

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
 Data File : BF132728.D
 Acq On : 09 Mar 2023 20:39
 Operator : CG\JU
 Sample : 01828-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AVENEL-60

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.104	254	258	263	rVB	53785	65981	1.65%	0.190%
2	5.210	441	446	457	rVB	1559131	1984592	49.71%	5.729%
3	5.610	510	514	517	rBV	4025417	3783214	94.77%	10.921%
4	5.993	576	579	584	rBV	53208	52558	1.32%	0.152%
5	6.610	679	684	687	rBV	4052531	3783576	94.78%	10.922%
6	6.798	713	716	720	rBV	77895	62915	1.58%	0.182%
7	6.975	743	746	750	rBV	1191561	1039837	26.05%	3.002%
8	7.387	813	816	823	rVB2	48510	53408	1.34%	0.154%
9	7.510	834	837	839	rBV	76699	69665	1.75%	0.201%
10	7.540	839	842	846	rVB	2680882	2465549	61.76%	7.117%
11	8.263	961	965	968	rBV	1721184	1320419	33.08%	3.812%
12	9.339	1144	1148	1151	rBV	4929633	3992122	100.00%	11.524%
13	9.481	1169	1172	1179	rVB	50878	47373	1.19%	0.137%
14	9.675	1202	1205	1208	rVB2	58144	52750	1.32%	0.152%
15	9.939	1246	1250	1254	rVB2	50032	52844	1.32%	0.153%
16	10.022	1261	1264	1268	rBV	1684005	1384803	34.69%	3.998%
17	10.733	1382	1385	1389	rVB	822741	740319	18.54%	2.137%
18	10.816	1395	1399	1403	rBV	2516853	2220323	55.62%	6.409%
19	10.928	1413	1418	1426	rVB7	51795	85886	2.15%	0.248%
20	11.045	1435	1438	1443	rBV	42951	48459	1.21%	0.140%
21	11.516	1515	1518	1521	rBV	1295604	1196725	29.98%	3.455%
22	11.539	1521	1522	1526	rVB	151149	125698	3.15%	0.363%
23	12.033	1602	1606	1612	rBV2	236981	299764	7.51%	0.865%
24	12.739	1723	1726	1729	rBV	318197	286324	7.17%	0.827%
25	12.775	1729	1732	1735	rVB	154384	138825	3.48%	0.401%
26	12.974	1760	1766	1771	rVV	259671	308959	7.74%	0.892%
27	13.022	1771	1774	1777	rVB3	40595	48907	1.23%	0.141%
28	13.110	1785	1789	1792	rBV	3694678	3124254	78.26%	9.019%
29	13.245	1810	1812	1815	rVB	210446	160804	4.03%	0.464%
30	13.539	1860	1862	1866	rVB3	67188	67070	1.68%	0.194%
31	13.610	1871	1874	1879	rVB	219489	212993	5.34%	0.615%
32	13.998	1937	1940	1951	rVB3	284901	491363	12.31%	1.418%
33	14.139	1961	1964	1966	rBV	85113	71827	1.80%	0.207%
34	14.180	1966	1971	1974	rBV	1217567	1246007	31.21%	3.597%
35	14.204	1974	1975	1978	rVB	118705	64645	1.62%	0.187%
36	14.269	1982	1986	1991	rBV	415359	459397	11.51%	1.326%

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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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.627	2044	2047	2049	rBV	87306	94622	2.37%	0.273%
38	15.027	2113	2115	2123	rVB	105251	122033	3.06%	0.352%
39	15.263	2151	2155	2158	rBV	119193	183783	4.60%	0.531%
40	15.310	2160	2163	2168	rVB	347371	376135	9.42%	1.086%
41	15.651	2219	2221	2227	rVB	91158	105836	2.65%	0.306%
42	15.721	2228	2233	2249	rVB	846716	1248516	31.27%	3.604%
43	16.180	2307	2311	2317	rVB	235745	383560	9.61%	1.107%
44	17.939	2604	2610	2625	rVB	125000	516914	12.95%	1.492%

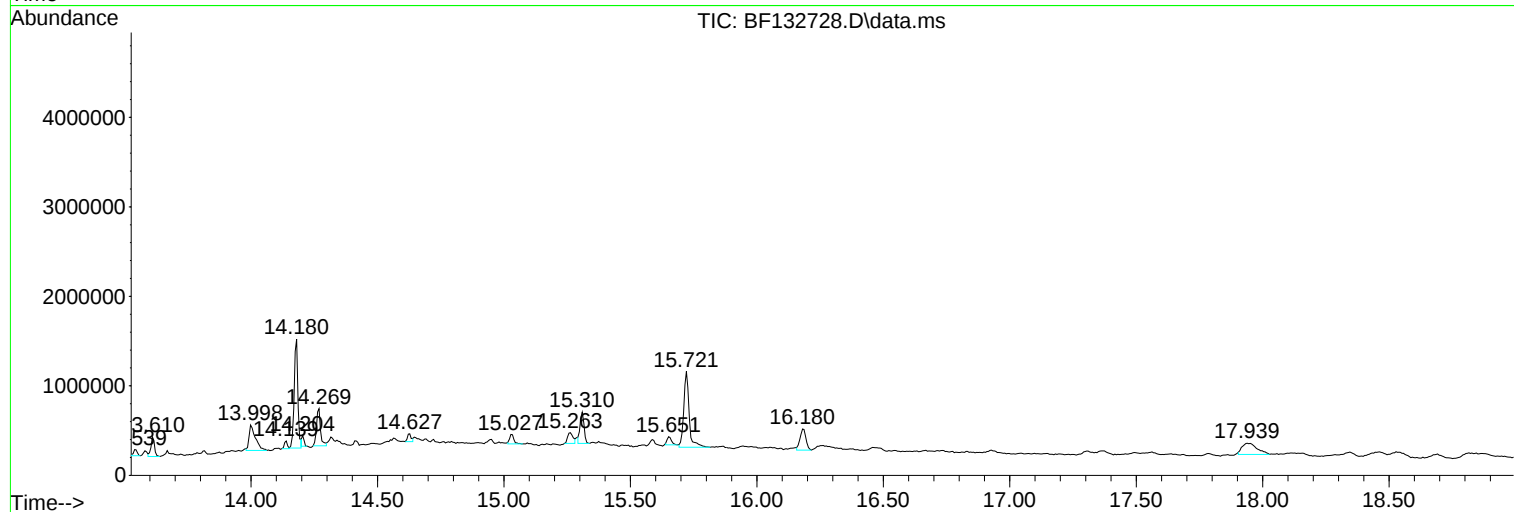
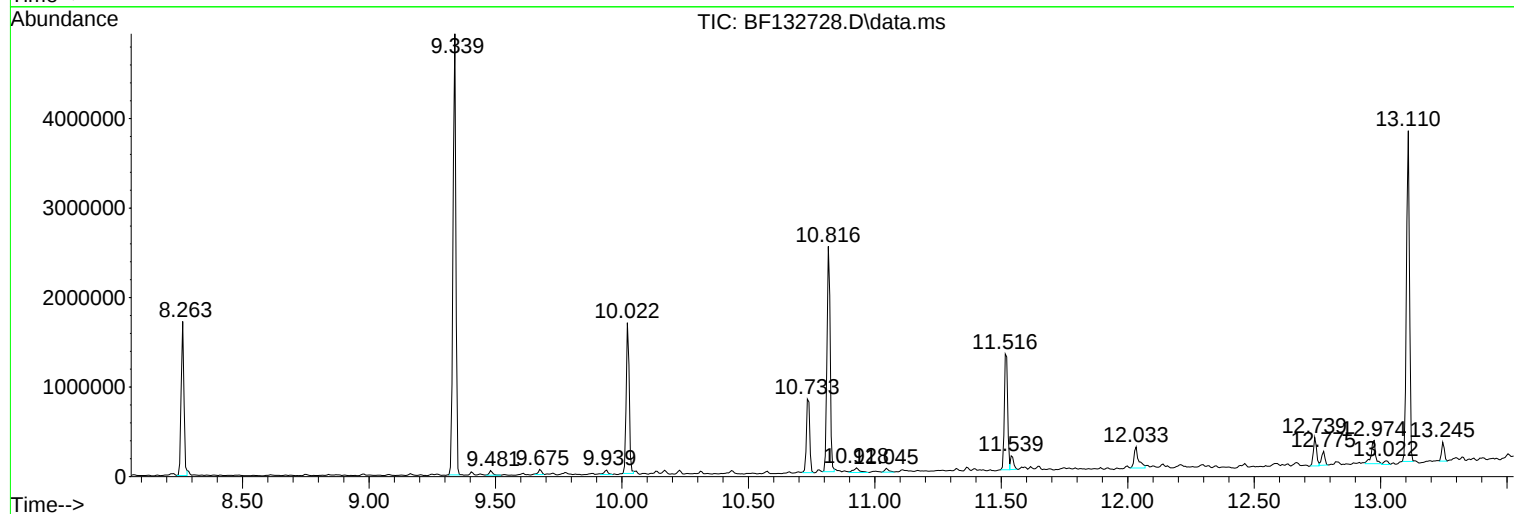
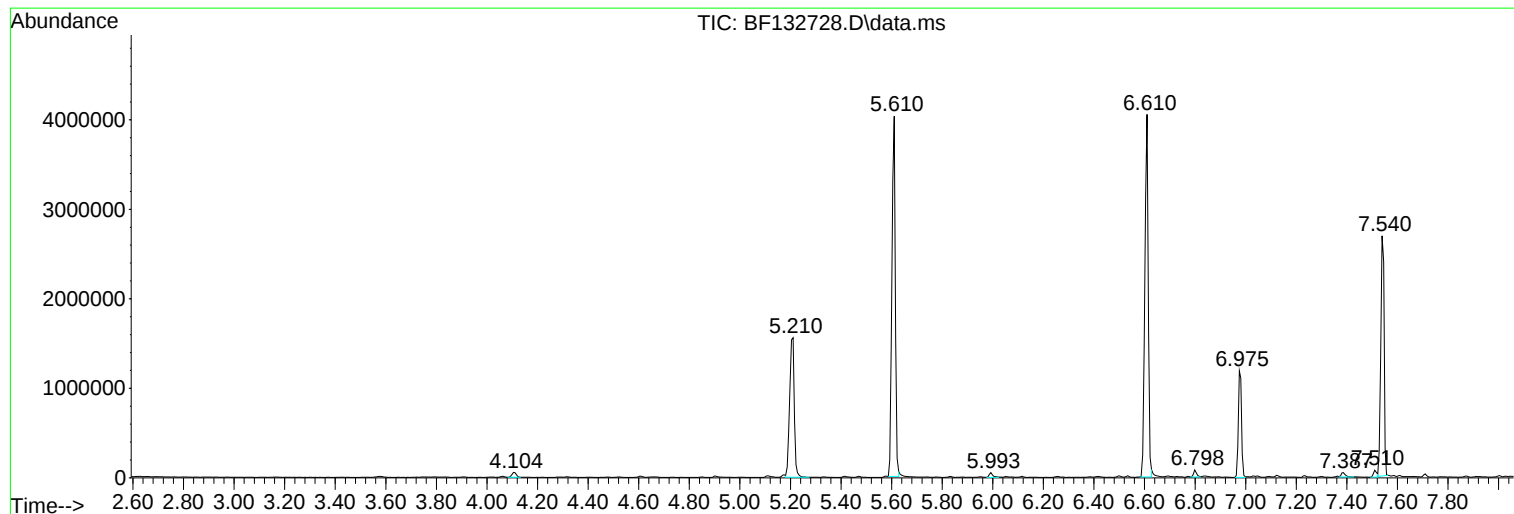
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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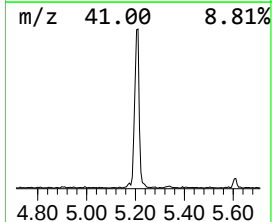
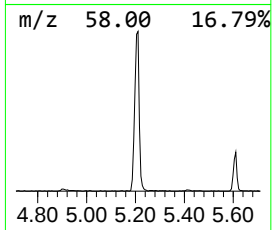
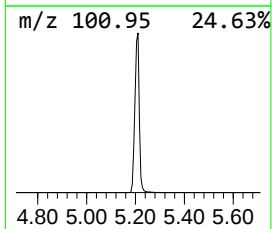
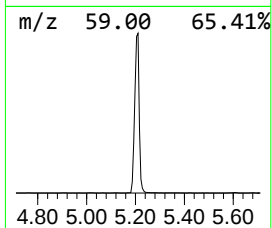
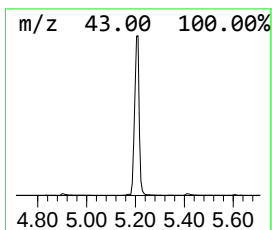
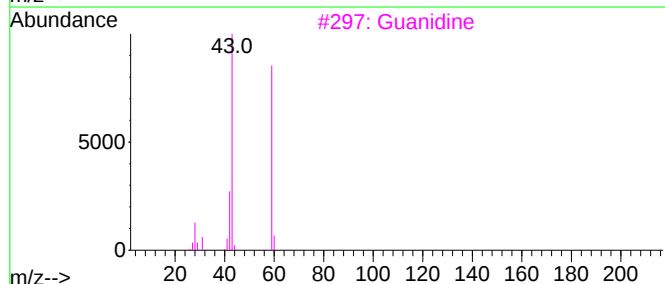
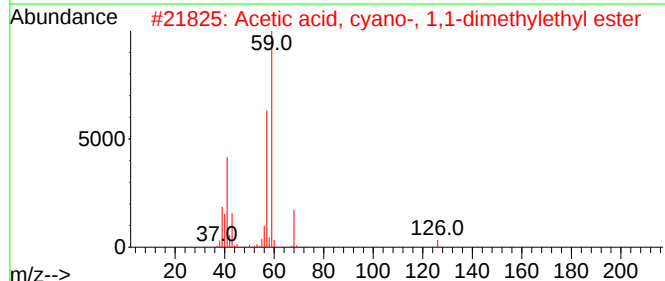
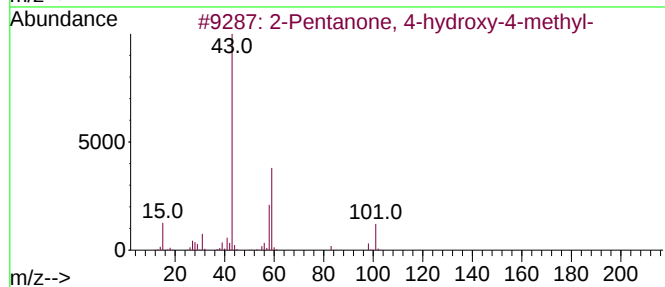
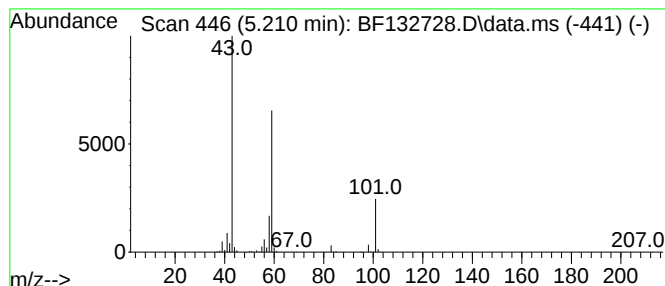
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	38.17 ng	1984590	1,4-Dichlorobenzene-d4	6.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Guanidine	59	CH5N3	000113-00-8	9
4			Acetone	58	C3H6O	000067-64-1	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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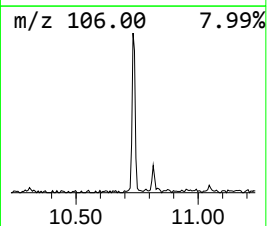
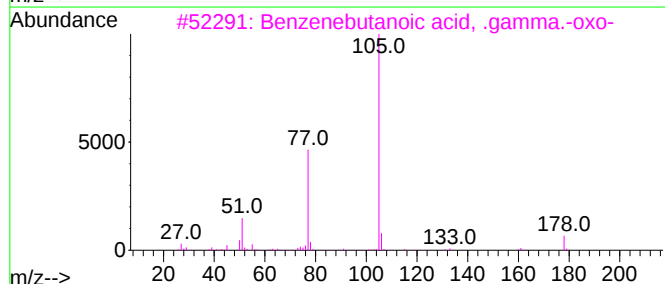
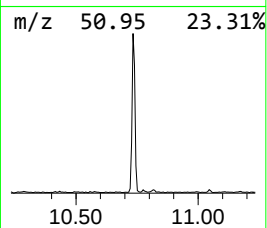
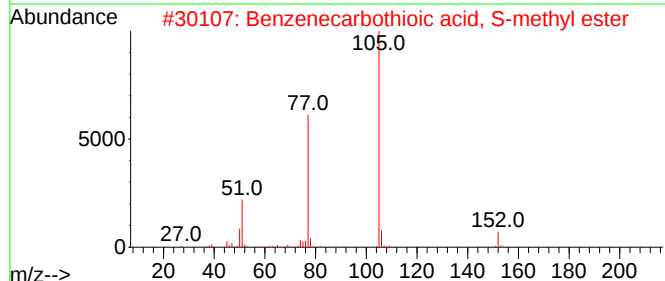
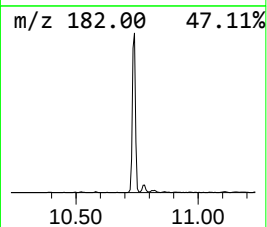
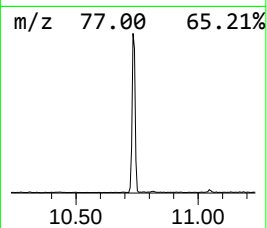
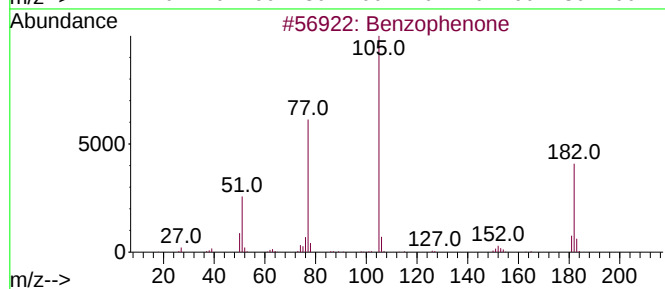
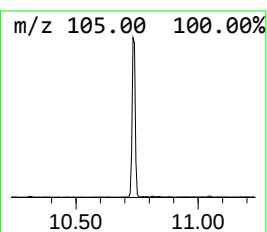
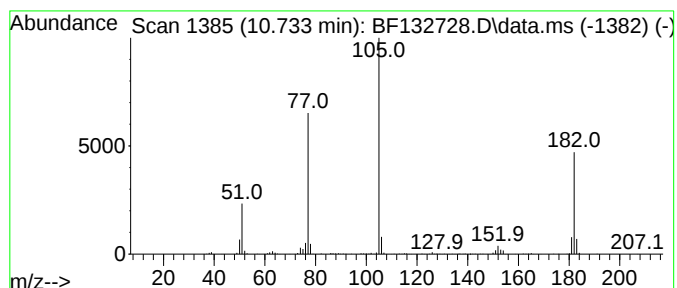
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	10.69 ng	740319	Acenaphthene-d10	10.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



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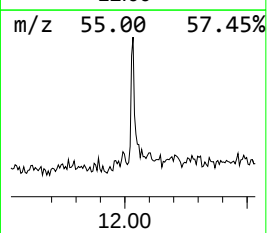
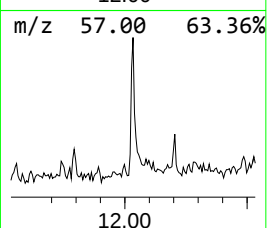
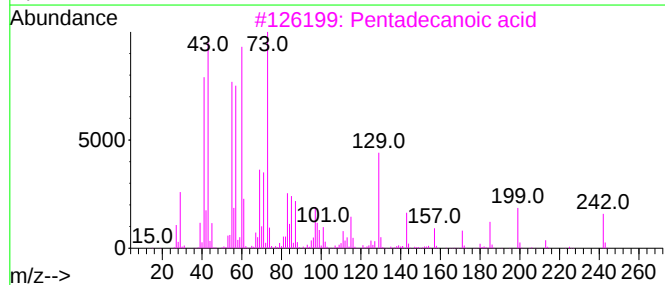
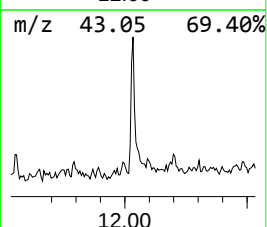
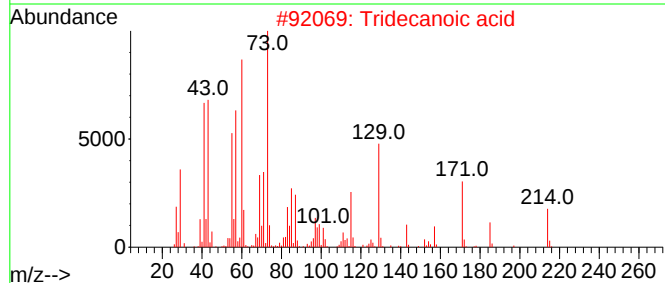
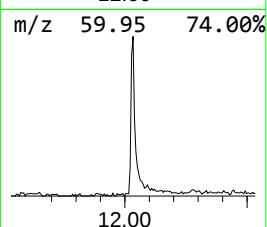
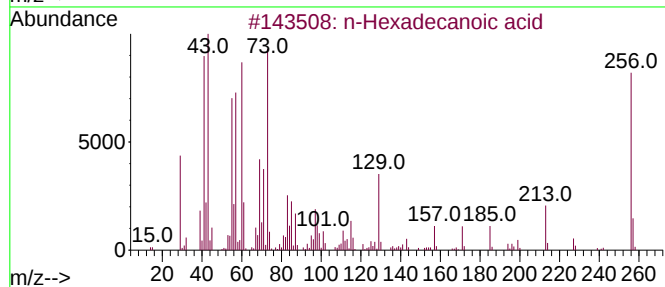
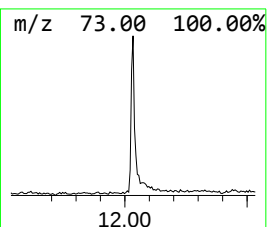
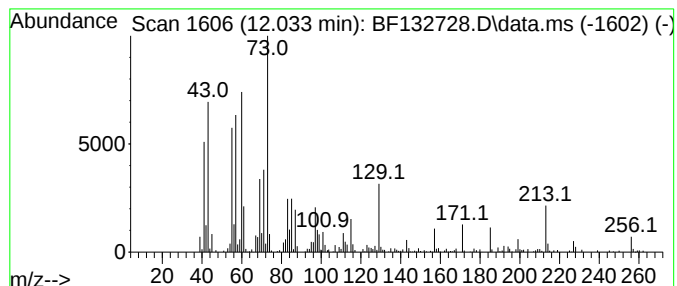
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.033	5.01 ng	299764	Phenanthrene-d10		11.522	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	70
5	Hexadecane, 1-chloro-		260	C16H33Cl	004860-03-1	25



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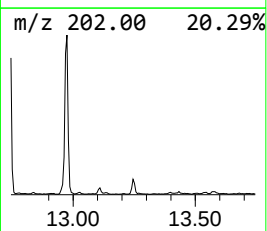
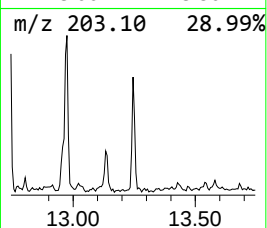
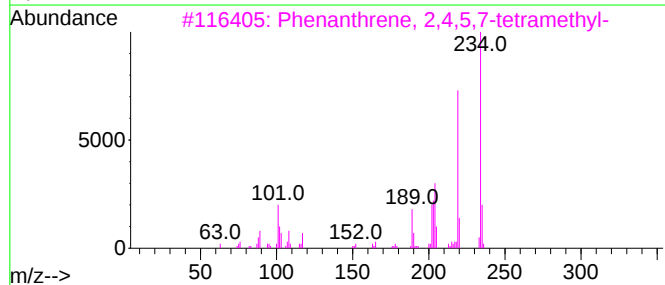
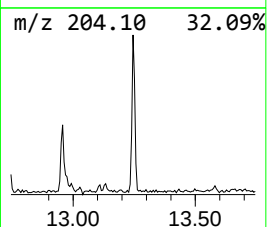
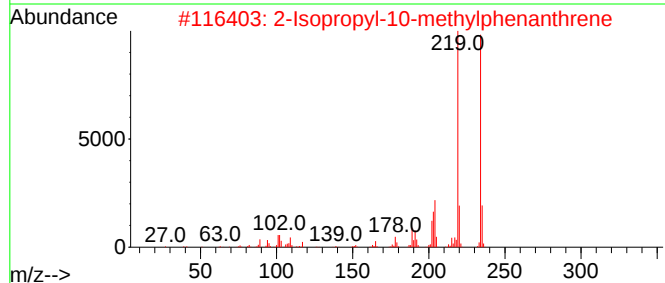
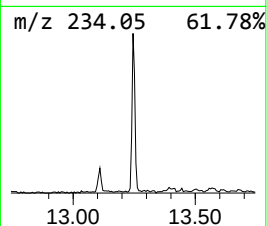
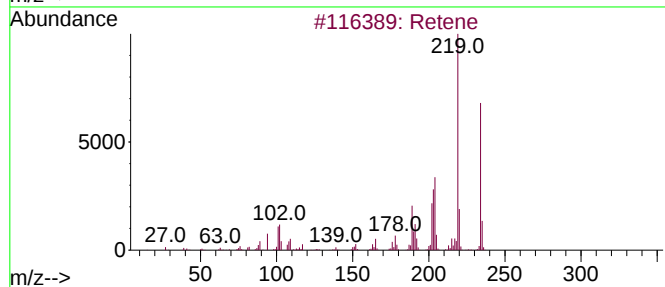
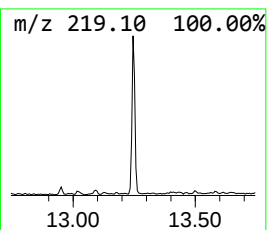
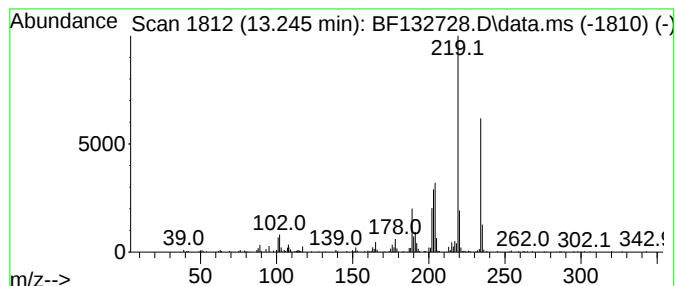
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Retene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.245	2.58 ng	160804	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Retene	234	C18H18	000483-65-8	98
2			2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	91
3			Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	86
4			Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	53
5			Ethanone, 1-(4,6-dihydroxy-2,3,5...	234	C13H14O4	021987-07-5	49



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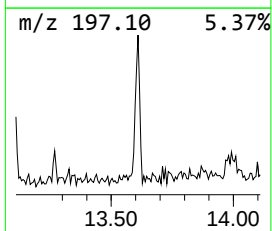
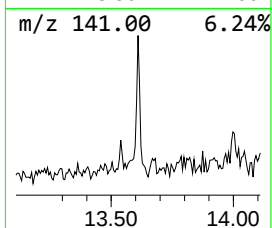
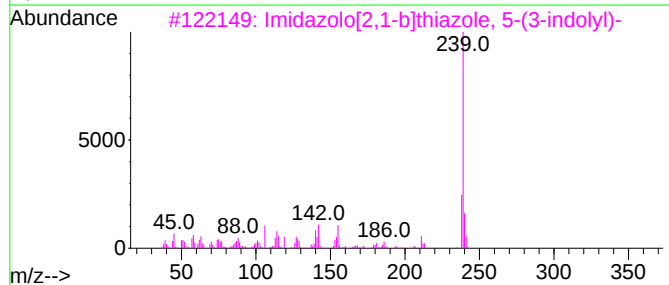
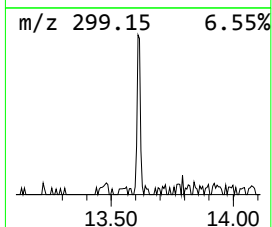
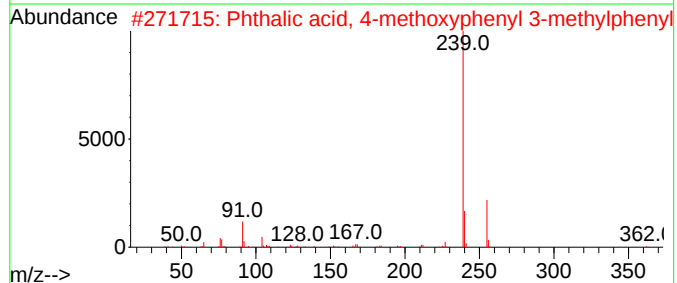
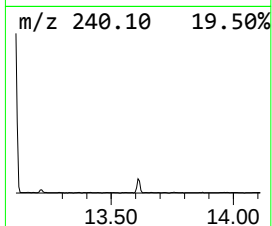
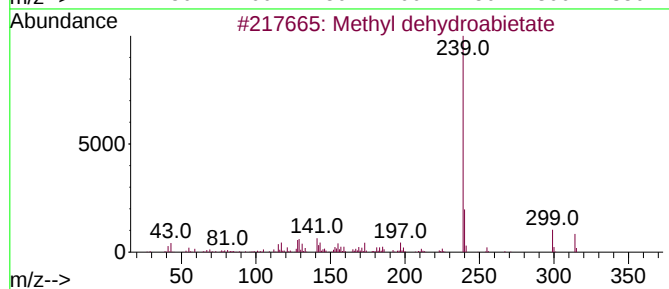
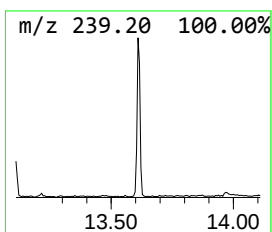
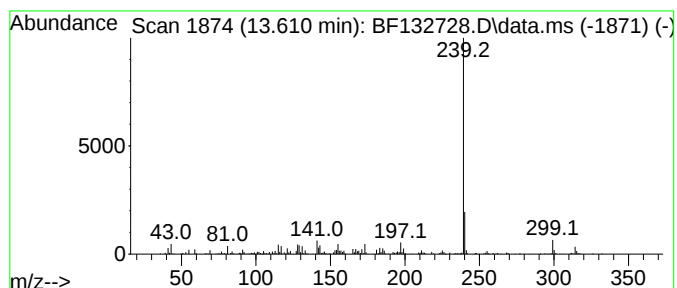
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl dehydroabietate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.610	3.42 ng	212993	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl dehydroabietate	314	C21H30O2	001235-74-1	90
2			Phthalic acid, 4-methoxyphenyl 3...	362	C22H18O5	1000315-68-0	64
3			Imidazolo[2,1-b]thiazole, 5-(3-i...	239	C13H9N3S	327097-37-0	64
4			trans-1,2-Bis(methyldichlorosily...	252	C4H8Cl4Si2	065899-10-7	49
5			Benzaldehyde, 3-[4-(1,1-dimethyl...	254	C17H18O2	069770-23-6	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132728.D
Acq On : 09 Mar 2023 20:39
Operator : CG\JU
Sample : 01828-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

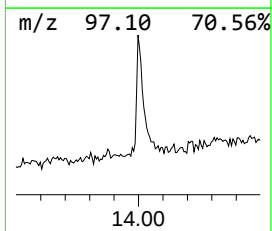
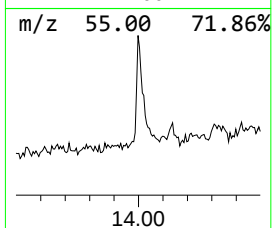
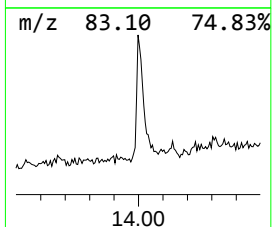
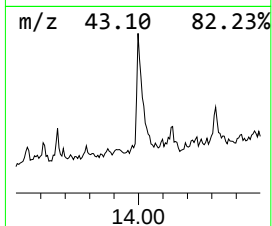
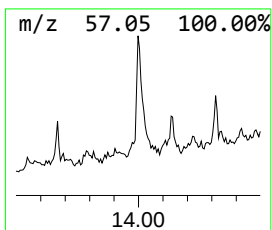
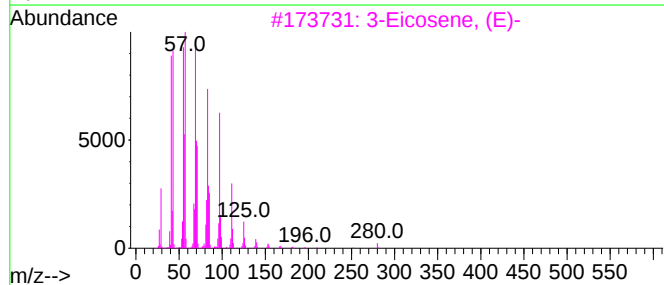
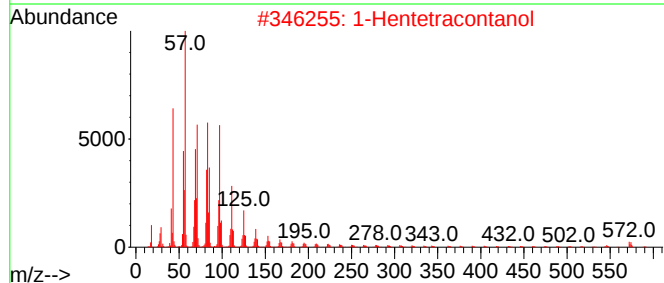
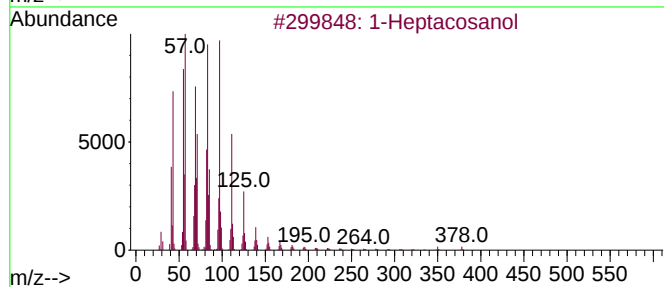
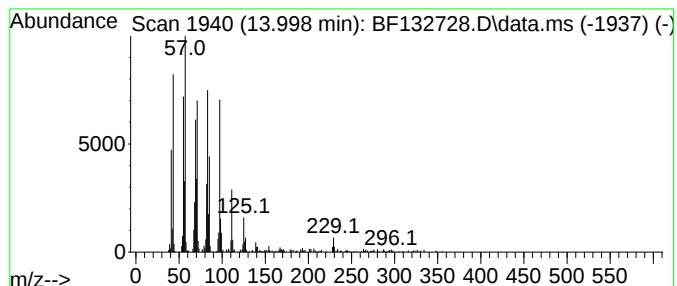
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.998	7.89 ng	491363	Chrysene-d12	14.180	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	90
2	1-Hentetracontanol	593	C41H84O	040710-42-7	90
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
4	1-Hexacosanol	382	C26H54O	000506-52-5	74
5	1-Heneicosanol	312	C21H44O	015594-90-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132728.D
Acq On : 09 Mar 2023 20:39
Operator : CG\JU
Sample : 01828-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AVENEL-60

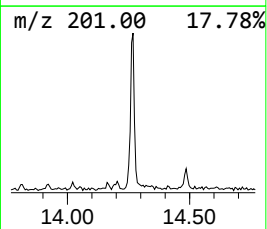
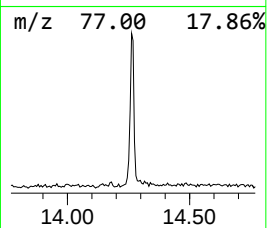
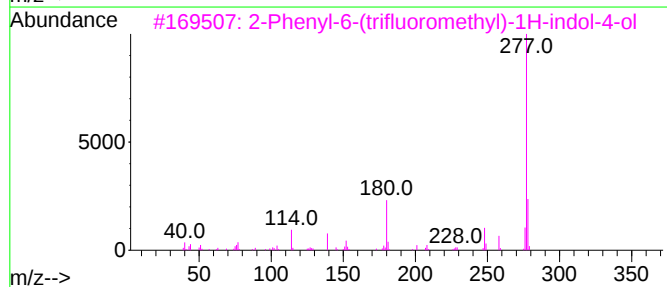
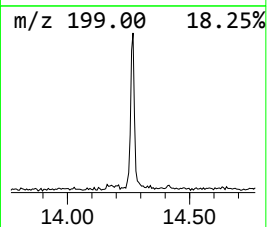
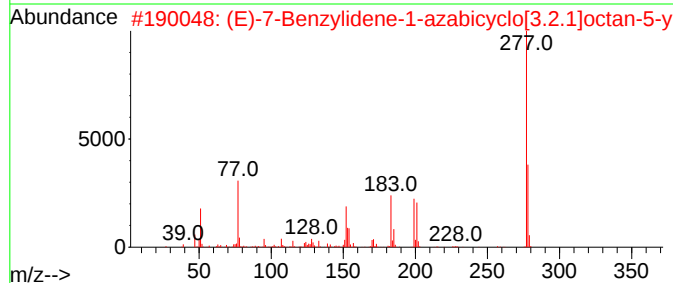
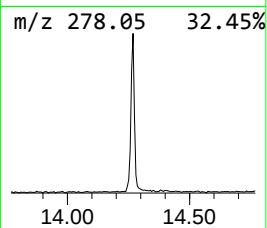
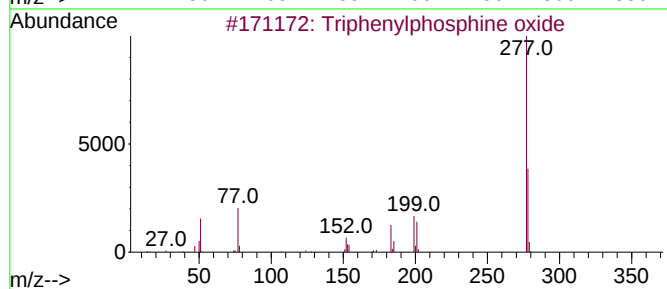
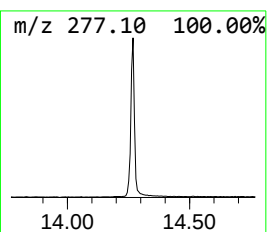
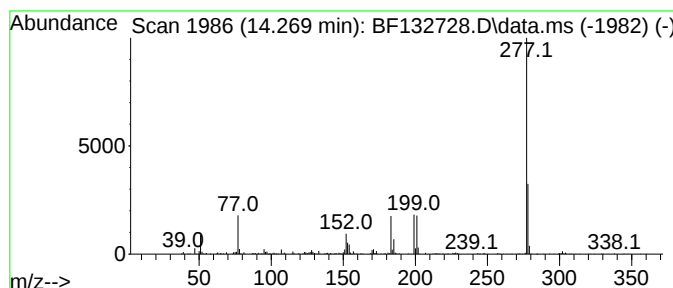
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	7.37 ng	459397	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	59
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	49
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132728.D
Acq On : 09 Mar 2023 20:39
Operator : CG\JU
Sample : 01828-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
AVENEL-60

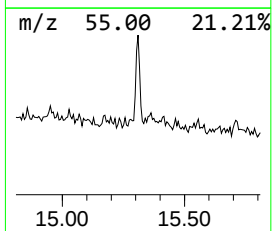
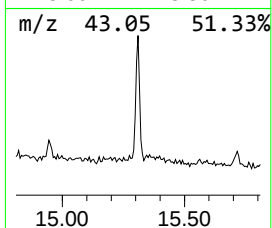
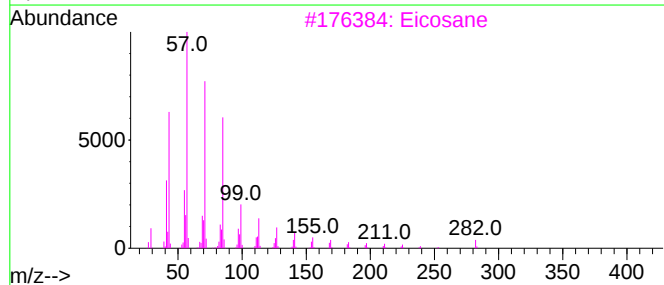
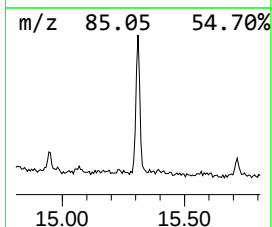
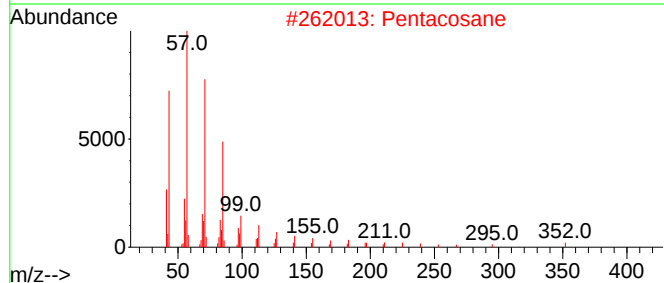
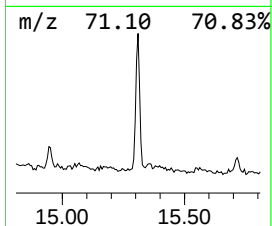
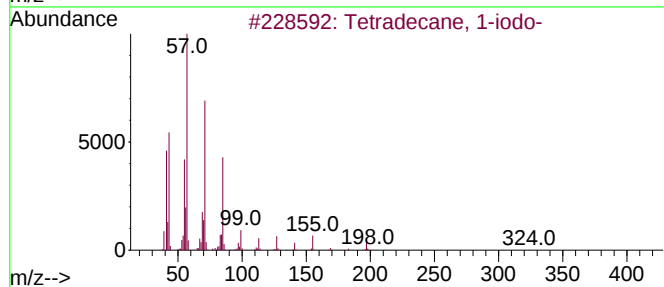
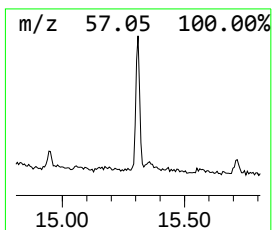
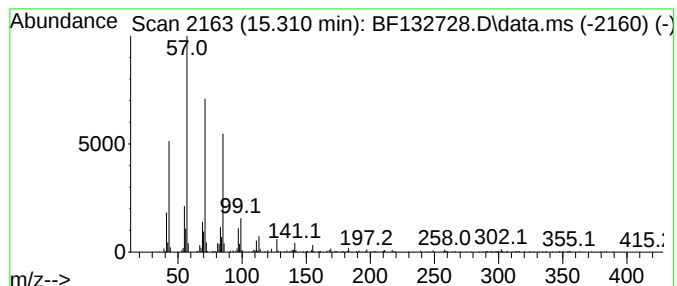
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	6.03 ng	376135	Perylene-d12	15.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	90
2			Pentacosane	352	C25H52	000629-99-2	90
3			Eicosane	282	C20H42	000112-95-8	90
4			Tetradecane	198	C14H30	000629-59-4	83
5			Hexacosane	366	C26H54	000630-01-3	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132728.D
Acq On : 09 Mar 2023 20:39
Operator : CG\JU
Sample : 01828-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AVENEL-60

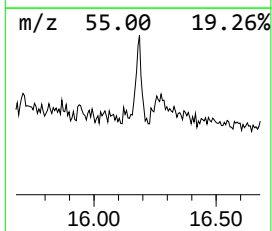
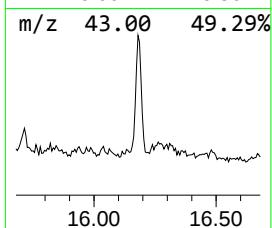
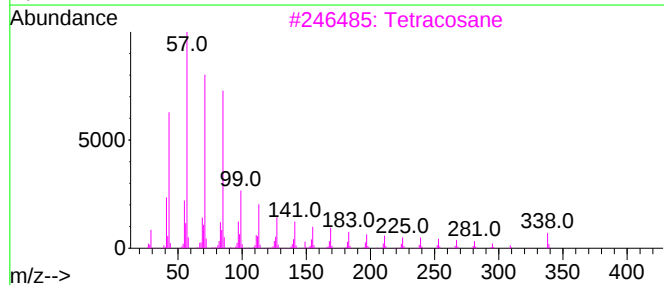
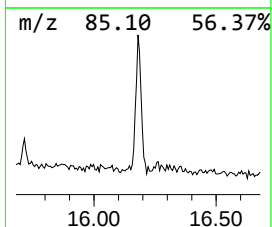
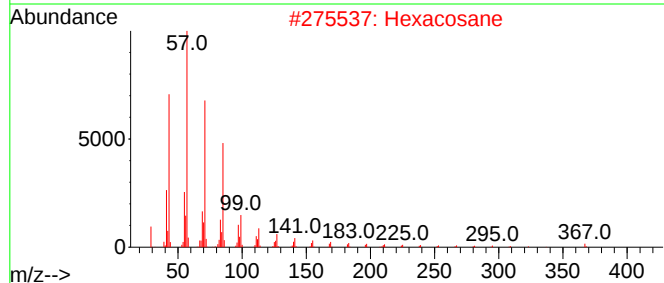
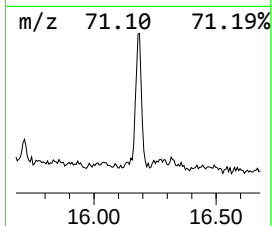
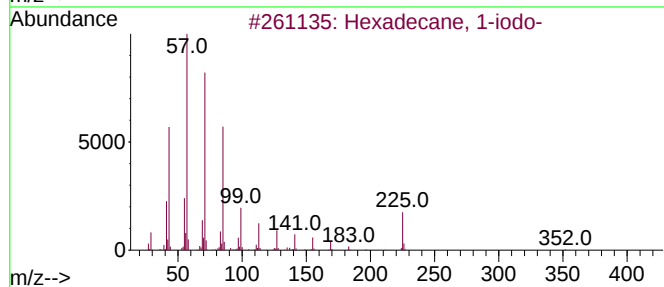
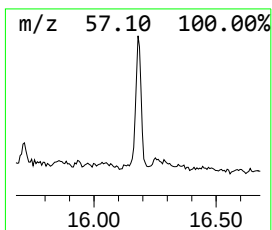
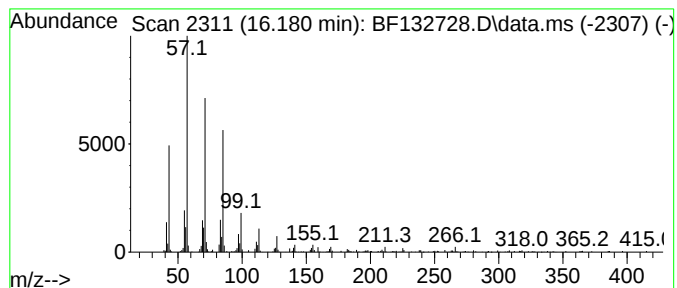
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	6.14 ng	383560	Perylene-d12	15.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heneicosane	296	C21H44	000629-94-7	87
5			Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132728.D
Acq On : 09 Mar 2023 20:39
Operator : CG\JU
Sample : 01828-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

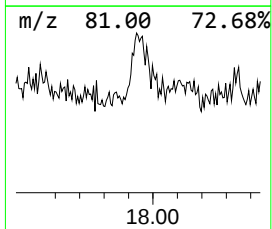
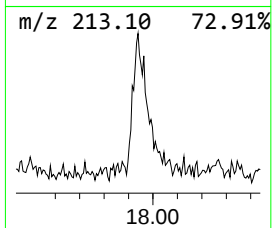
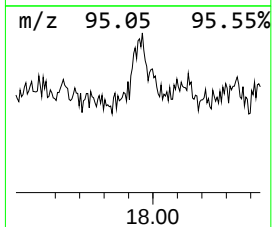
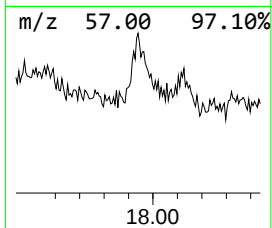
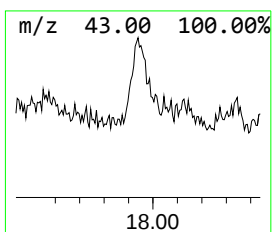
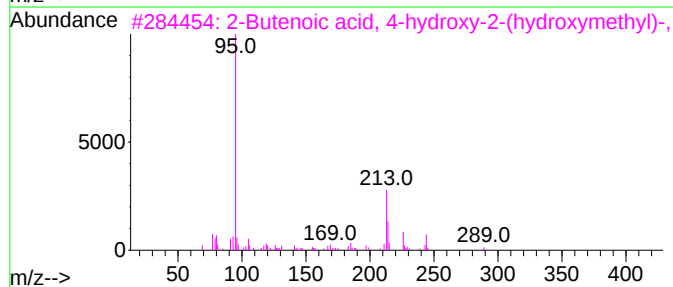
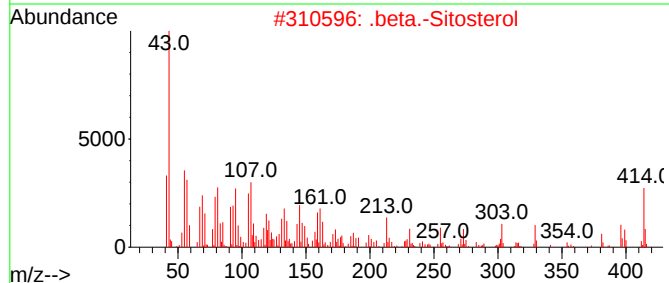
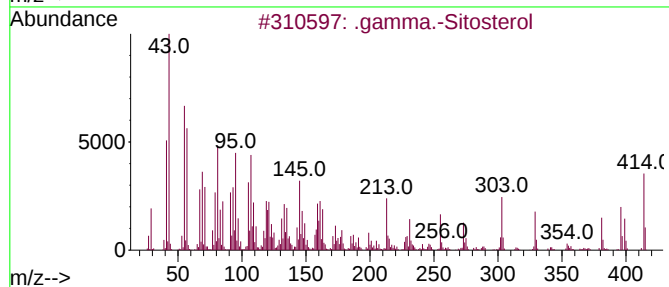
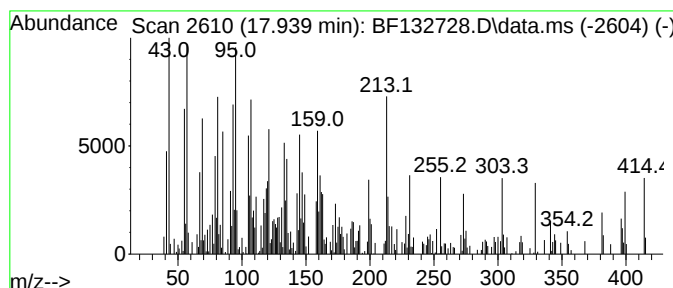
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	8.28 ng	516914	Perylene-d12	15.721
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		.gamma.-Sitosterol	414 C29H50O	000083-47-6 90
2		.beta.-Sitosterol	414 C29H50O	000083-46-5 86
3		2-Butenoic acid, 4-hydroxy-2-(hy...	376 C20H24O7	024268-45-9 35
4		cis-4-Acetoxy-trans-1-(m-methoxy...	273 C16H19NO3	1000241-10-4 25
5		17-(1,5-Dimethylhexyl)-10,13-dim...	414 C29H50O	1000210-86-9 22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132728.D
Acq On : 09 Mar 2023 20:39
Operator : CG\JU
Sample : 01828-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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
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Benzophenone	10.733	10.7	ng	740319	3	10.022	1384800	20.0
n-Hexadecanoic ...	12.033	5.0	ng	299764	4	11.522	1196730	20.0
Retene	13.245	2.6	ng	160804	5	14.180	1246010	20.0
Methyl dehydroa...	13.610	3.4	ng	212993	5	14.180	1246010	20.0
1-Heptacosanol	13.998	7.9	ng	491363	5	14.180	1246010	20.0
Triphenylphosph...	14.269	7.4	ng	459397	5	14.180	1246010	20.0
Tetradecane, 1-...	15.310	6.0	ng	376135	6	15.721	1248520	20.0
Hexadecane, 1-i...	16.180	6.1	ng	383560	6	15.721	1248520	20.0
.gamma.-Sitosterol	17.939	8.3	ng	516914	6	15.721	1248520	20.0