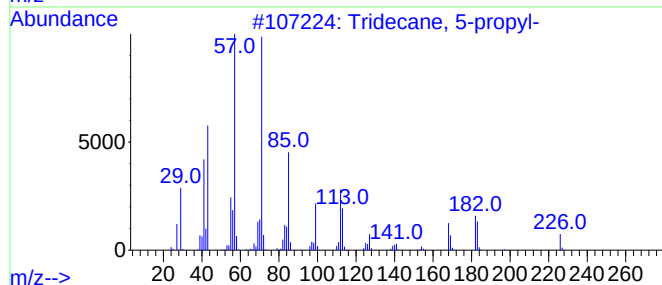
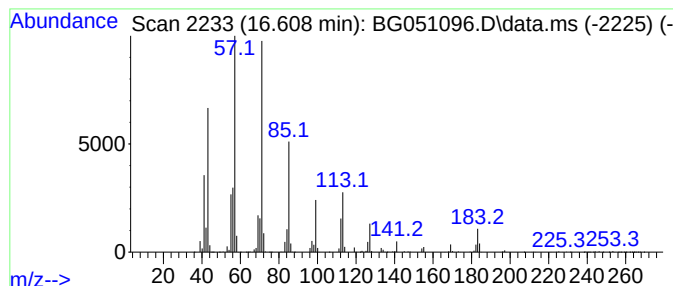
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.608	20.00 ng	15838300	Phenanthrene-d10	17.648

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	78
2			Hexadecane	226	C16H34	000544-76-3	72
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	64
4			Octane, 2-methyl-	128	C9H20	003221-61-2	59
5			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
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Sample : M4673-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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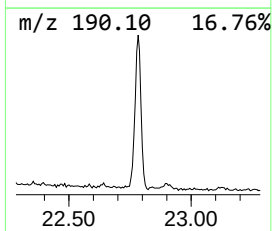
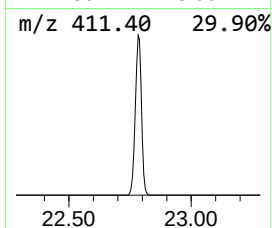
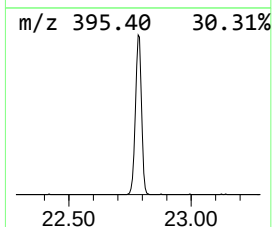
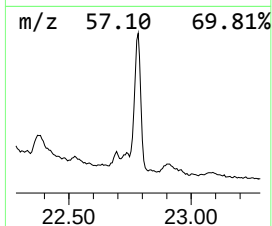
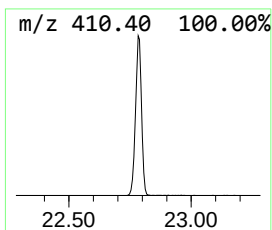
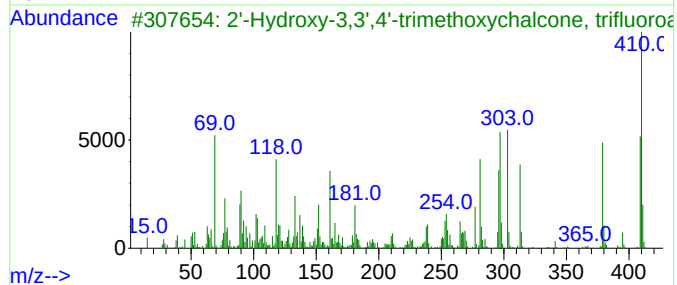
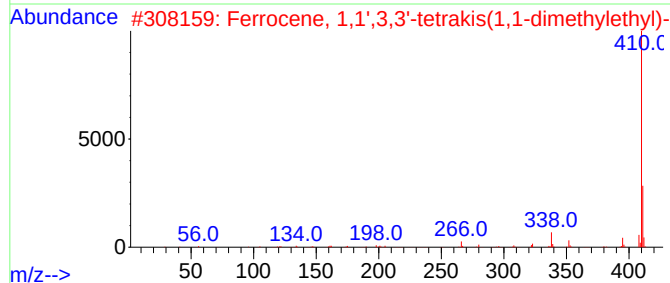
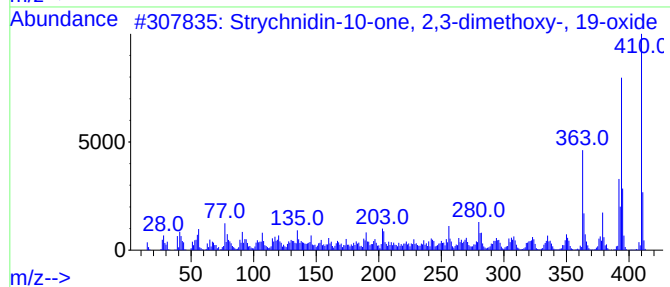
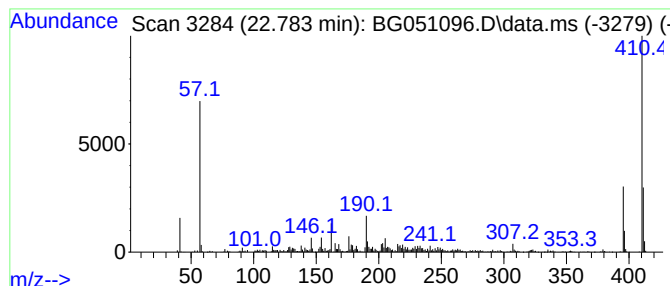
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Strychnidin-10-one, 2,3-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.783	20.00 ng	1590580	Chrysene-d12	21.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Strychnidin-10-one, 2,3-dimethox...	410	C23H26N2O5	017301-81-4	72
2			Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	52
3			2'-Hydroxy-3,3',4'-trimethoxycha...	410	C20H17F3O6	1010453-84-8	49
4			3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	42
5			Di(trimethylene-1-naphthyl)siloxane	410	C26H26OSi2	093241-94-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
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Sample : M4673-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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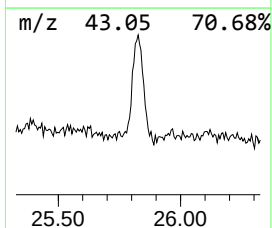
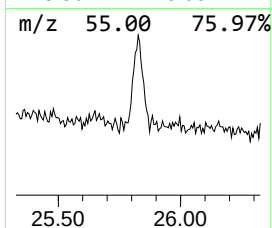
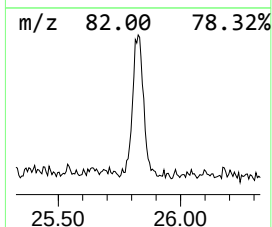
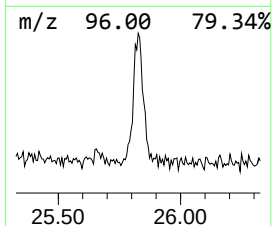
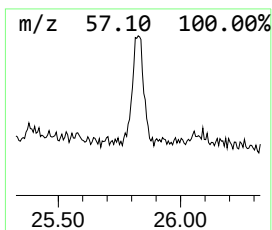
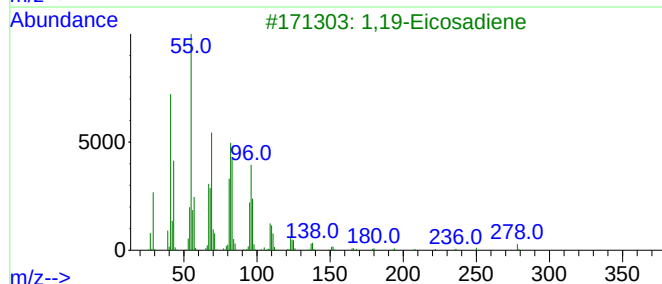
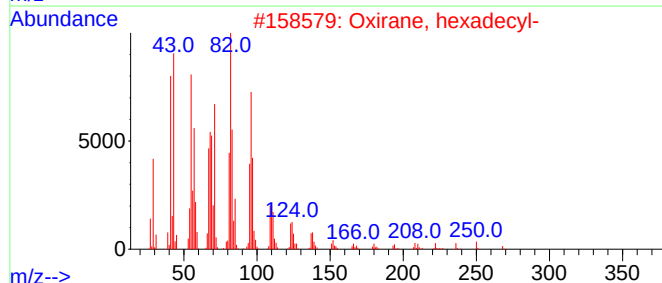
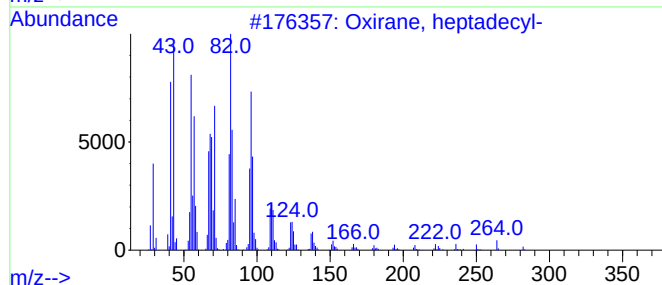
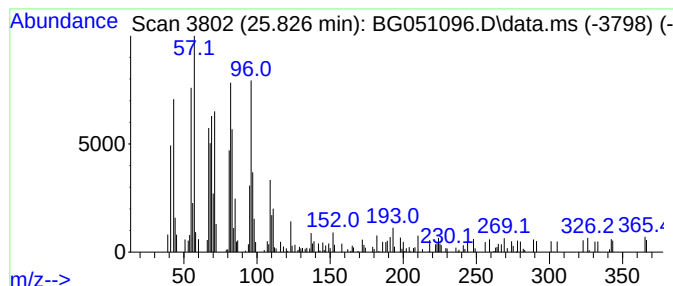
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.826	12.62 ng	195038	Perylene-d12	25.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	96
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3			1,19-Eicosadiene	278	C20H38	014811-95-1	89
4			Tetracosanal	352	C24H48O	057866-08-7	87
5			Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
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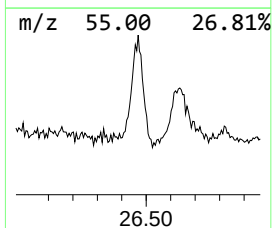
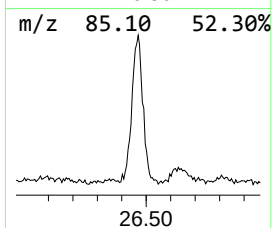
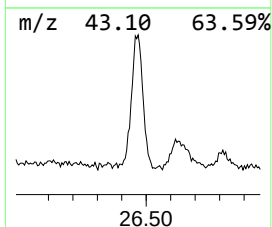
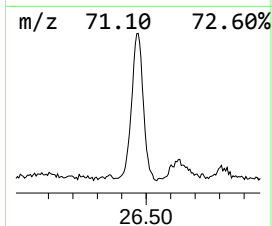
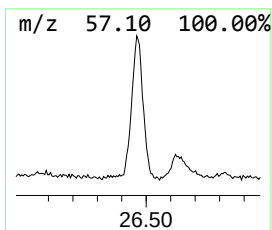
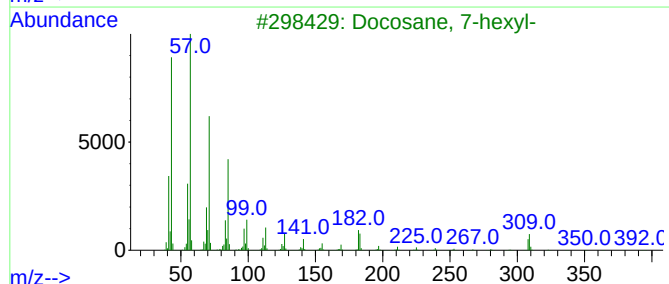
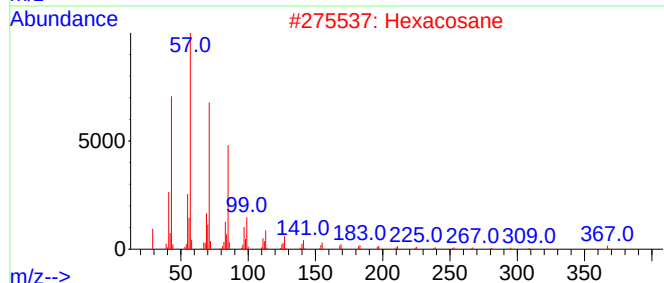
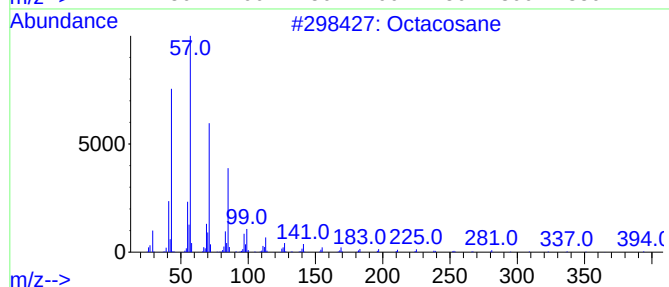
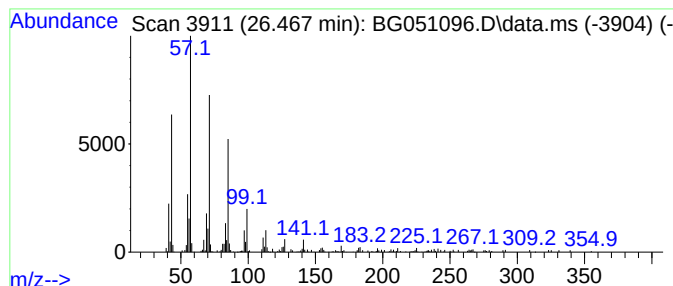
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.467	26.21 ng	404965	Perylene-d12	25.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Hexacosane	366	C26H54	000630-01-3	87
3			Docosane, 7-hexyl-	394	C28H58	055373-86-9	86
4			Hexatriacontane	507	C36H74	000630-06-8	83
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111721\
Data File : BG051096.D
Acq On : 17 Nov 2021 17:41
Operator : CG/JU
Sample : M4673-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-72-11933

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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
Dodecane, 2,7,1...	13.359	3.0	ng	494632	3	14.863	3257550	20.0
unknown13.635	13.635	4.9	ng	803851	3	14.863	3257550	20.0
unknown14.275	14.275	14.2	ng	2314870	3	14.863	3257550	20.0
Dodecane, 4-met...	14.310	6.5	ng	1054400	3	14.863	3257550	20.0
Decahydro-1,1,4...	14.592	15.8	ng	2570110	3	14.863	3257550	20.0
unknown14.681	14.681	22.9	ng	3723660	3	14.863	3257550	20.0
1-Decanol, 2-he...	15.356	9.7	ng	1585290	3	14.863	3257550	20.0
unknown15.656	15.656	22.7	ng	3691650	3	14.863	3257550	20.0
Tridecane, 5-pr...	16.608	20.0	ng	15838300	4	17.648	15838300	20.0
Strychnidin-10-...	22.783	20.0	ng	1590580	5	21.937	1590580	20.0
Oxirane, heptad...	25.826	12.6	ng	195038	6	25.321	309054	20.0
Octacosane	26.467	26.2	ng	404965	6	25.321	309054	20.0