

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
 Data File : BF132339.D
 Acq On : 06 Feb 2023 15:48
 Operator : CG\JU
 Sample : 01440-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-1

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_F\Methods\8270-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132339.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.690	308	315	321	rBV	69827	72854	1.31%	0.208%
2	5.284	408	416	425	rBV	553789	615036	11.09%	1.759%
3	5.672	477	482	485	rBV	2040513	2018541	36.40%	5.773%
4	6.660	645	650	661	rVB	1475586	1309106	23.61%	3.744%
5	7.048	713	716	720	rVB	1192268	973948	17.56%	2.785%
6	7.613	807	812	816	rBV	2525384	2743021	49.47%	7.845%
7	8.336	931	935	938	rBV	1714506	1329320	23.97%	3.802%
8	9.419	1114	1119	1122	rBV	5904641	5544948	100.00%	15.858%
9	10.101	1231	1235	1238	rBV	1936559	1552838	28.00%	4.441%
10	10.283	1260	1266	1273	rBV	98180	105211	1.90%	0.301%
11	10.813	1354	1356	1360	rVB	291124	254478	4.59%	0.728%
12	10.895	1365	1370	1373	rBV	4138046	3806276	68.64%	10.886%
13	11.236	1422	1428	1435	rBV3	94654	105399	1.90%	0.301%
14	11.601	1486	1490	1493	rBV	1717041	1569203	28.30%	4.488%
15	11.695	1501	1506	1511	rVB2	87086	119475	2.15%	0.342%
16	12.118	1570	1578	1581	rBV	1686610	1926950	34.75%	5.511%
17	12.360	1615	1619	1622	rBV2	55212	58167	1.05%	0.166%
18	12.818	1695	1697	1705	rVB	112988	141102	2.54%	0.404%
19	12.901	1705	1711	1724	rBV	785415	770514	13.90%	2.204%
20	13.195	1756	1761	1764	rBV	5861137	5518716	99.53%	15.783%
21	13.407	1794	1797	1807	rBV2	80603	103692	1.87%	0.297%
22	13.748	1851	1855	1858	rBV2	93923	98471	1.78%	0.282%
23	14.089	1909	1913	1932	rVB2	443773	1043524	18.82%	2.984%
24	14.260	1938	1942	1945	rBV	1122873	1002548	18.08%	2.867%
25	14.401	1962	1966	1969	rBV	126015	108764	1.96%	0.311%
26	14.712	2015	2019	2022	rBV	122577	114586	2.07%	0.328%
27	15.048	2070	2076	2082	rVB2	93665	133782	2.41%	0.383%
28	15.136	2084	2091	2095	rBV	479081	508453	9.17%	1.454%
29	15.389	2126	2134	2135	rBV5	49758	98905	1.78%	0.283%
30	15.418	2136	2139	2151	rVB	94014	177202	3.20%	0.507%
31	15.836	2204	2210	2219	rVB	728972	980538	17.68%	2.804%
32	16.448	2307	2314	2316	rBV7	25263	59981	1.08%	0.172%

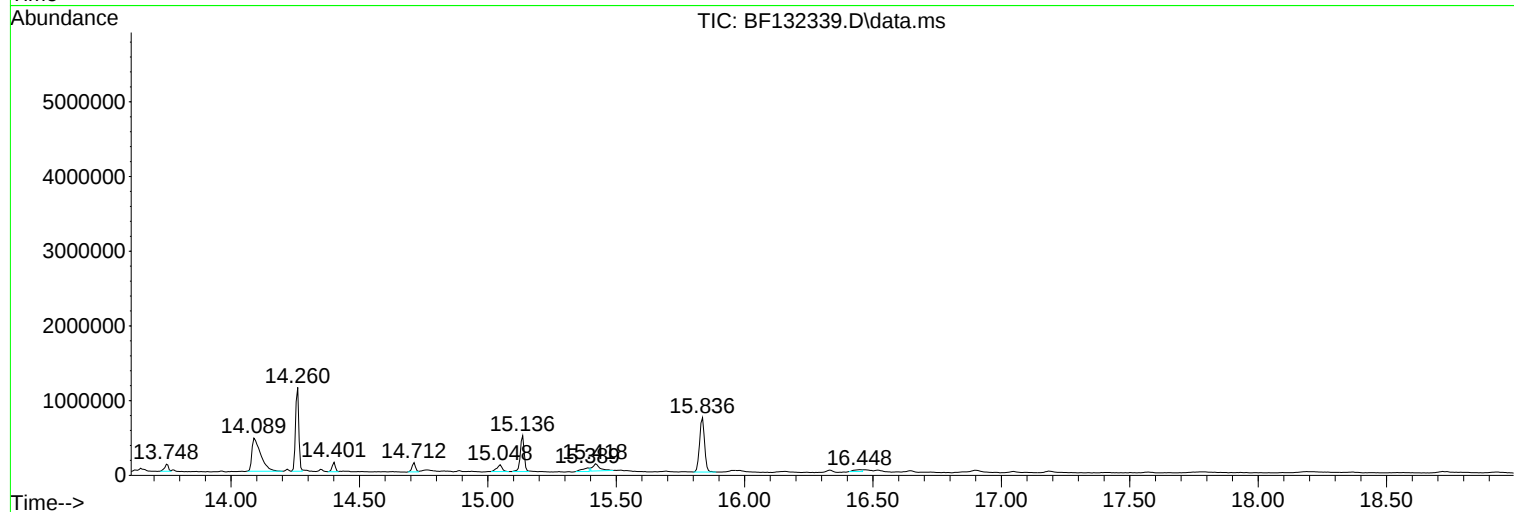
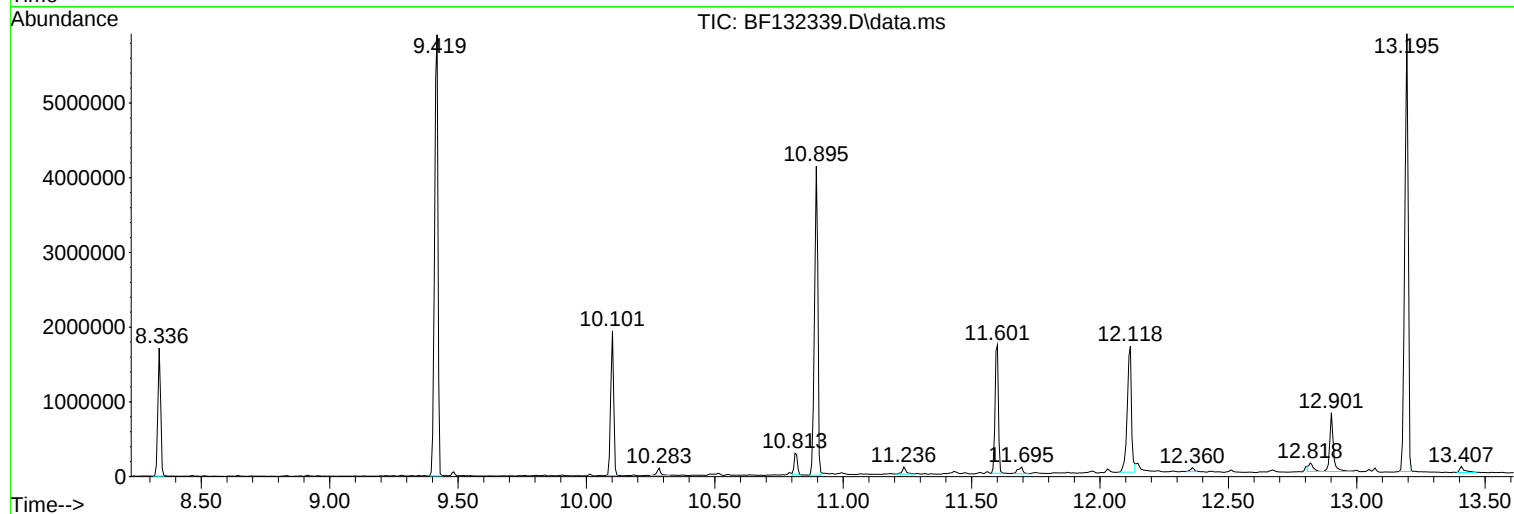
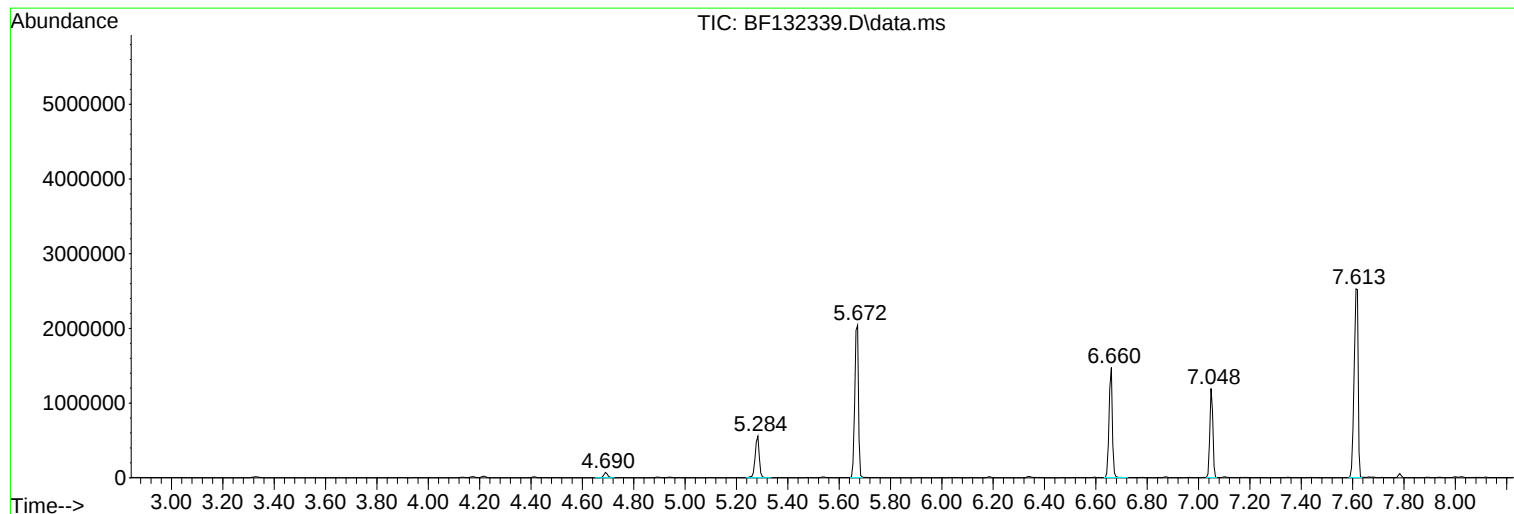
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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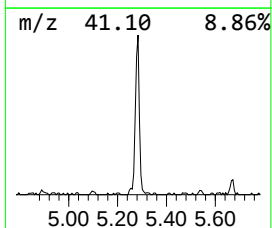
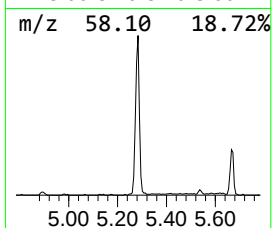
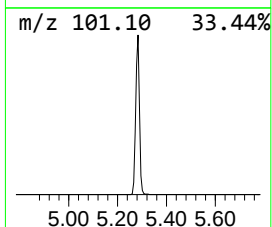
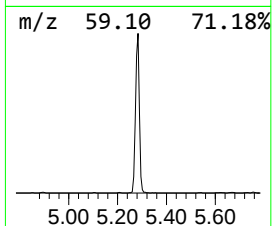
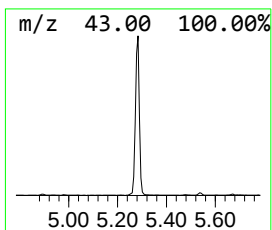
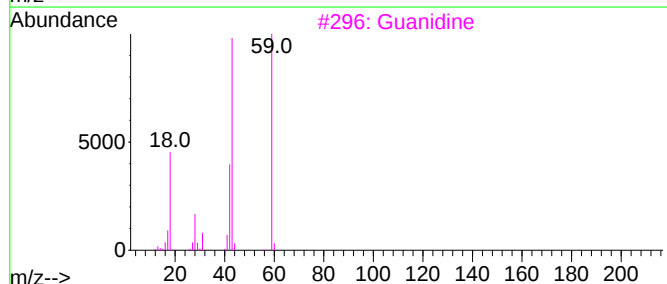
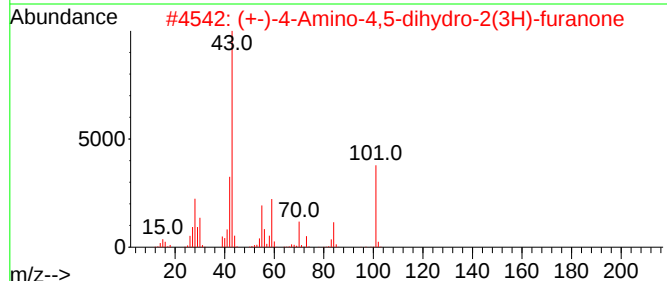
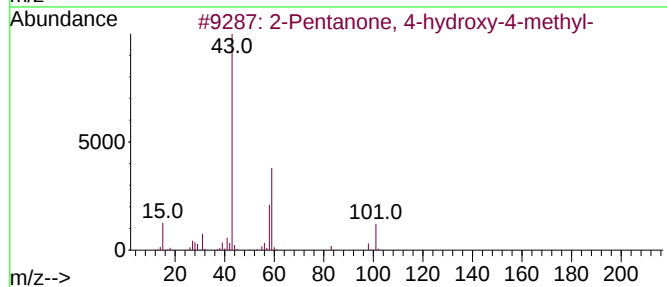
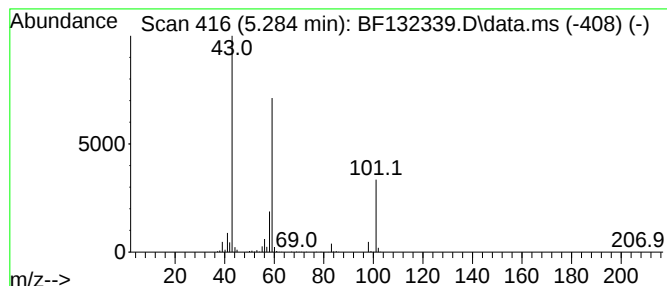
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.284	12.63 ng	615036	1,4-Dichlorobenzene-d4	7.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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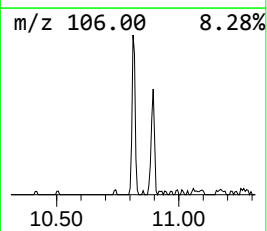
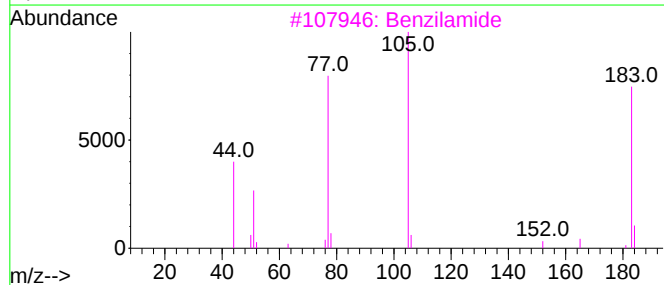
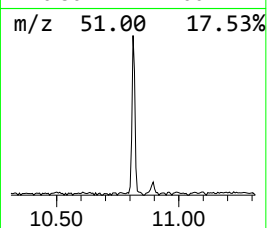
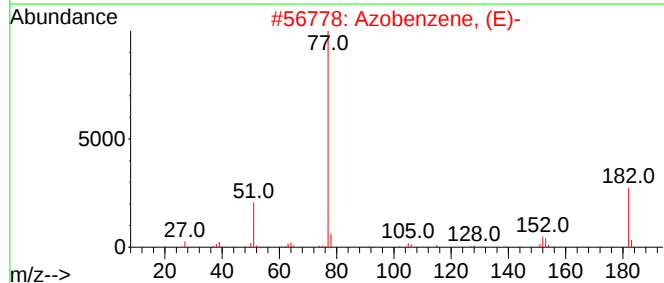
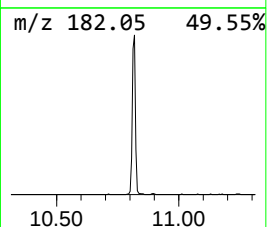
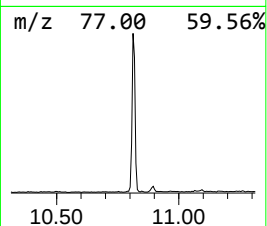
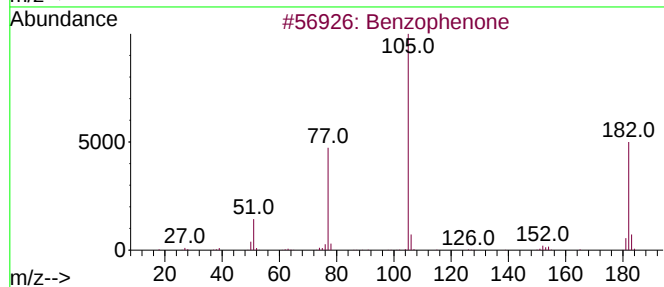
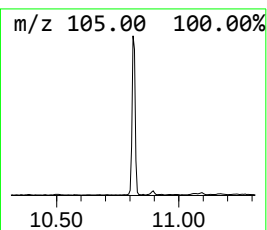
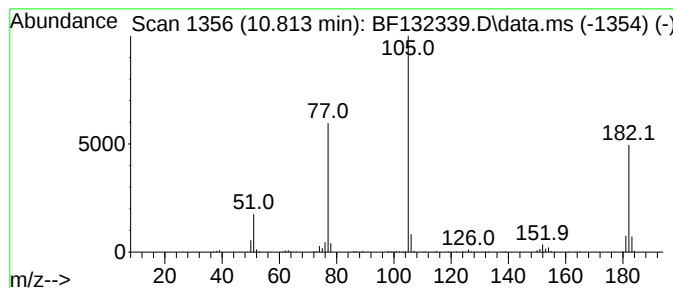
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Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.813	3.28 ng	254478	Acenaphthene-d10	10.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
3			Benzilamide	227	C14H13NO2	004746-87-6	47
4			Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	43
5			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	43



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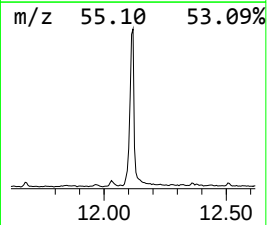
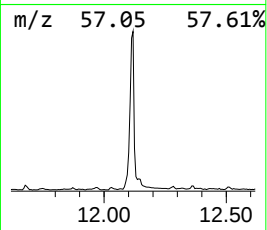
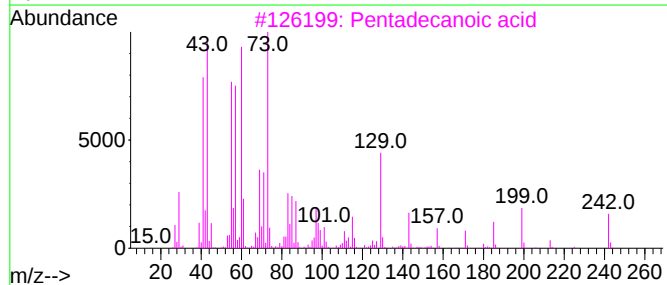
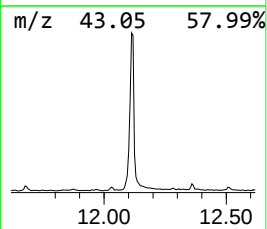
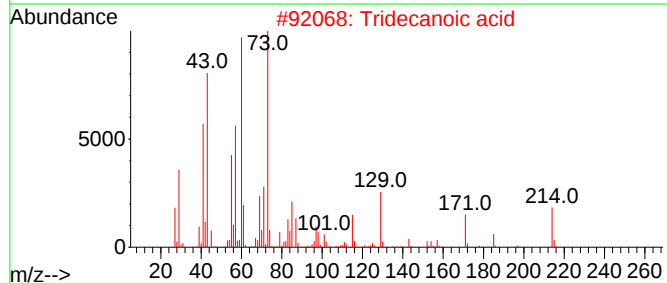
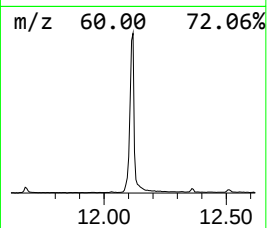
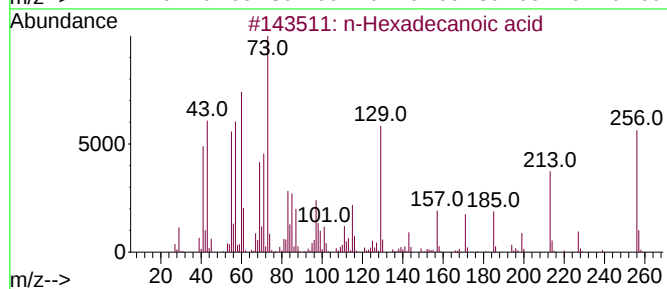
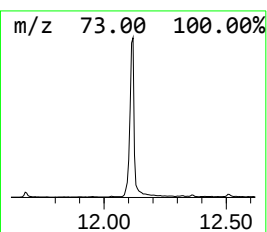
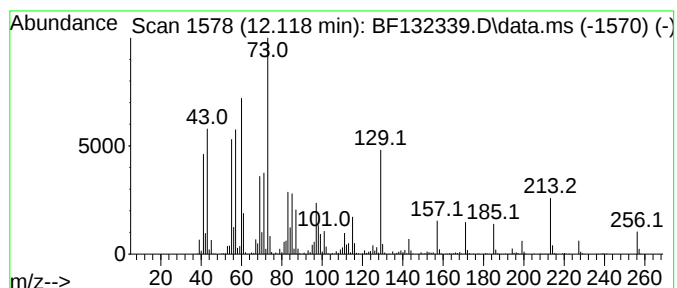
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.118	24.56 ng	1926950	Phenanthrene-d10		11.601	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	72
4	Dodecanoic acid		200	C12H24O2	000143-07-7	47
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	43



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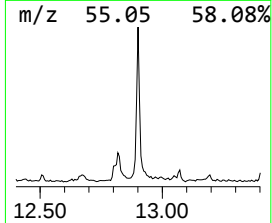
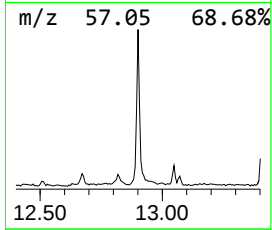
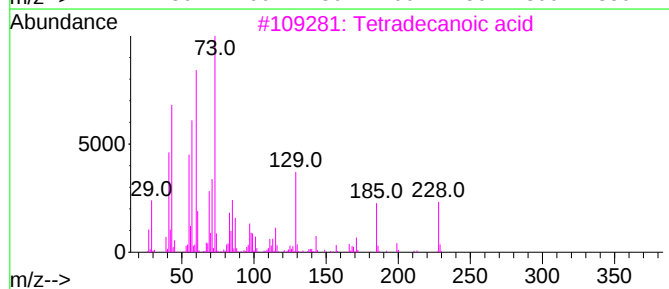
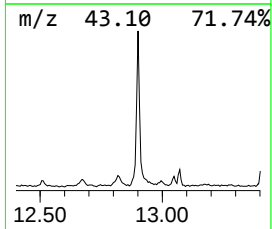
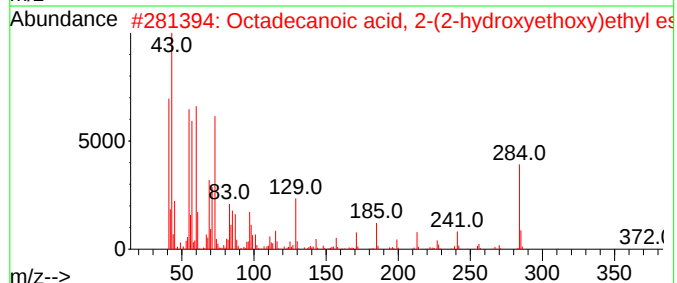
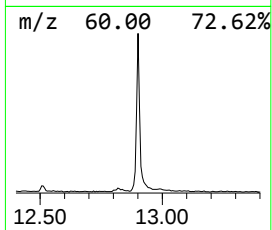
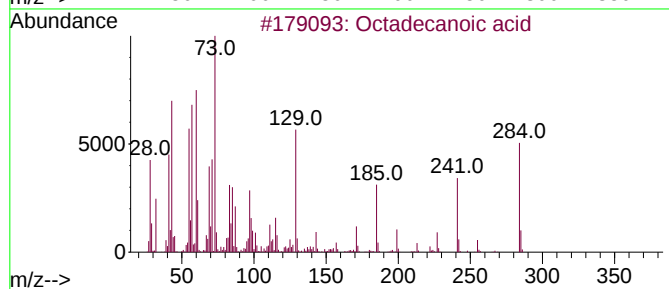
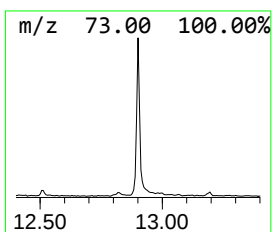
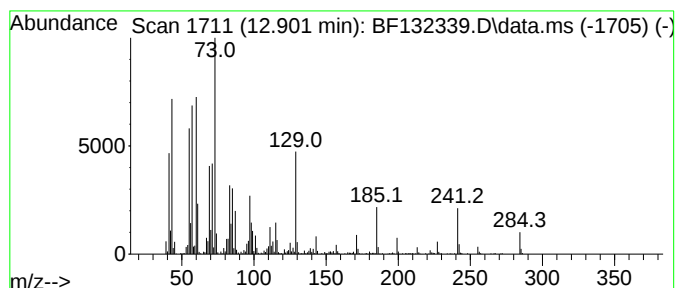
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.901	9.82 ng	770514	Phenanthrene-d10		11.601	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	86
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	81
4	Tridecanoic acid		214	C13H26O2	000638-53-9	70
5	Dodecanoic acid		200	C12H24O2	000143-07-7	52



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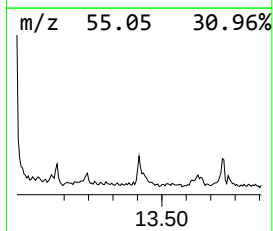
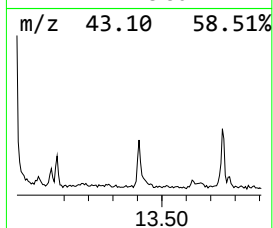
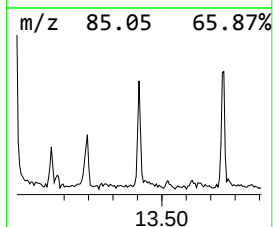
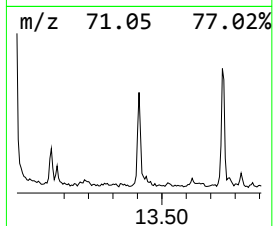
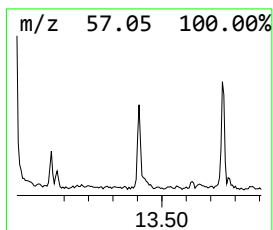
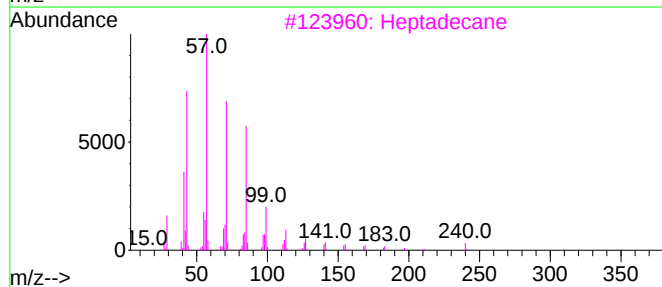
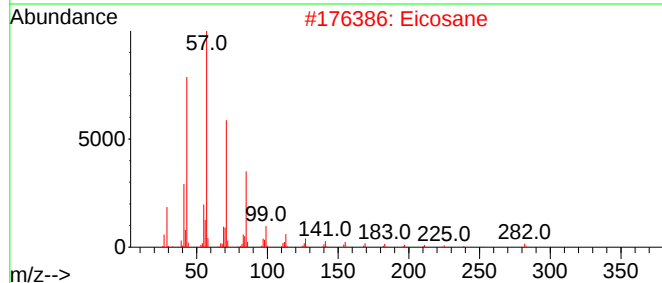
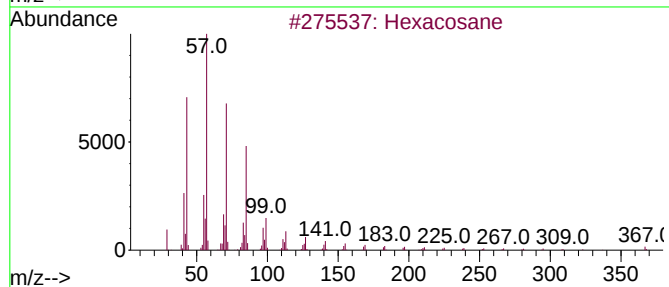
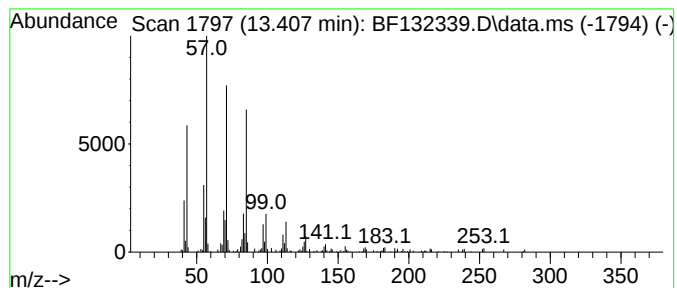
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Peak Number 5 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.407	2.07 ng	103692	Chrysene-d12	14.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Eicosane	282	C20H42	000112-95-8	91
3			Heptadecane	240	C17H36	000629-78-7	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			Heneicosane	296	C21H44	000629-94-7	90



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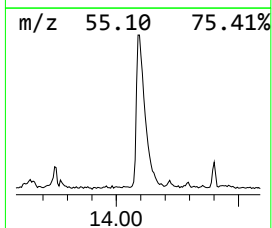
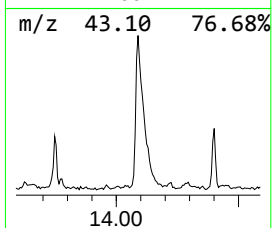
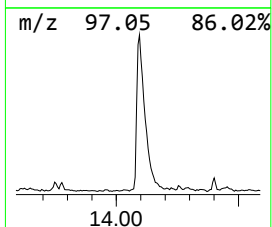
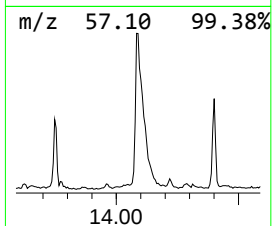
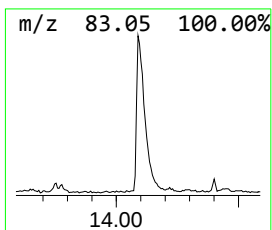
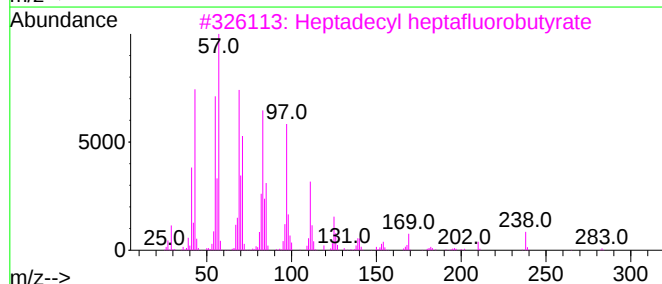
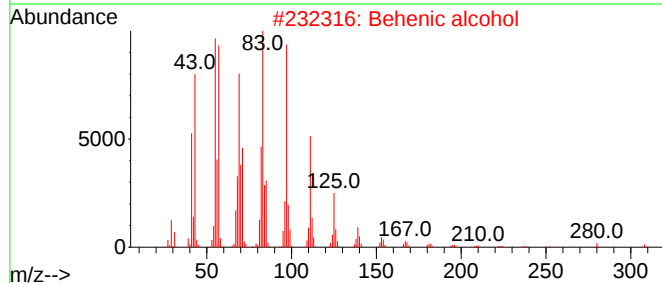
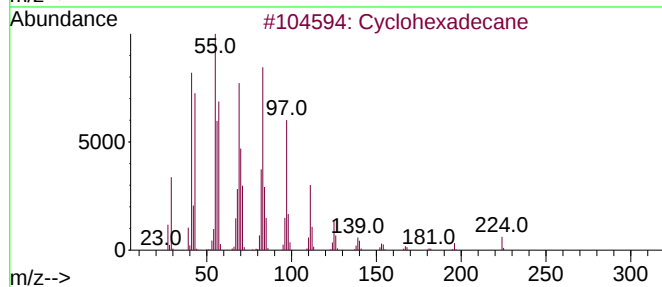
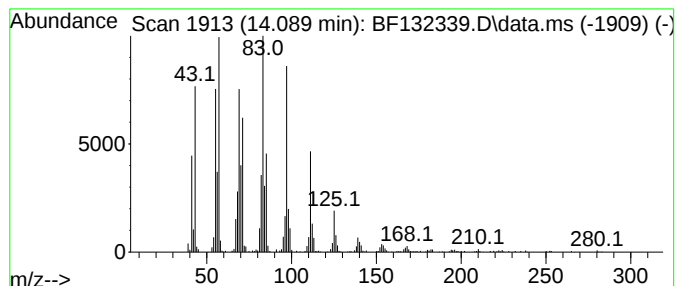
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	20.82 ng	1043520	Chrysene-d12	14.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
Data File : BF132339.D
Acq On : 06 Feb 2023 15:48
Operator : CG\JU
Sample : 01440-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1

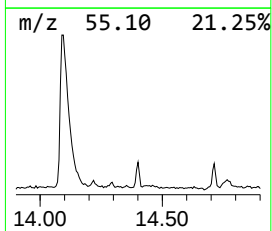
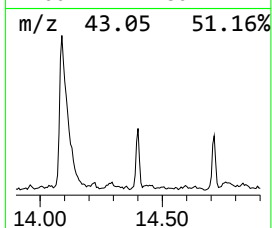
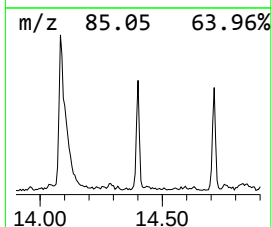
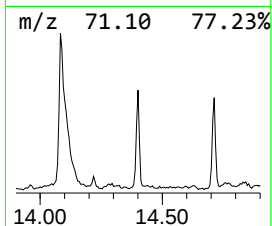
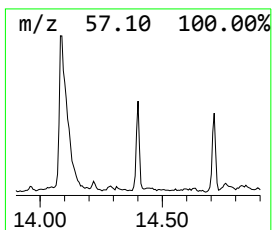
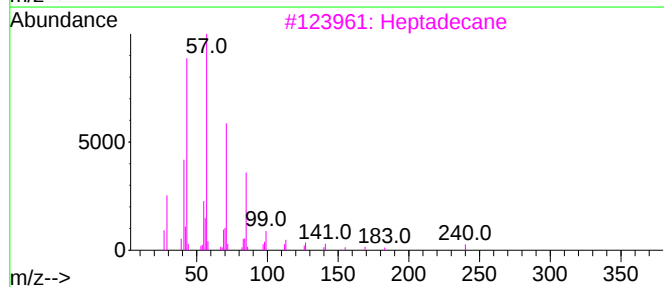
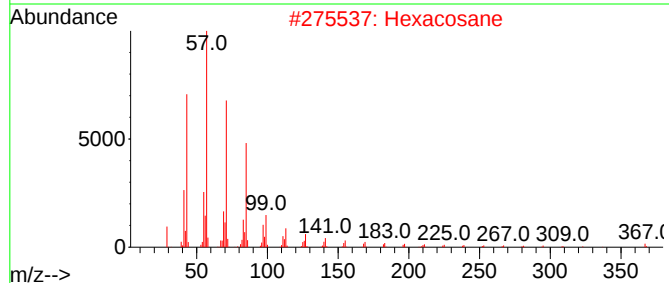
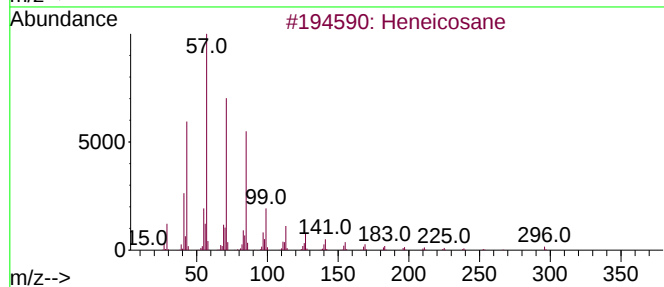
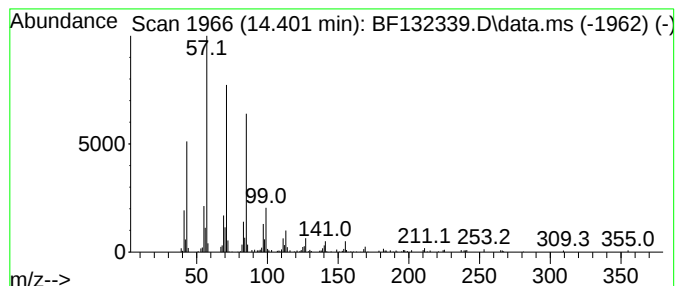
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.401	2.17 ng	108764	Chrysene-d12	14.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heptadecane	240	C17H36	000629-78-7	87
4			Octacosane	394	C28H58	000630-02-4	86
5			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
Data File : BF132339.D
Acq On : 06 Feb 2023 15:48
Operator : CG\JU
Sample : 01440-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MH-1

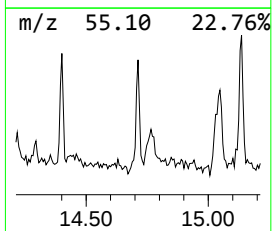
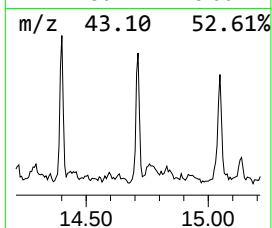
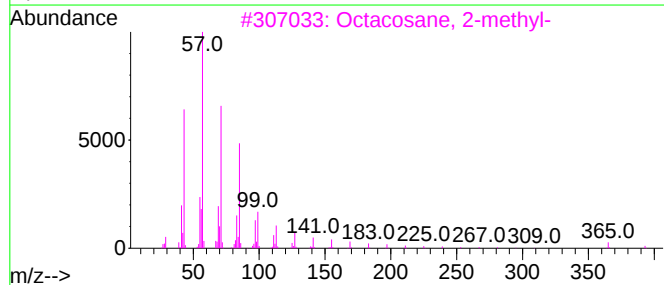
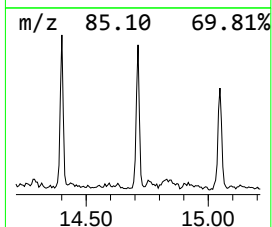
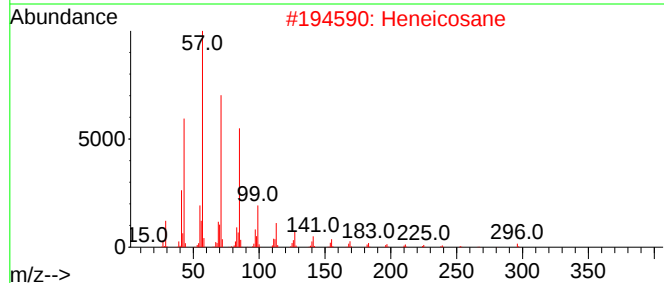
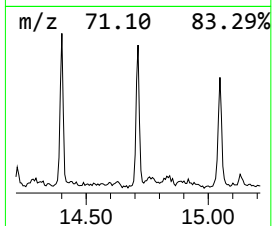
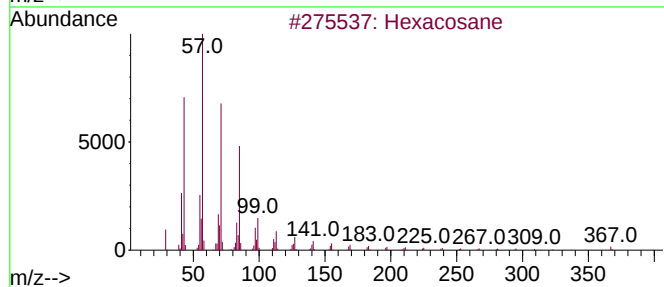
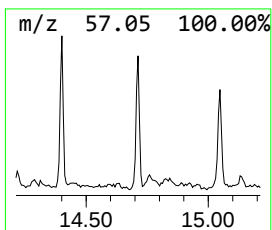
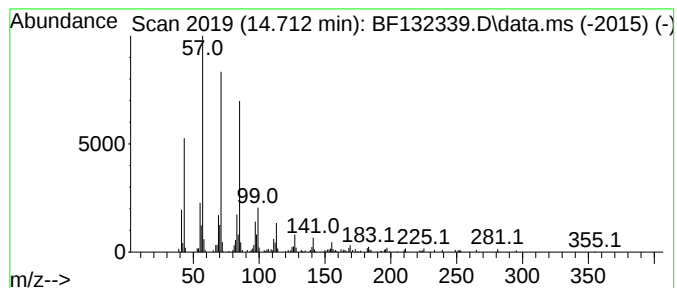
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.712	2.29 ng	114586	Chrysene-d12	14.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Pentacosane	352	C25H52	000629-99-2	90
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
Data File : BF132339.D
Acq On : 06 Feb 2023 15:48
Operator : CG\JU
Sample : 01440-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

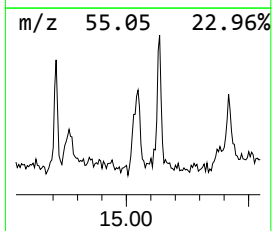
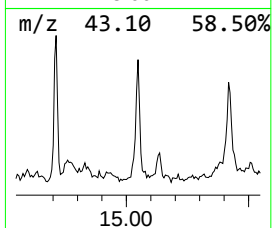
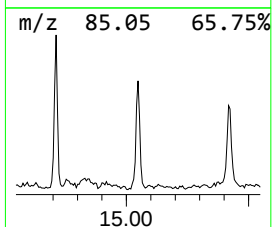
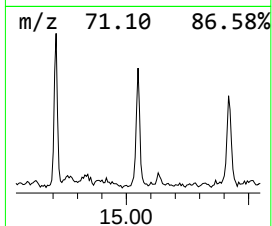
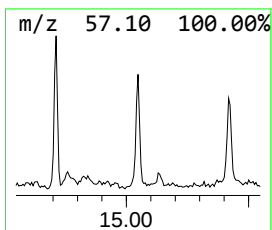
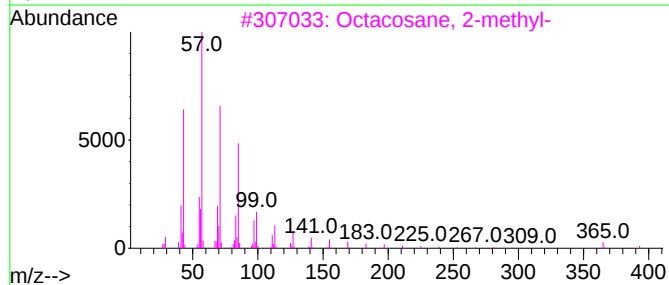
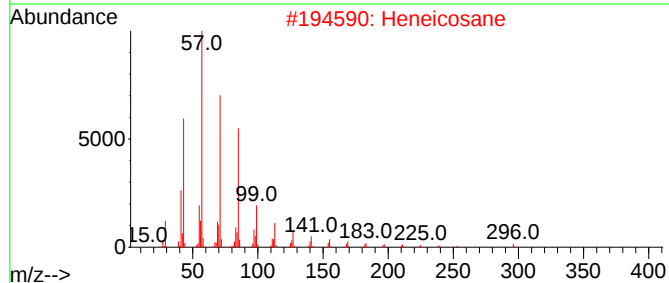
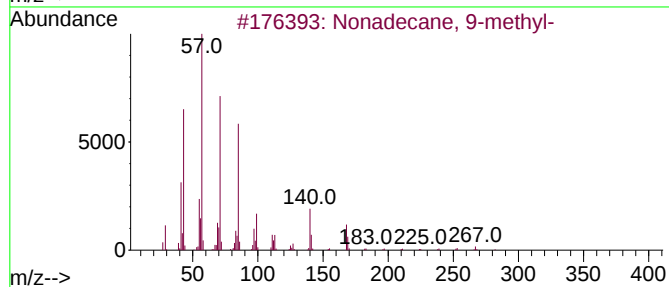
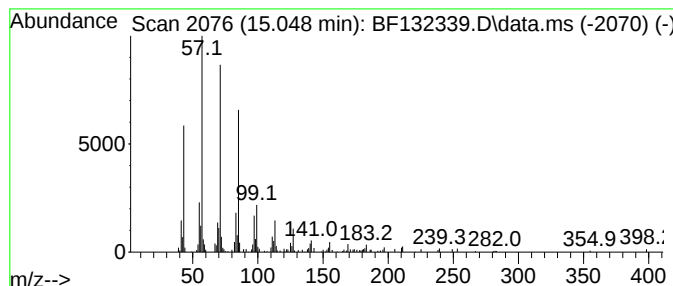
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.048	2.73 ng	133782	Perylene-d12	15.836	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	2-Methyltetracosane	352	C25H52	001560-78-7	91
5	Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
Data File : BF132339.D
Acq On : 06 Feb 2023 15:48
Operator : CG\JU
Sample : 01440-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MH-1

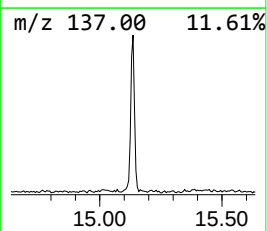
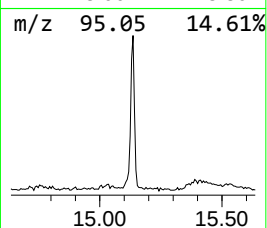
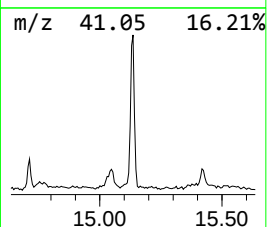
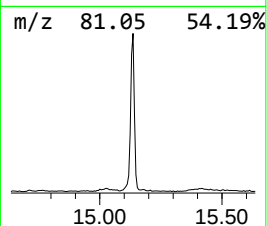
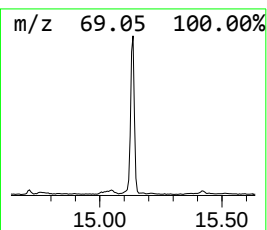
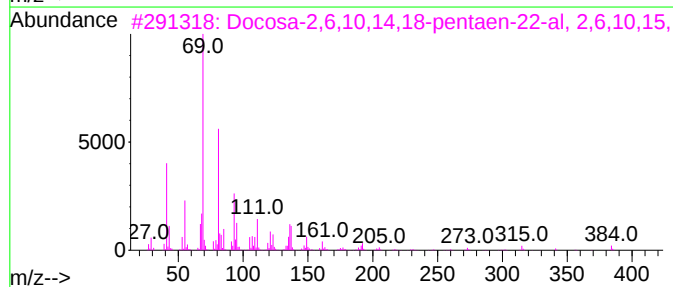
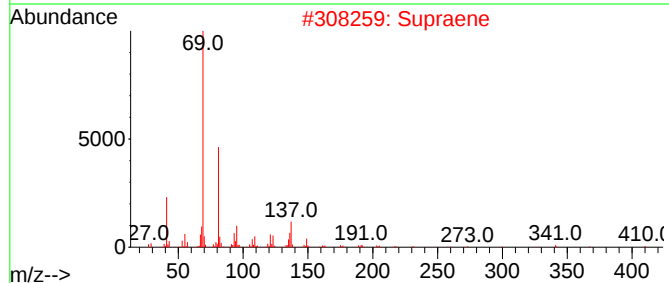
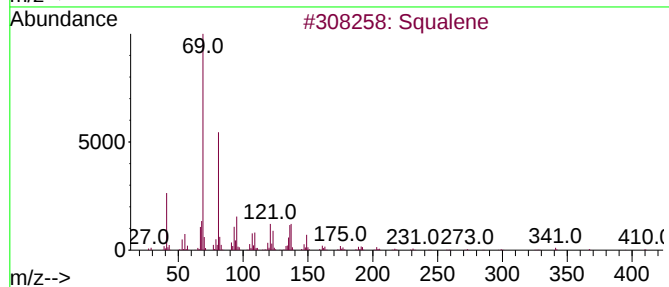
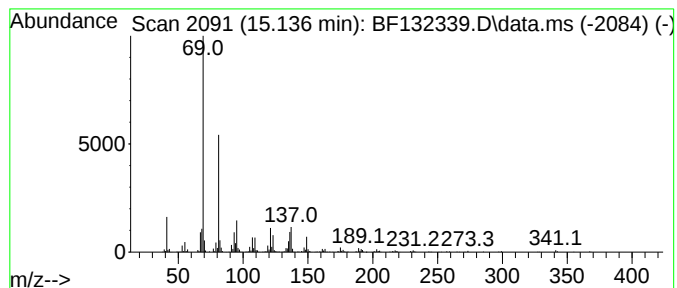
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.136	10.37 ng	508453	Perylene-d12	15.836

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
Data File : BF132339.D
Acq On : 06 Feb 2023 15:48
Operator : CG\JU
Sample : 01440-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

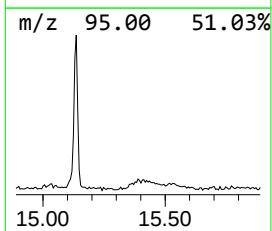
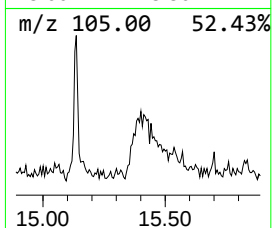
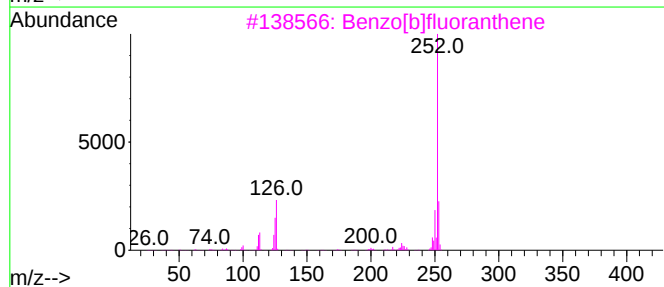
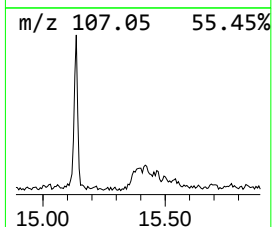
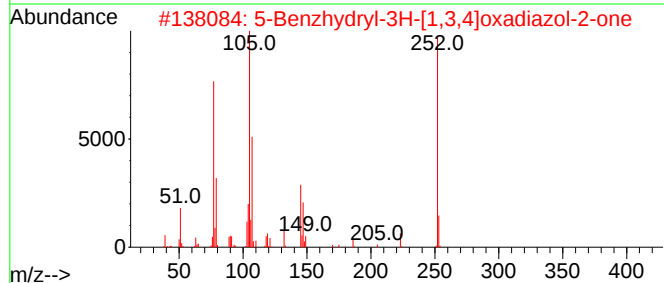
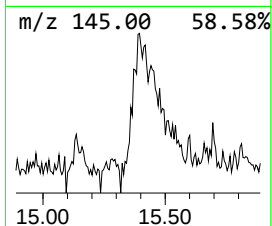
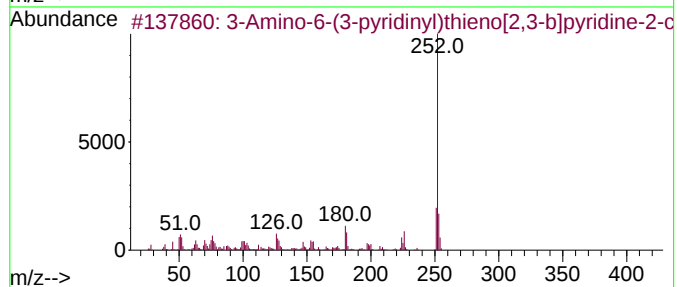
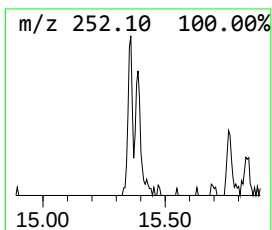
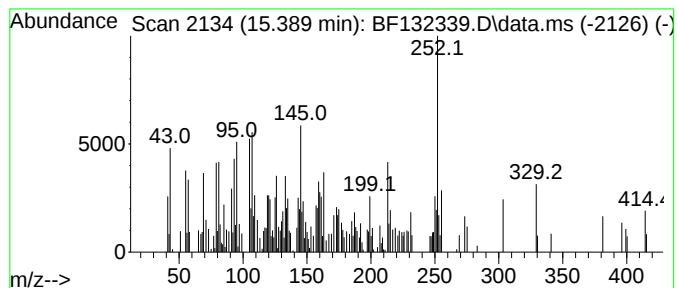
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TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.389

Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.389	2.02 ng	98905	Perylene-d12	15.836

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Amino-6-(3-pyridinyl)thieno[2,...	252	C13H8N4S	118947-66-3	35
2		5-Benzhydryl-3H-[1,3,4]oxadiazol...	252	C15H12N2O2	1000318-50-4	30
3		Benzo[b]fluoranthene	252	C20H12	000205-99-2	25
4		p-(Adamantyl-1)phenylcyclopropane	252	C19H24	1000140-46-1	25
5		4-Methyl-5-thiatetracyclo[10.4.0...	252	C16H12OS	1000445-13-3	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
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Sample : 01440-01
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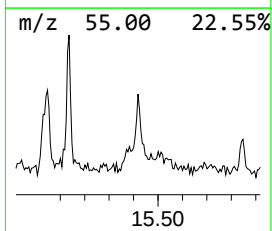
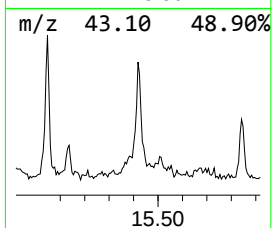
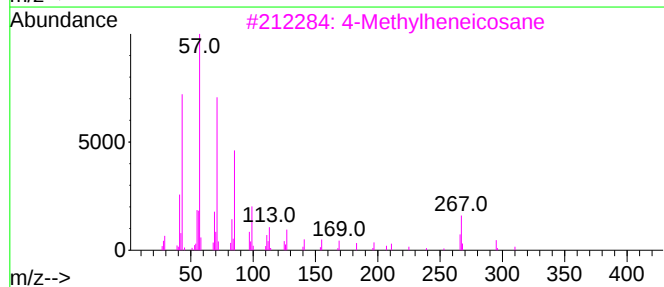
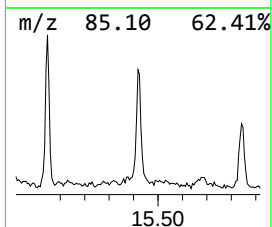
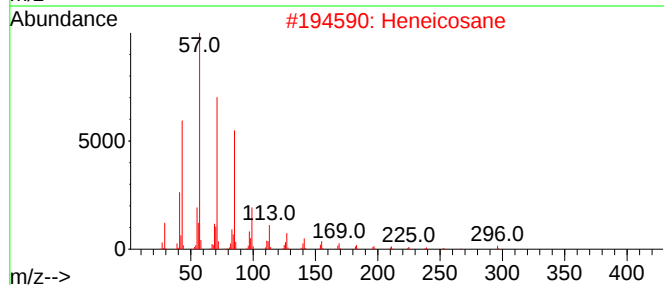
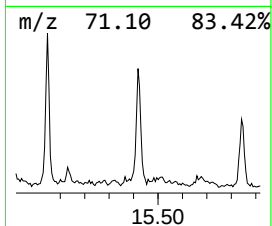
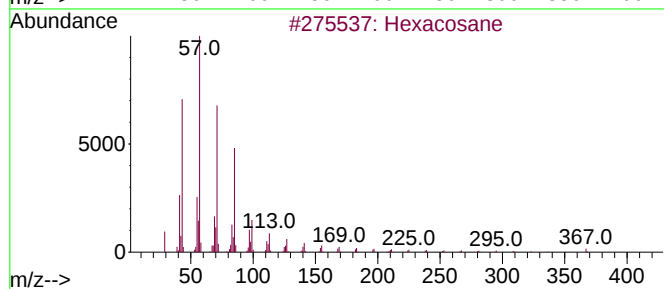
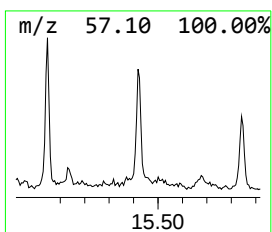
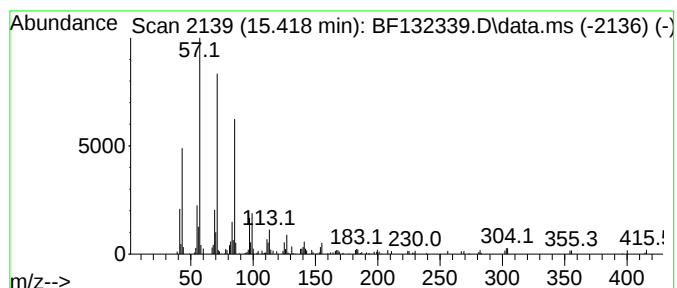
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 4-Methylheneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.418	3.61 ng	177202	Perylene-d12	15.836	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	4-Methylheneicosane	310	C22H46	025117-29-7	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020623\
Data File : BF132339.D
Acq On : 06 Feb 2023 15:48
Operator : CG\JU
Sample : 01440-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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-...	5.284	12.6	ng	615036	1	7.048	973948	20.0
Benzophenone	10.813	3.3	ng	254478	3	10.101	1552840	20.0
n-Hexadecanoic ...	12.118	24.6	ng	1926950	4	11.601	1569200	20.0
Octadecanoic acid	12.901	9.8	ng	770514	4	11.601	1569200	20.0
Hexacosane	13.407	2.1	ng	103692	5	14.259	1002550	20.0
Cyclohexadecane	14.089	20.8	ng	1043520	5	14.259	1002550	20.0
Heneicosane	14.401	2.2	ng	108764	5	14.259	1002550	20.0
Octacosane, 2-m...	14.712	2.3	ng	114586	5	14.259	1002550	20.0
Nonadecane, 9-m...	15.048	2.7	ng	133782	6	15.836	980538	20.0
Squalene	15.136	10.4	ng	508453	6	15.836	980538	20.0
unknown15.389	15.389	2.0	ng	98905	6	15.836	980538	20.0
4-Methylheneico...	15.418	3.6	ng	177202	6	15.836	980538	20.0