

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
 Data File : BF133538.D
 Acq On : 31 May 2023 14:38
 Operator : CG\JU
 Sample : 02972-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-11-0A

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	497	503	511	rBV	135267	186910	5.12%	0.595%
2	5.445	565	571	574	rBV	3069816	3003224	82.27%	9.562%
3	6.457	737	743	746	rBV	2887761	3055540	83.70%	9.728%
4	6.828	803	806	810	rBV	885473	708351	19.40%	2.255%
5	7.392	897	902	905	rBV	2127085	1993884	54.62%	6.348%
6	8.110	1021	1024	1028	rBV	1137832	951828	26.07%	3.030%
7	9.192	1204	1208	1211	rBV	4015442	3384498	92.71%	10.775%
8	9.869	1319	1323	1326	rBV	1345015	1049551	28.75%	3.342%
9	10.163	1370	1373	1378	rVB	73394	62922	1.72%	0.200%
10	10.416	1412	1416	1421	rBV7	18676	39027	1.07%	0.124%
11	10.580	1441	1444	1447	rVB	142368	127734	3.50%	0.407%
12	10.657	1452	1457	1460	rBV	2599906	2317140	63.47%	7.377%
13	11.357	1572	1576	1579	rBV	1252066	1162207	31.84%	3.700%
14	11.580	1609	1614	1618	rBV	48072	66311	1.82%	0.211%
15	11.886	1660	1666	1669	rBV	431564	460938	12.63%	1.468%
16	11.922	1669	1672	1675	rVB	74556	74184	2.03%	0.236%
17	12.027	1678	1690	1694	rBV3	205041	543935	14.90%	1.732%
18	12.563	1775	1781	1785	rBV	65764	99012	2.71%	0.315%
19	12.669	1794	1799	1808	rBV2	192171	228187	6.25%	0.726%
20	12.792	1813	1820	1823	rBV	74978	105732	2.90%	0.337%
21	12.945	1841	1846	1850	rBV	3606426	3650516	100.00%	11.622%
22	13.245	1890	1897	1911	rVB2	307914	702541	19.24%	2.237%
23	13.421	1923	1927	1934	rVB	144943	145012	3.97%	0.462%
24	13.863	1998	2002	2015	rVB2	150464	324968	8.90%	1.035%
25	13.998	2018	2025	2032	rBV4	1335915	2038262	55.83%	6.489%
26	14.515	2109	2113	2116	rBV	35117	41496	1.14%	0.132%
27	14.586	2119	2125	2131	rBV2	464395	834716	22.87%	2.658%
28	14.763	2152	2155	2157	rBV	58439	66554	1.82%	0.212%
29	14.933	2180	2184	2194	rVB10	29990	64351	1.76%	0.205%
30	15.121	2212	2216	2217	rBV3	35244	39231	1.07%	0.125%
31	15.162	2217	2223	2238	rVB	300165	634756	17.39%	2.021%
32	15.451	2267	2272	2277	rBV	672221	770282	21.10%	2.452%
33	15.821	2327	2335	2343	rVB2	201447	492903	13.50%	1.569%
34	16.209	2393	2401	2418	rBV6	180507	760364	20.83%	2.421%
35	16.568	2454	2462	2472	rBV	158508	449010	12.30%	1.430%
36	16.904	2513	2519	2535	rVB4	70917	217249	5.95%	0.692%

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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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.468	2607	2615	2623	rBV2	111887	313766	8.60%	0.999%
38	18.509	2785	2792	2803	rVB3	78212	242375	6.64%	0.772%

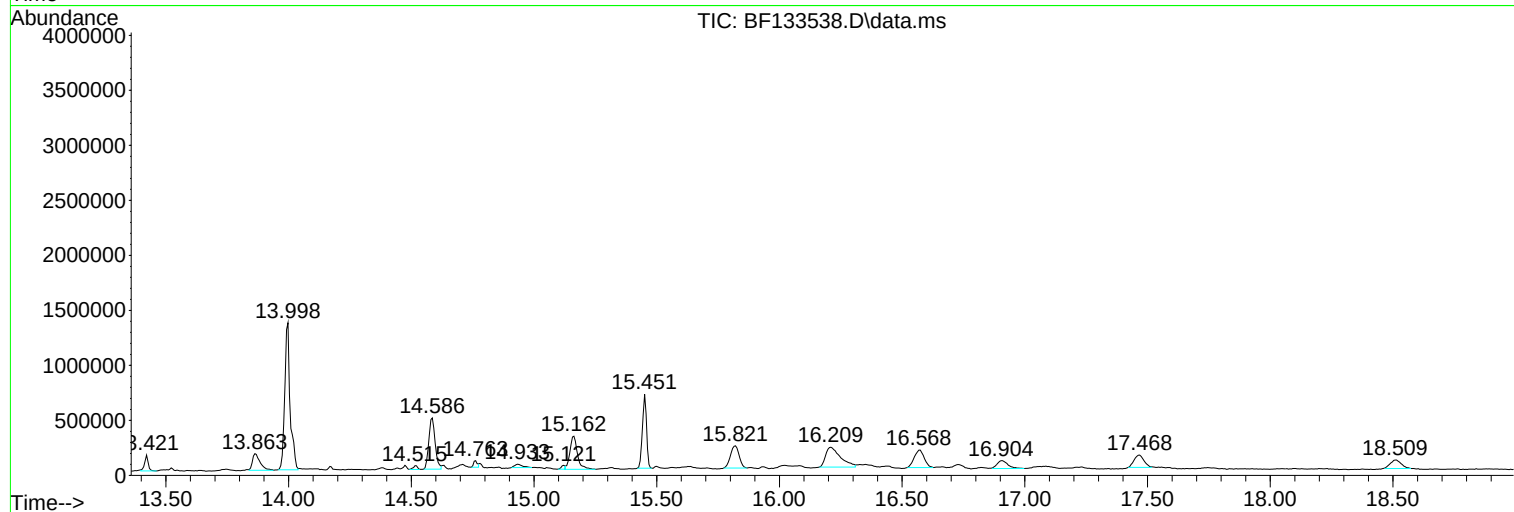
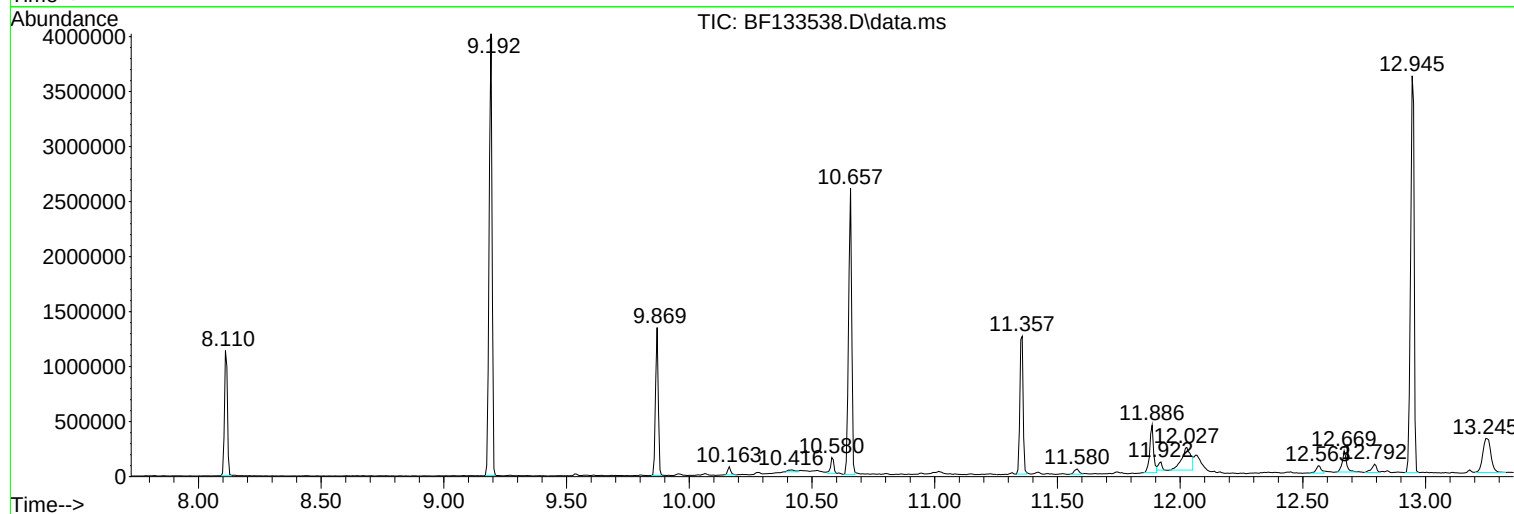
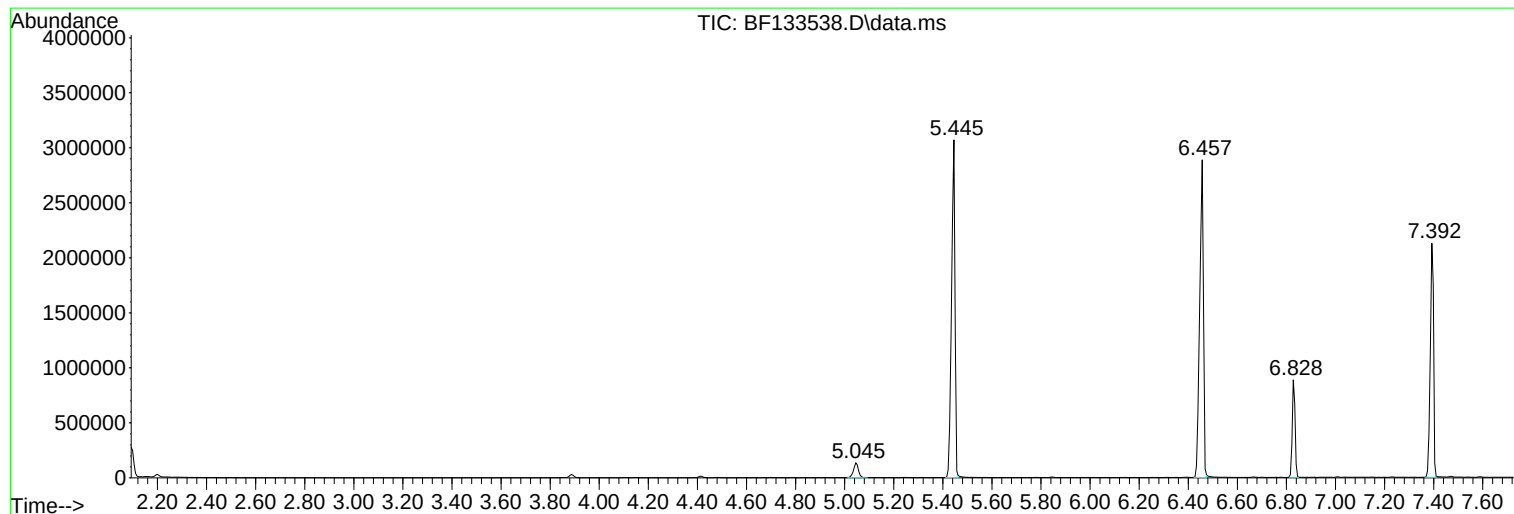
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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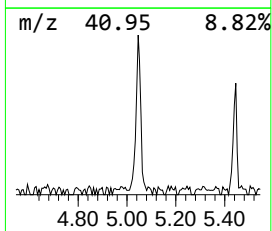
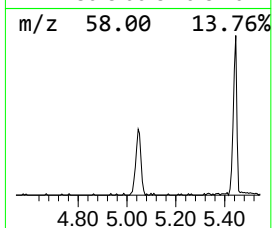
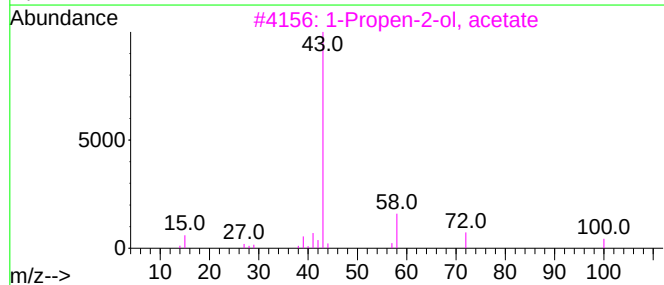
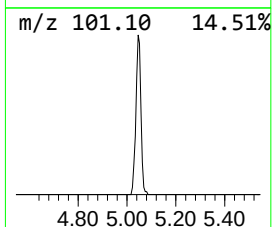
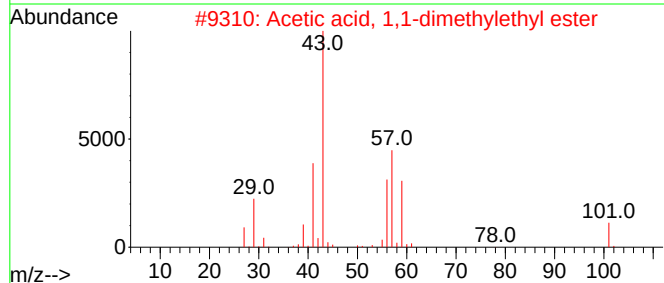
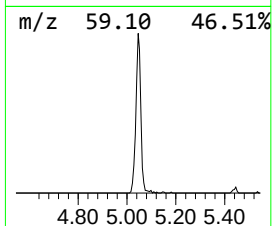
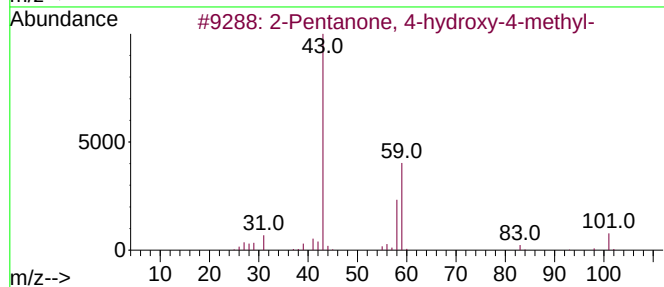
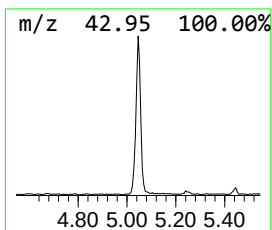
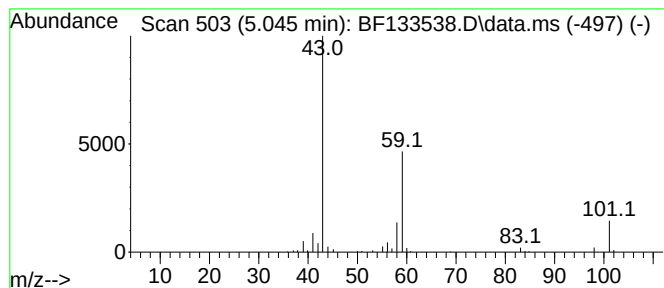
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	5.28 ng	186910	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9		



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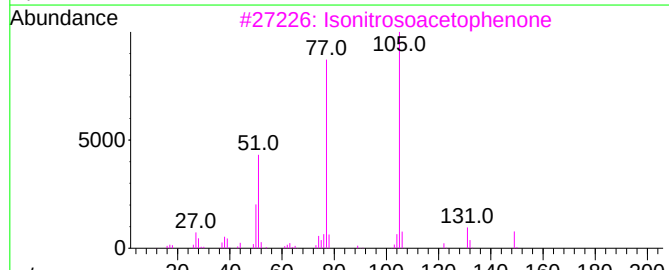
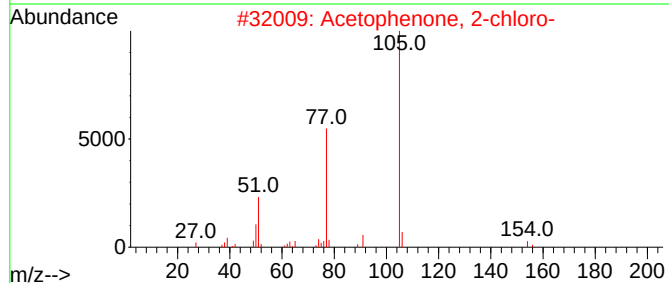
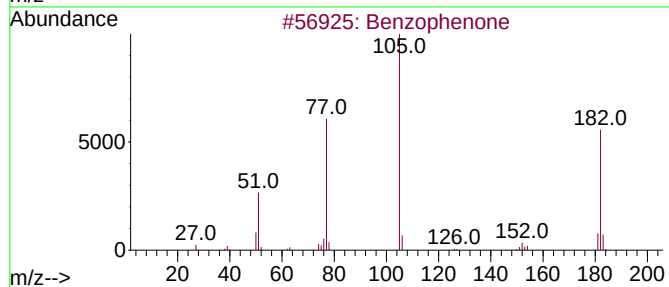
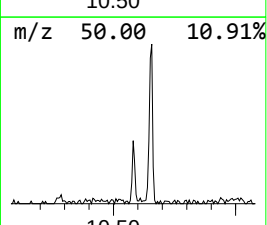
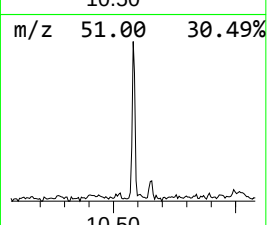
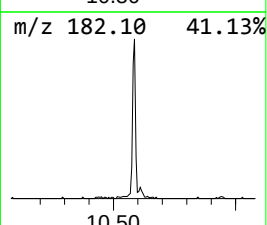
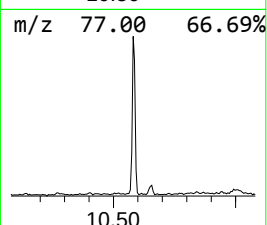
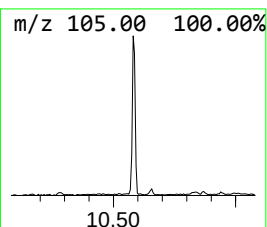
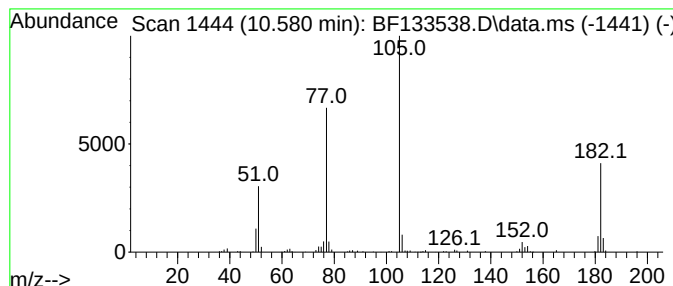
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Peak Number 2 Benzophenone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	2.43 ng	127734	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
3			Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	50
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50



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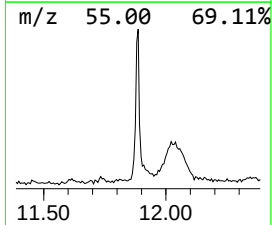
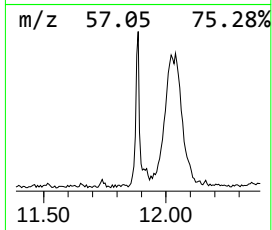
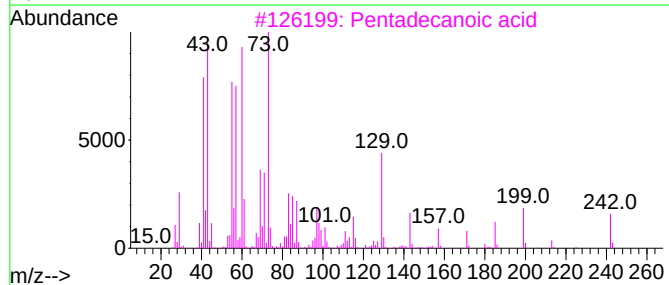
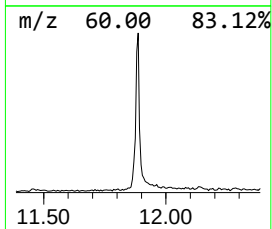
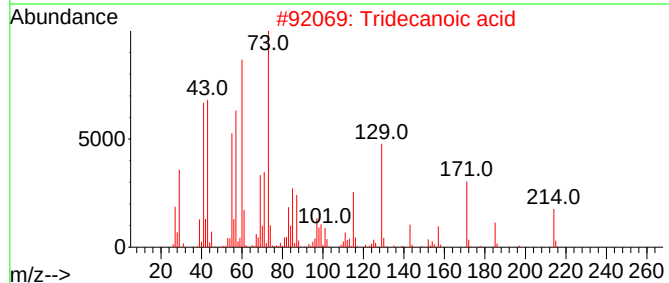
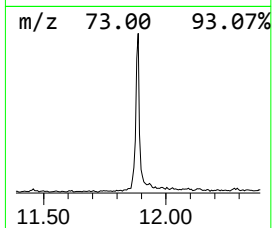
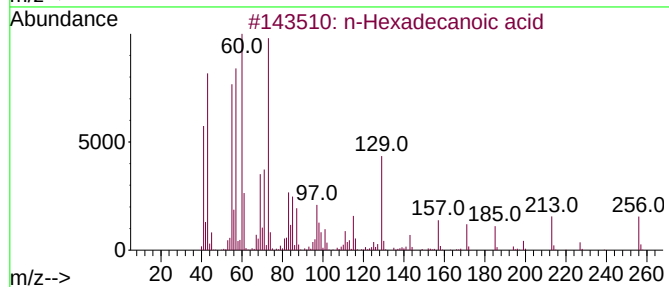
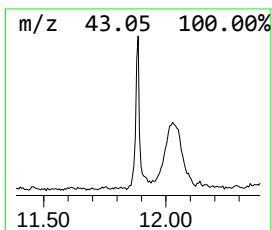
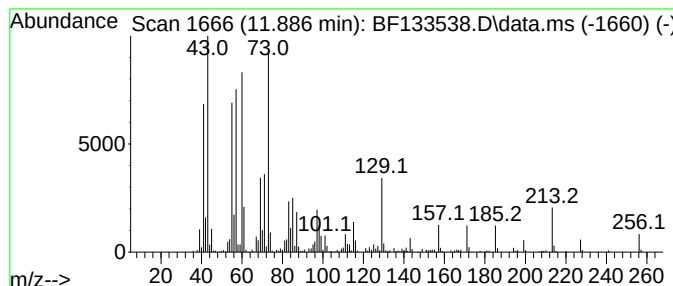
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	7.93 ng	460938	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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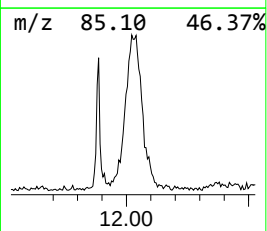
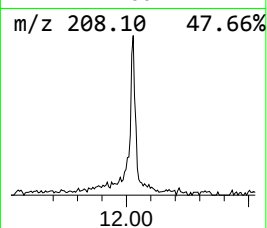
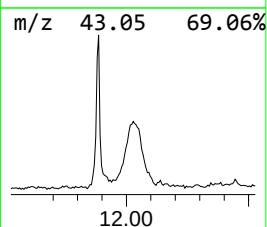
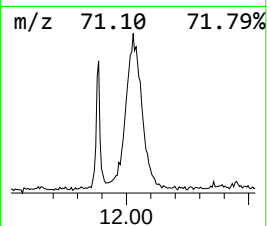
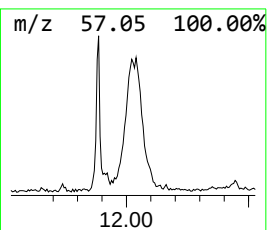
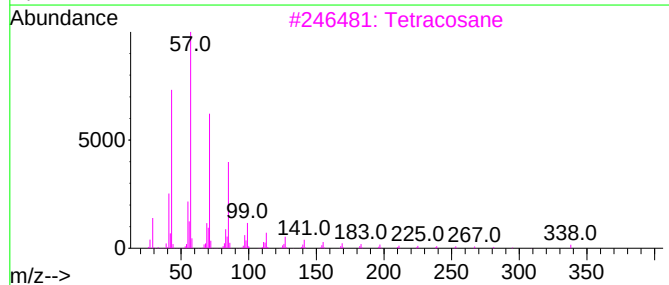
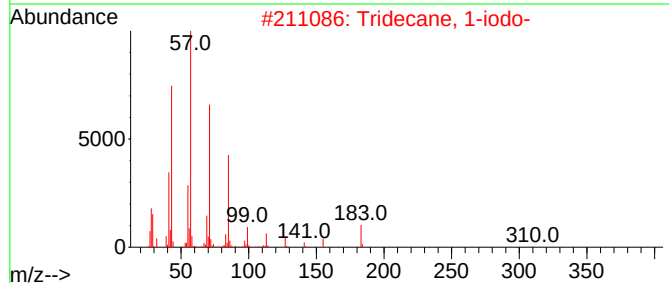
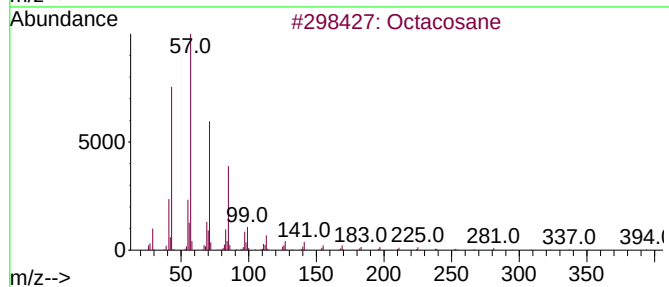
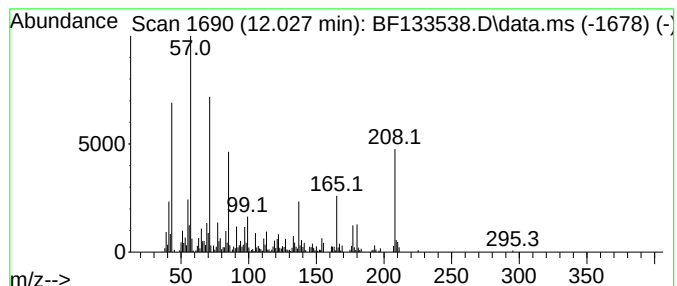
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.027	9.36 ng	543935	Phenanthrene-d10	11.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	46
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	41
3		Tetracosane	338	C24H50	000646-31-1	41
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	41
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	41



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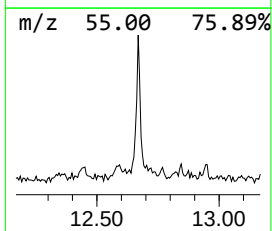
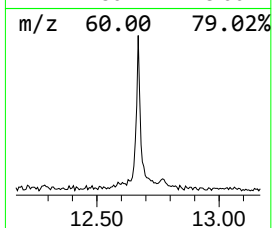
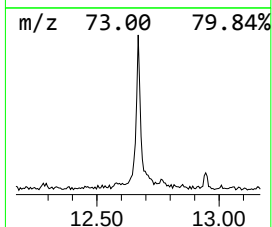
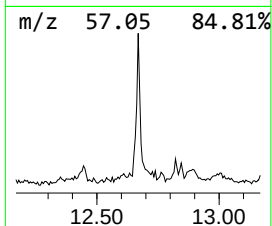
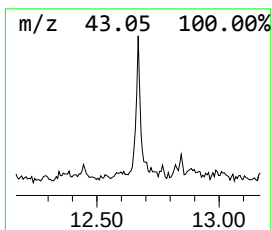
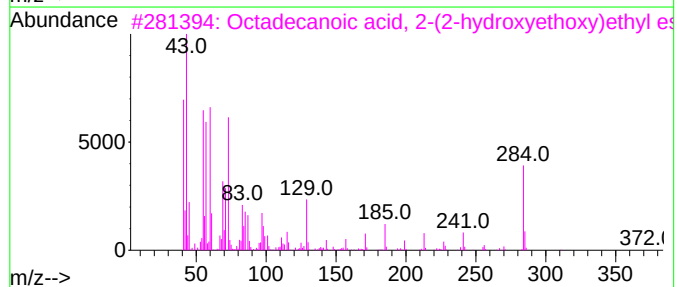
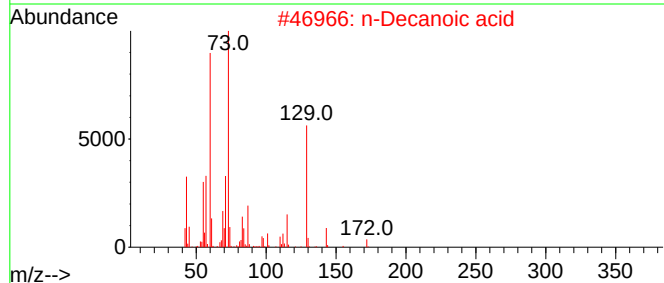
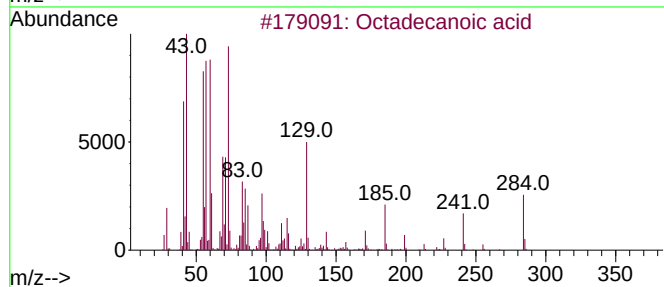
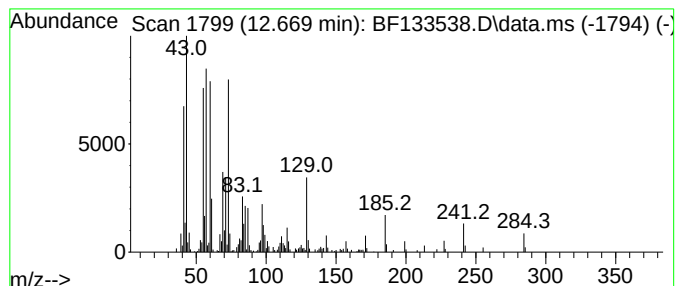
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	3.93 ng	228187	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86



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Acq On : 31 May 2023 14:38
Operator : CG\JU
Sample : 02972-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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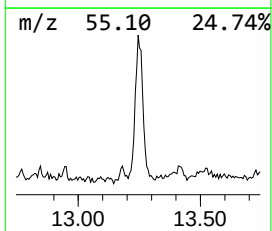
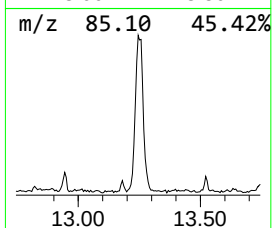
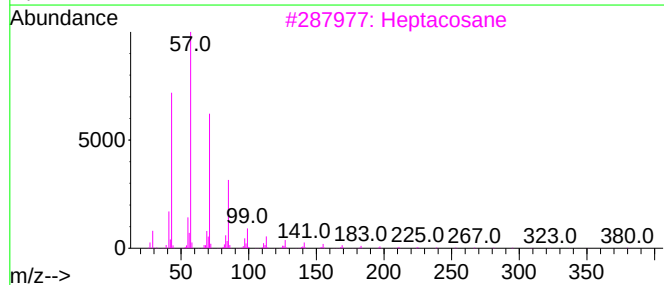
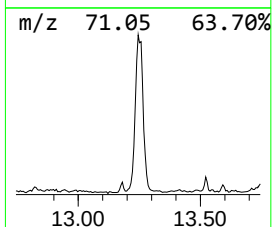
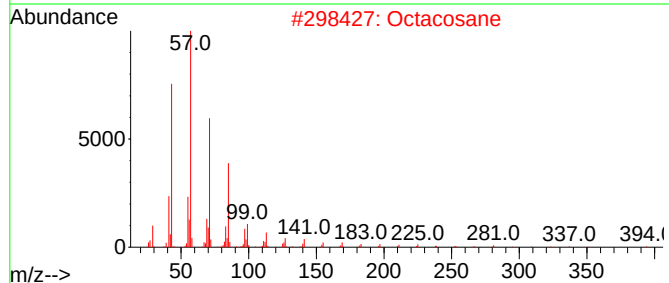
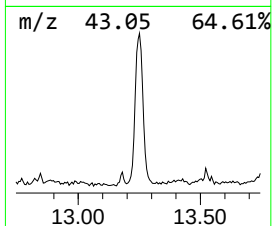
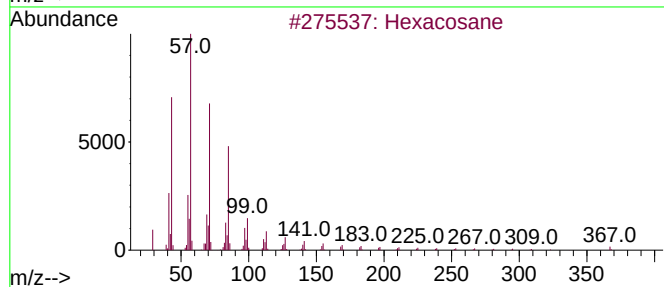
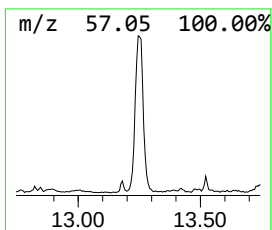
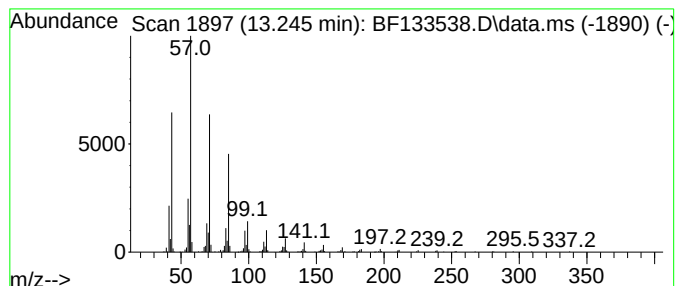
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.245	6.89 ng	702541	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
Data File : BF133538.D
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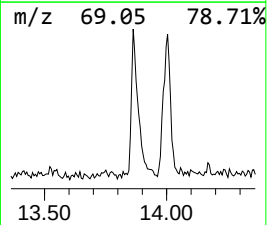
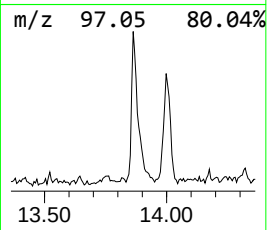
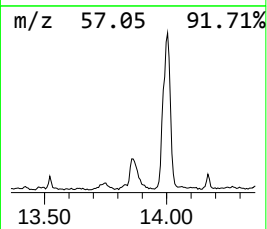
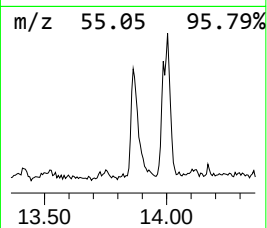
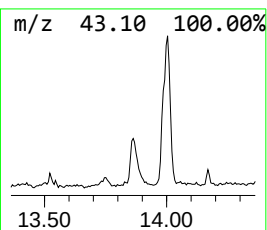
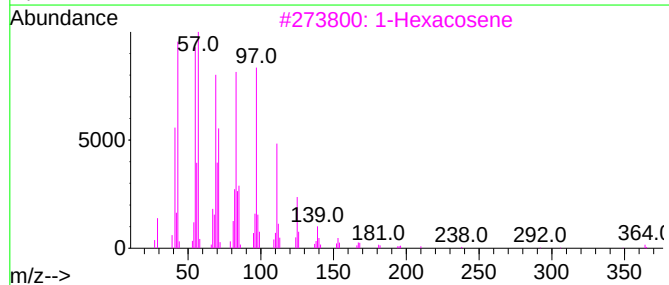
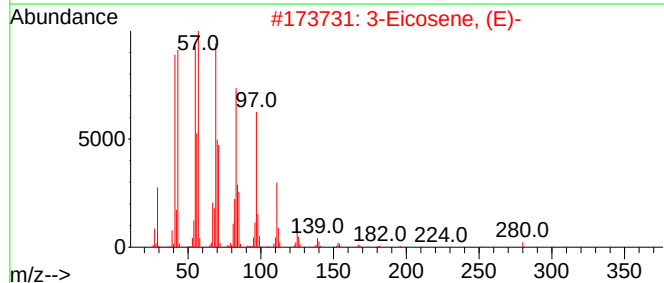
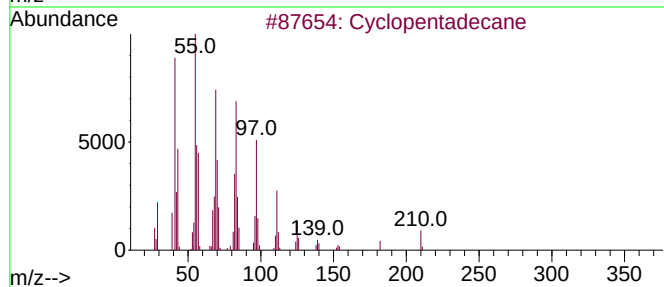
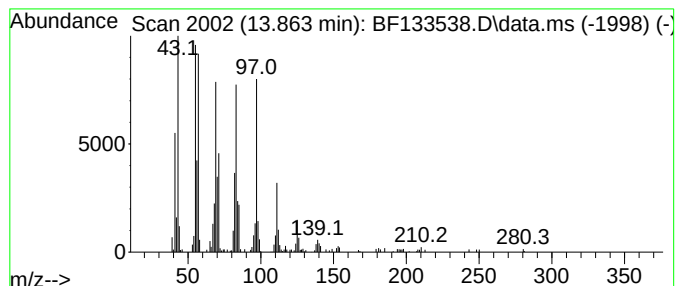
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	3.19 ng	324968	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	95
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	95
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
Data File : BF133538.D
Acq On : 31 May 2023 14:38
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ALS Vial : 5 Sample Multiplier: 1

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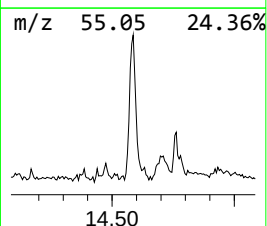
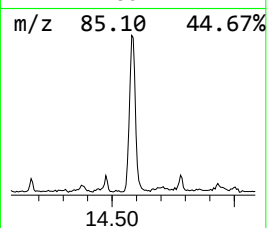
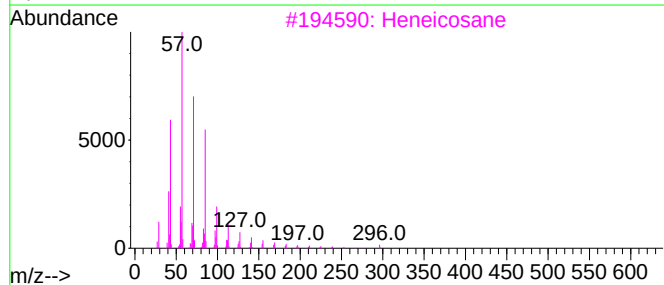
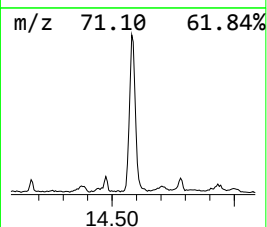
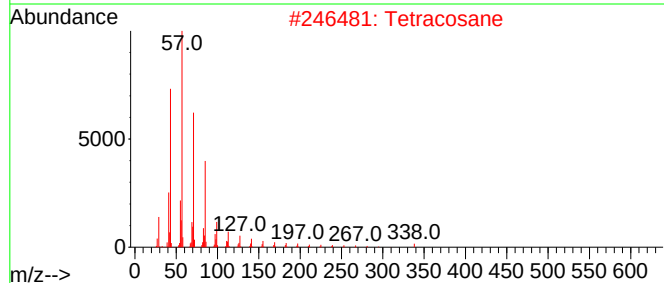
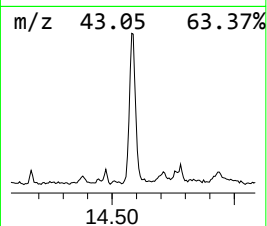
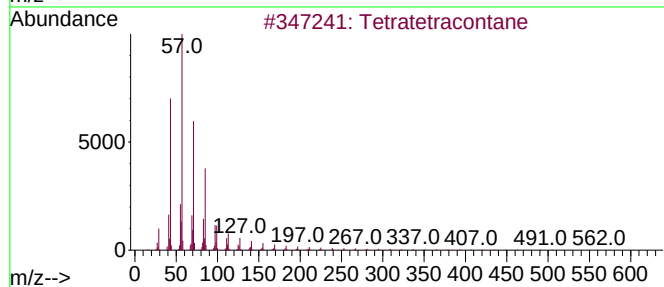
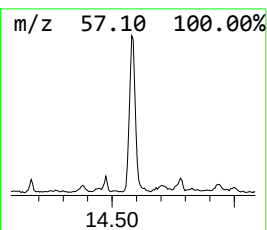
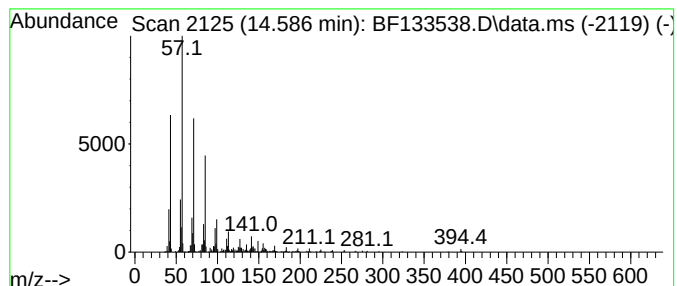
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	8.19 ng	834716	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Tetracosane	338	C24H50	000646-31-1	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
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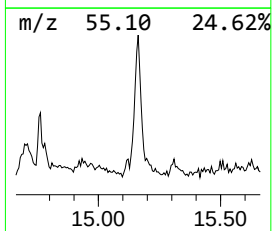
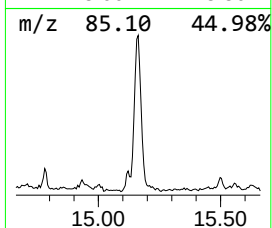
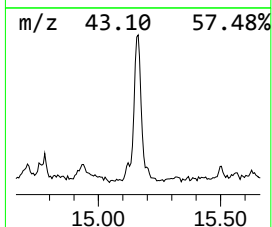
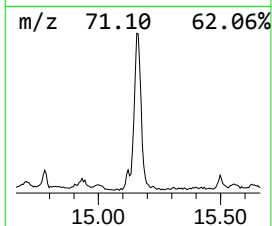
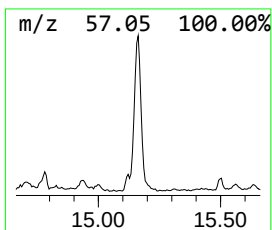
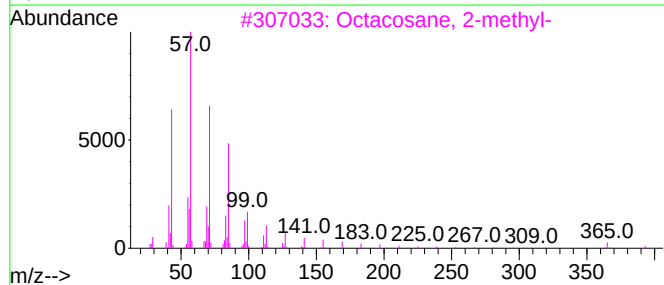
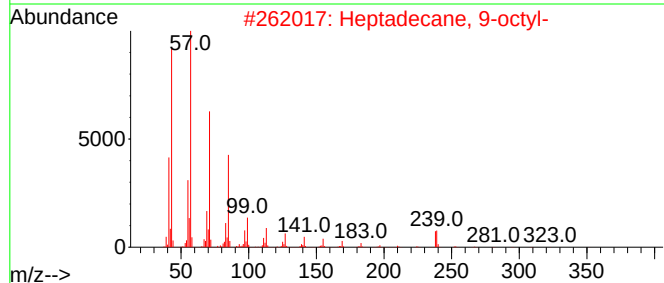
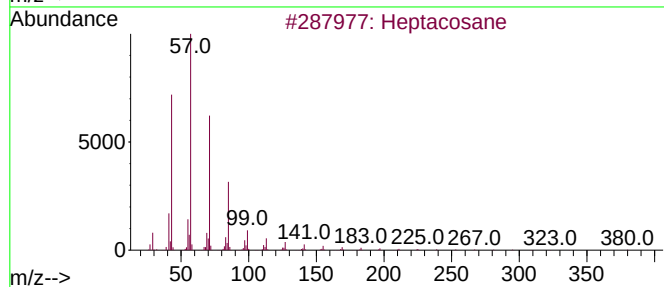
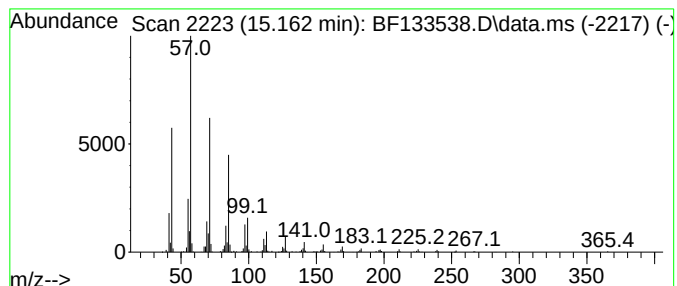
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.163	16.48 ng	634756	Perylene-d12	15.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
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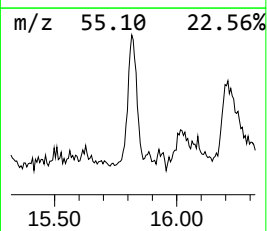
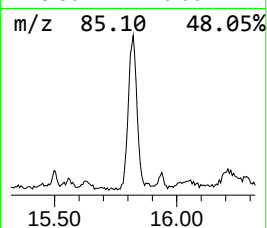
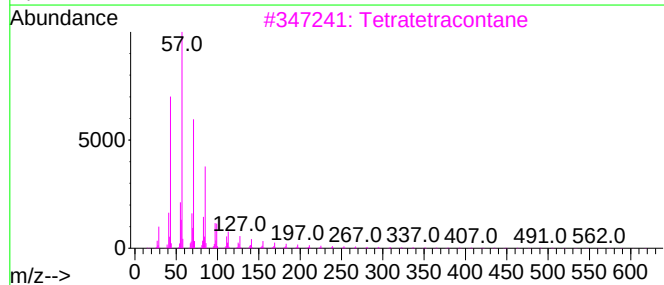
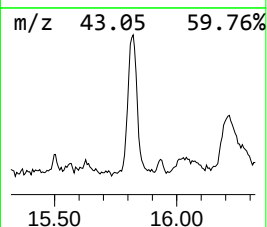
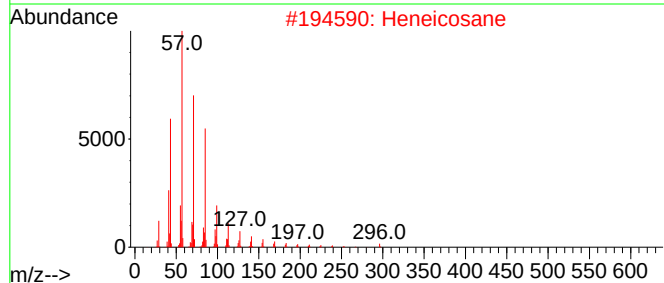
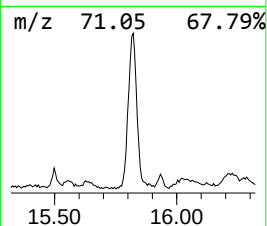
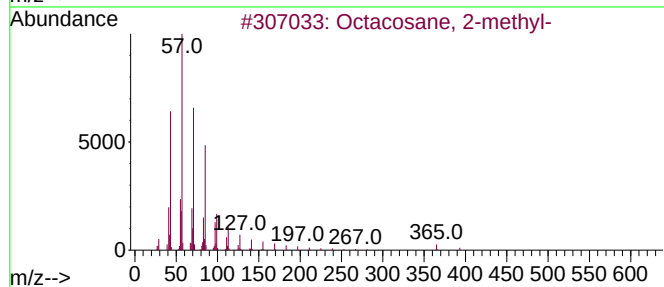
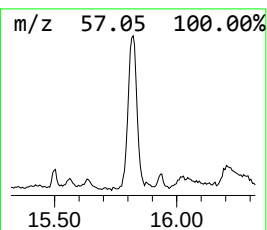
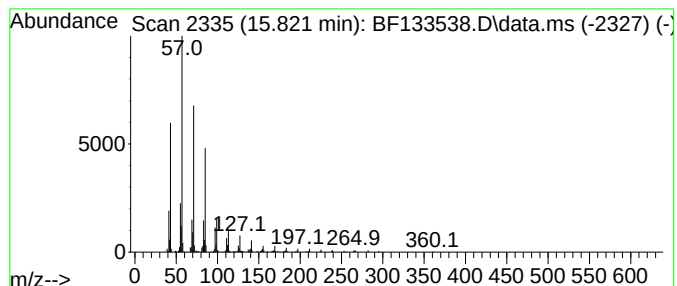
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.821	12.80 ng	492903	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



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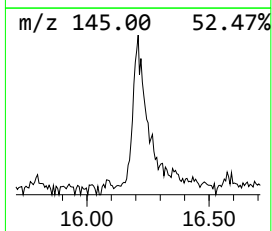
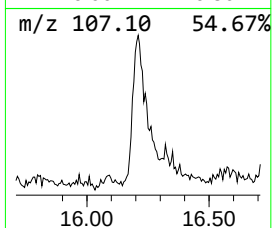
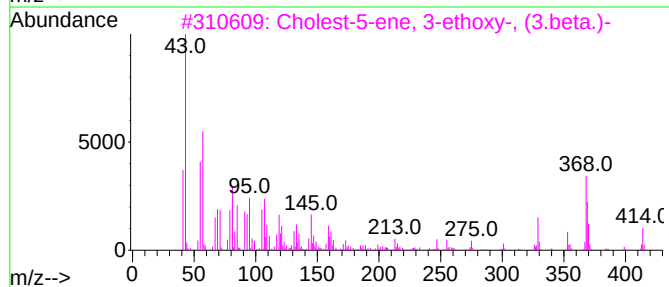
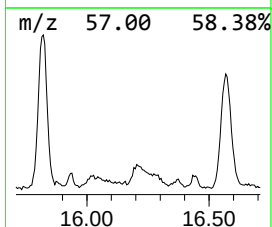
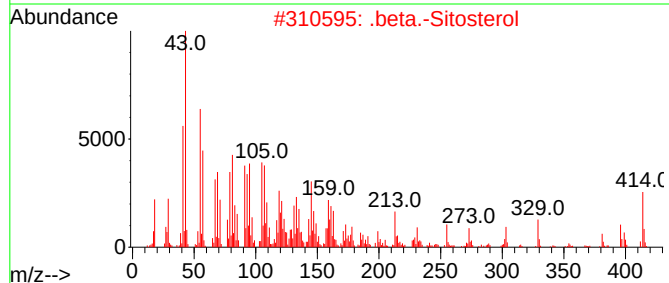
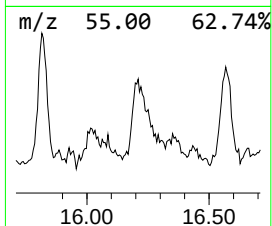
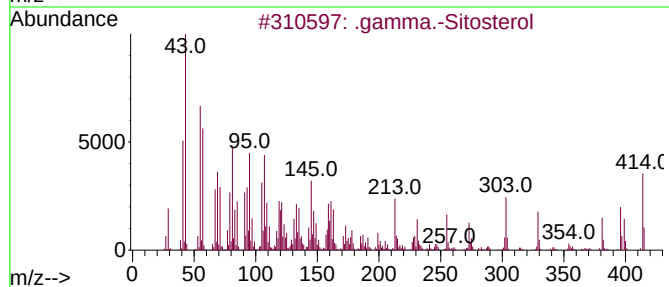
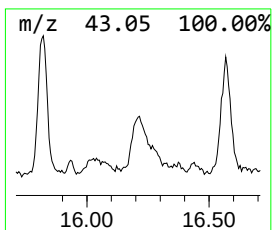
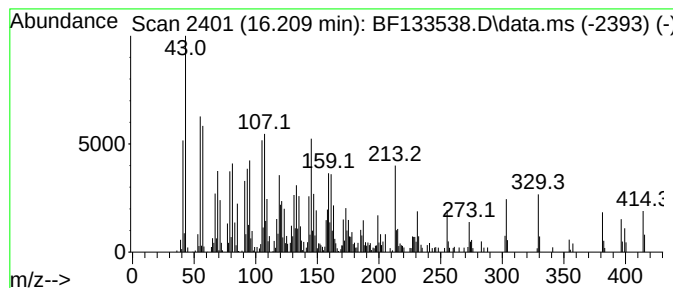
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	19.74 ng	760364	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2			.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3			Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	78
4			Campesterol	400	C28H48O	000474-62-4	49
5			(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
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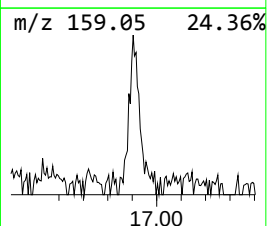
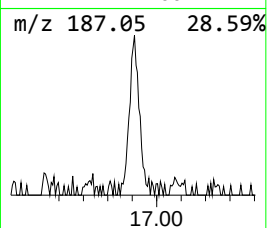
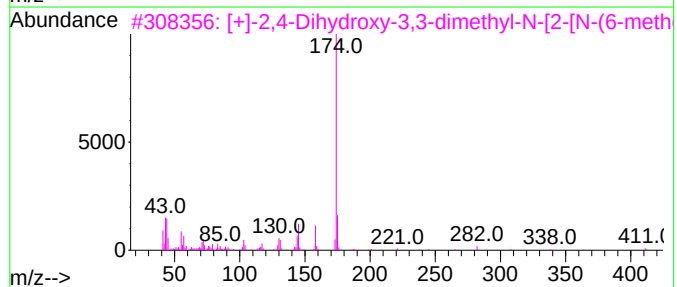
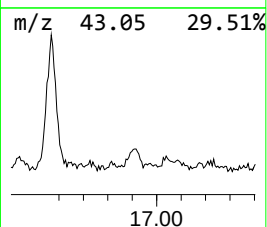
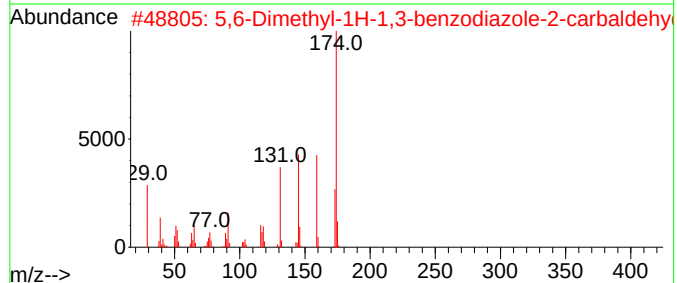
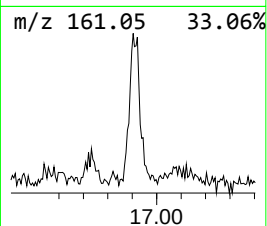
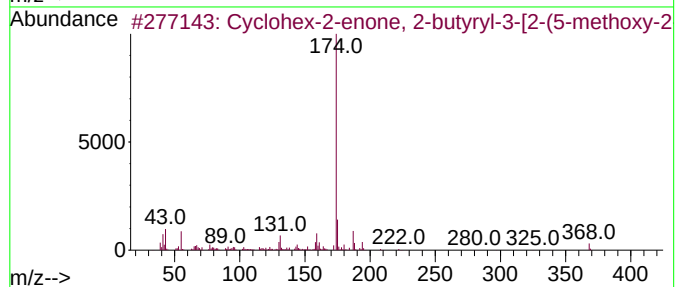
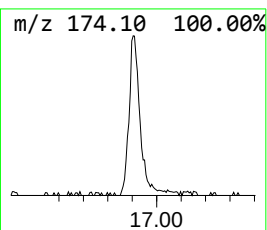
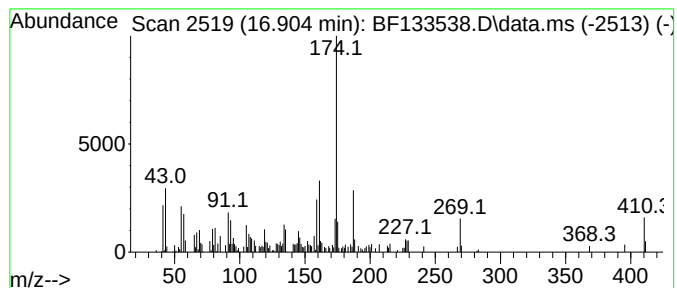
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.904 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.904	5.64 ng	217249	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohex-2-enone, 2-butyryl-3-[2...	368	C22H28N2O3	1000302-14-0	49
2			5,6-Dimethyl-1H-1,3-benzodiazole...	174	C10H10N2O	920484-85-1	47
3			[+]-2,4-Dihydroxy-3,3-dimethyl-N...	411	C18H25N3O6S	028124-68-7	43
4			2,2,4-Trimethyl-1,2-dihydro-quin...	189	C12H15NO	117330-56-0	38
5			2-(3-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-16-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
Data File : BF133538.D
Acq On : 31 May 2023 14:38
Operator : CG\JU
Sample : 02972-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-0A

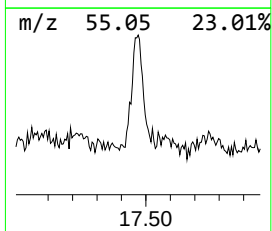
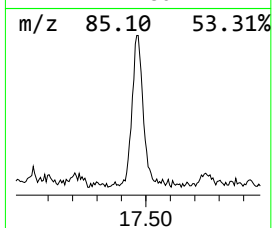
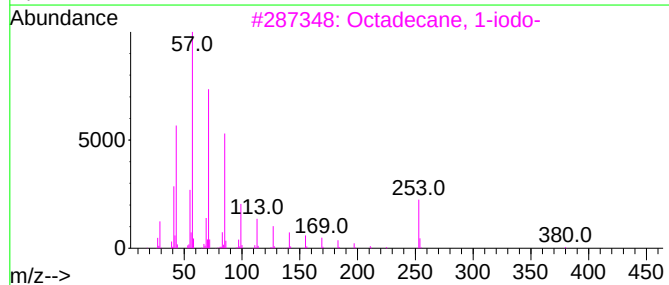
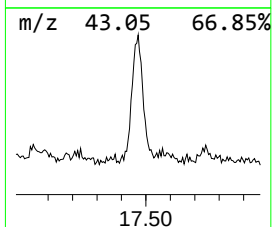
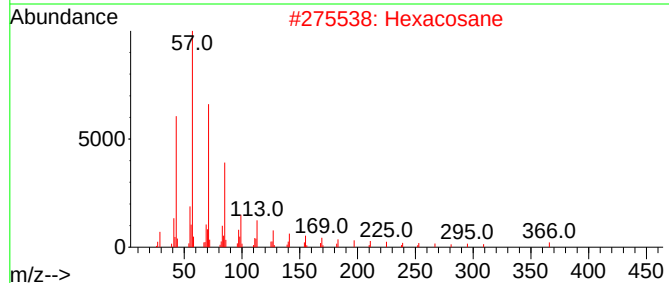
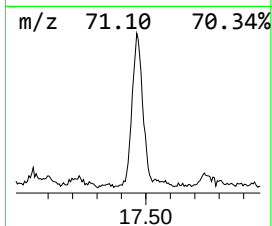
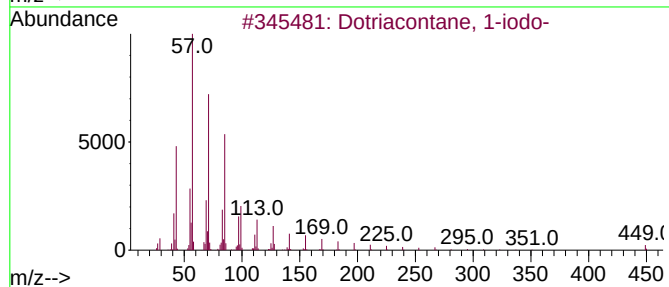
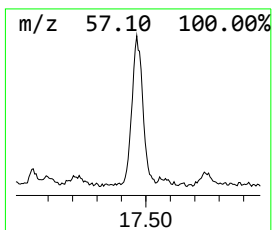
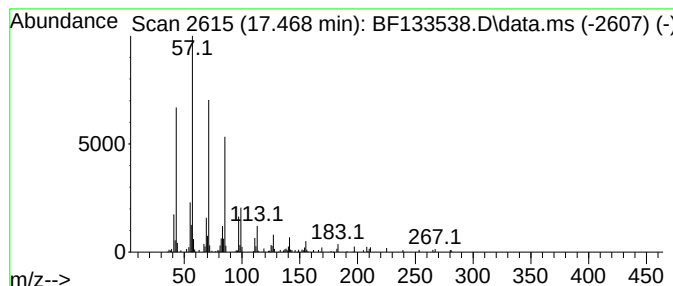
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Dotriacontane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.468	8.15 ng	313766	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4			Heptacosane	380	C27H56	000593-49-7	83
5			Tridecane, 3-methyl-	198	C14H30	006418-41-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
Data File : BF133538.D
Acq On : 31 May 2023 14:38
Operator : CG\JU
Sample : 02972-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

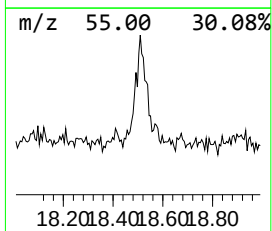
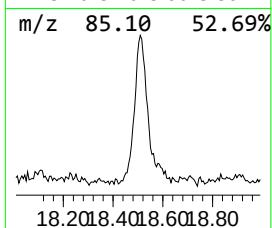
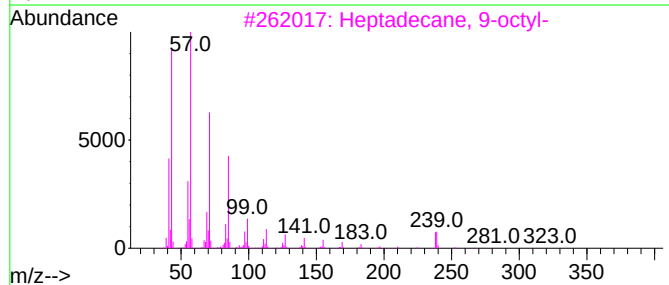
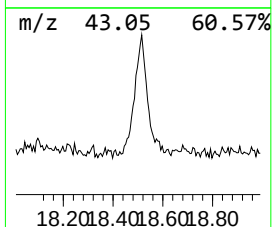
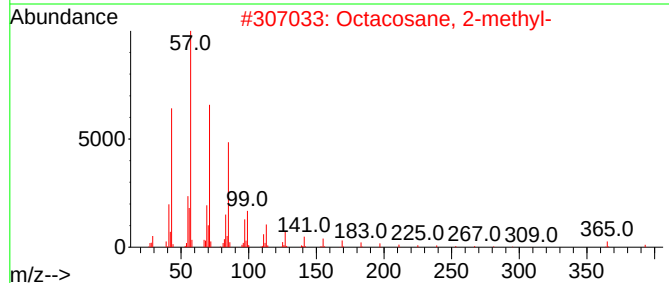
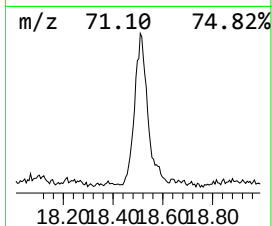
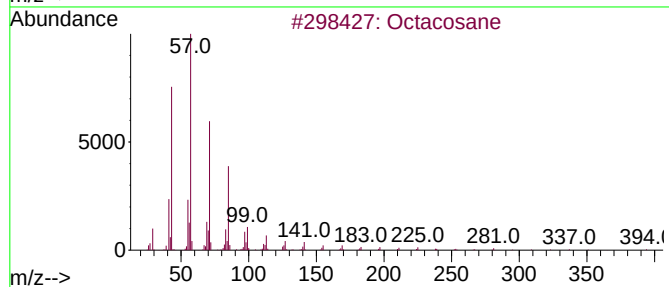
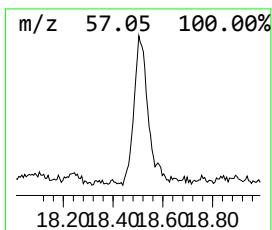
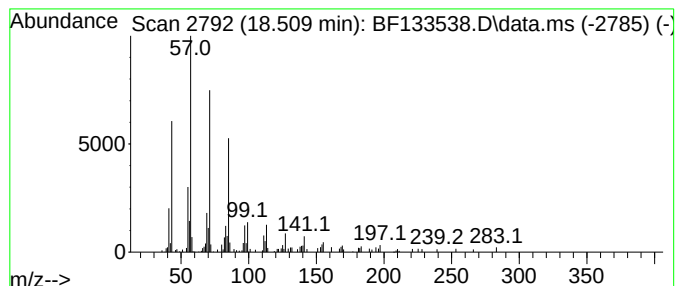
Instrument :
BNA_F
ClientSampleId :
TP-11-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.509	6.29 ng	242375	Perylene-d12	15.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
Data File : BF133538.D
Acq On : 31 May 2023 14:38
Operator : CG\JU
Sample : 02972-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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-...	5.045	5.3	ng	186910	1	6.828	708351	20.0
Benzophenone	10.580	2.4	ng	127734	3	9.869	1049550	20.0
n-Hexadecanoic ...	11.886	7.9	ng	460938	4	11.357	1162210	20.0
Octacosane	12.027	9.4	ng	543935	4	11.357	1162210	20.0
Octadecanoic acid	12.669	3.9	ng	228187	4	11.357	1162210	20.0
Hexacosane	13.245	6.9	ng	702541	5	13.998	2038260	20.0
Cyclopentadecane	13.863	3.2	ng	324968	5	13.998	2038260	20.0
Tetratetracontane	14.586	8.2	ng	834716	5	13.998	2038260	20.0
Heptacosane	15.163	16.5	ng	634756	6	15.451	770282	20.0
Octacosane, 2-m...	15.821	12.8	ng	492903	6	15.451	770282	20.0
.gamma.-Sitosterol	16.209	19.7	ng	760364	6	15.451	770282	20.0
Triacontane	16.568	11.7	ng	449010	6	15.451	770282	20.0
unknown16.904	16.904	5.6	ng	217249	6	15.451	770282	20.0
Dotriacontane, ...	17.468	8.2	ng	313766	6	15.451	770282	20.0
Heptadecane, 9-...	18.509	6.3	ng	242375	6	15.451	770282	20.0