

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
 Data File : BF132713.D
 Acq On : 09 Mar 2023 12:24
 Operator : CG\JU
 Sample : 01829-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-01-20230306

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: BF132713.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.604	340	343	348	rBV	97765	100656	2.29%	0.290%
2	5.210	441	446	456	rVB	1532289	1941243	44.18%	5.597%
3	5.610	510	514	518	rBV	3857001	3838286	87.35%	11.067%
4	6.610	680	684	694	rBV	3689729	3851314	87.65%	11.104%
5	6.981	743	747	750	rBV	1303429	1104899	25.15%	3.186%
6	7.545	838	843	846	rBV	3013968	2545399	57.93%	7.339%
7	8.263	962	965	968	rBV	1752145	1425340	32.44%	4.110%
8	9.339	1144	1148	1151	rBV	5268068	4394100	100.00%	12.669%
9	9.604	1189	1193	1196	rBV	226975	182462	4.15%	0.526%
10	9.922	1243	1247	1249	rBV	80466	78285	1.78%	0.226%
11	10.027	1261	1265	1268	rBV	1921236	1651389	37.58%	4.761%
12	10.739	1381	1386	1391	rVB	602290	496697	11.30%	1.432%
13	10.822	1395	1400	1403	rBV	3197847	2784084	63.36%	8.027%
14	11.110	1446	1449	1453	rBV	99836	92237	2.10%	0.266%
15	11.369	1490	1493	1496	rVB	112466	91896	2.09%	0.265%
16	11.410	1496	1500	1502	rBV2	95178	79534	1.81%	0.229%
17	11.521	1515	1519	1522	rBV	1908355	1578322	35.92%	4.551%
18	12.033	1601	1606	1620	rBV2	840669	930955	21.19%	2.684%
19	12.745	1722	1727	1735	rBV	178263	240115	5.46%	0.692%
20	12.821	1737	1740	1751	rVV	316635	384028	8.74%	1.107%
21	12.974	1760	1766	1773	rBV	215811	290382	6.61%	0.837%
22	13.039	1774	1777	1779	rVB	116010	99689	2.27%	0.287%
23	13.110	1785	1789	1793	rBV	3994225	3564024	81.11%	10.276%
24	13.998	1937	1940	1953	rVB2	304152	433869	9.87%	1.251%
25	14.180	1967	1971	1974	rBV	1277572	1176078	26.76%	3.391%
26	14.204	1974	1975	1980	rVB2	101009	81168	1.85%	0.234%
27	14.768	2068	2071	2073	rBV	81084	86545	1.97%	0.250%
28	15.262	2152	2155	2158	rBV	77563	100267	2.28%	0.289%
29	15.721	2229	2233	2240	rVB2	799924	1059351	24.11%	3.054%

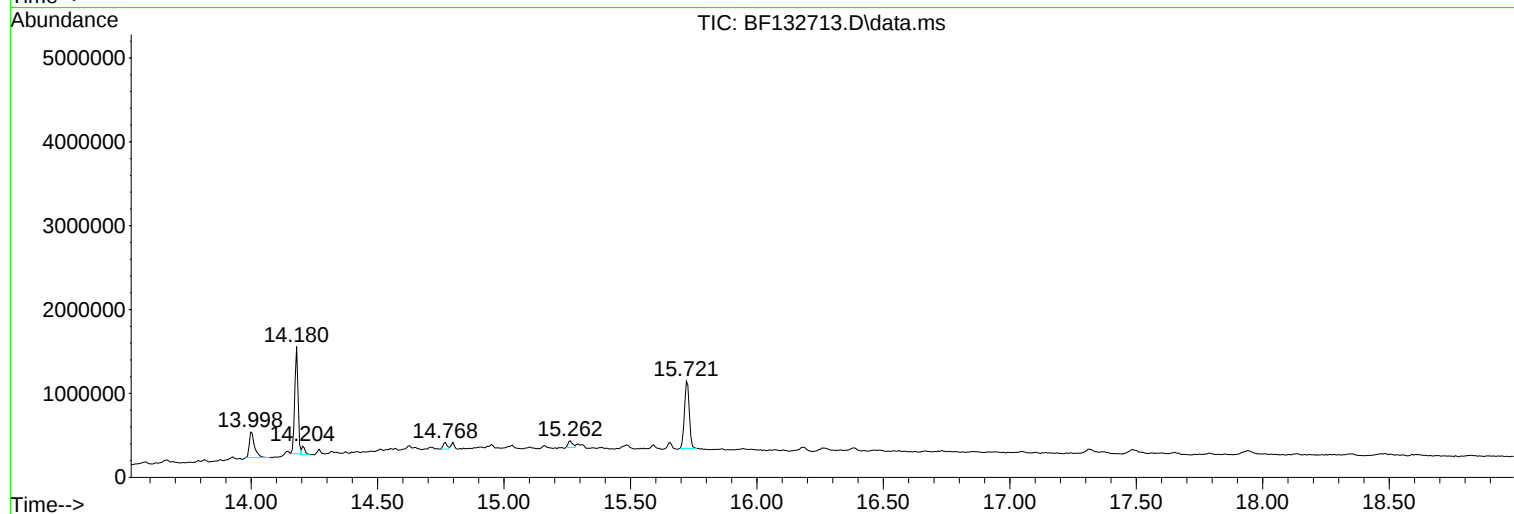
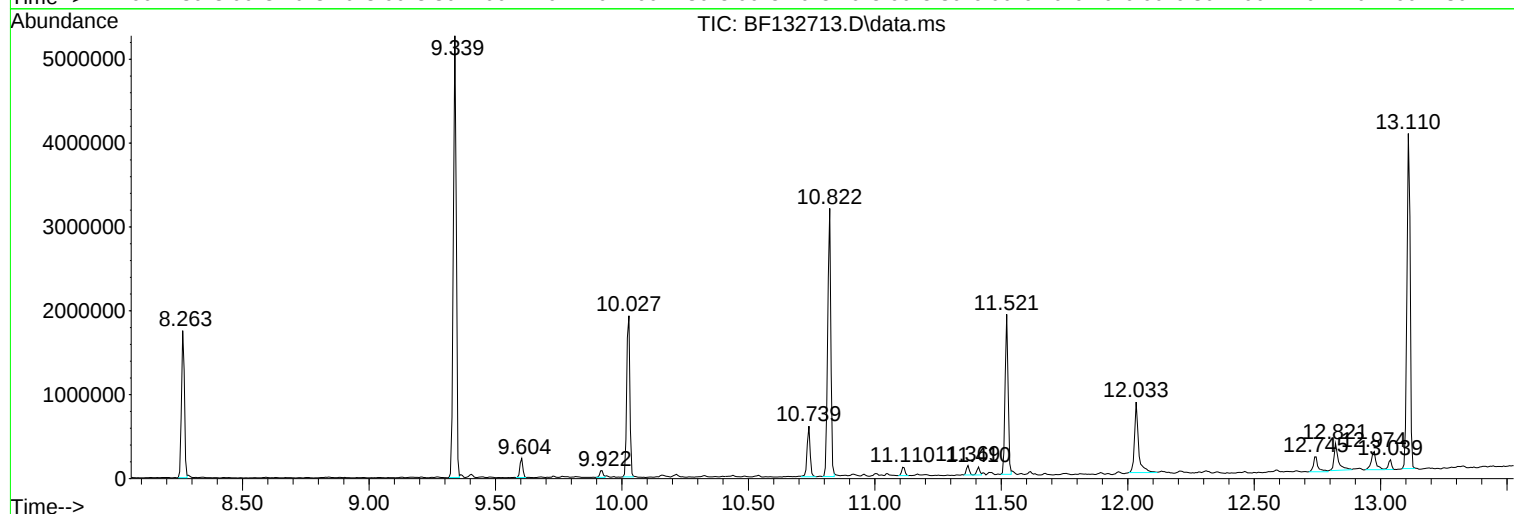
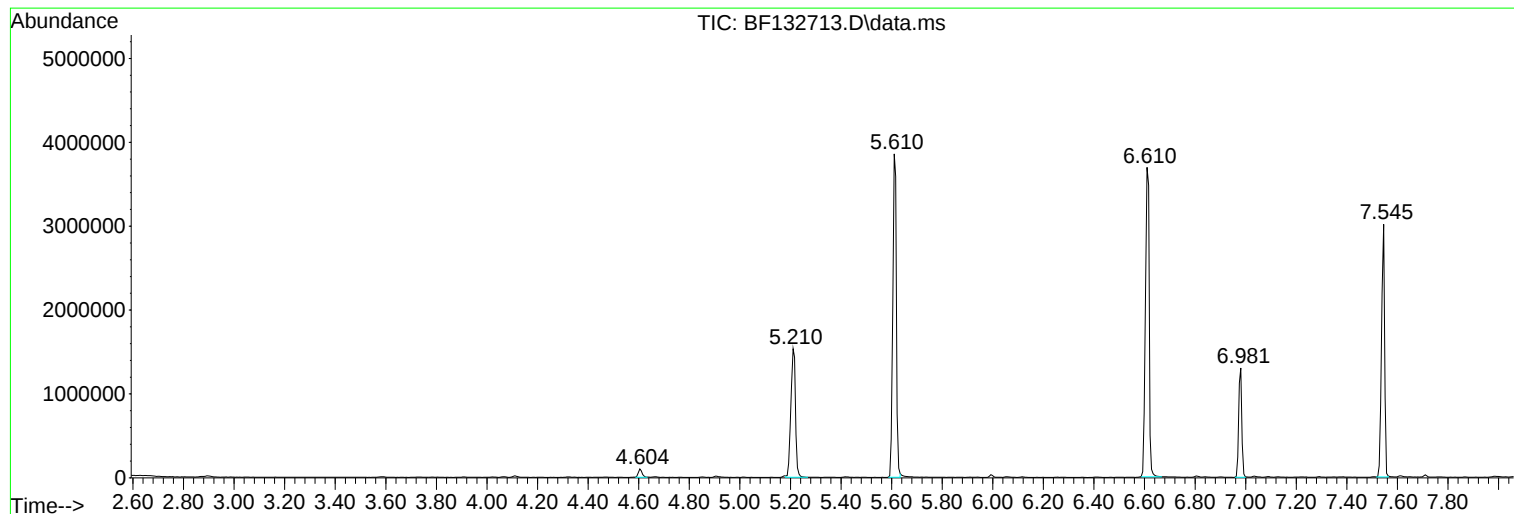
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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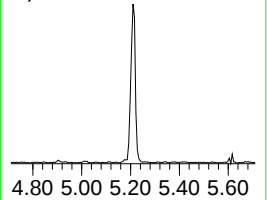
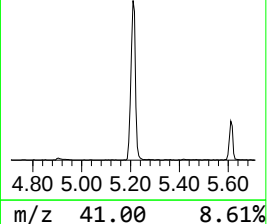
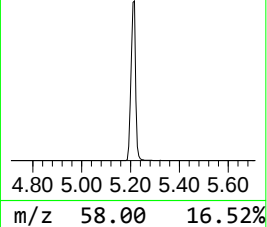
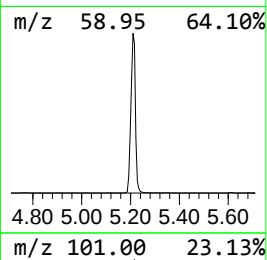
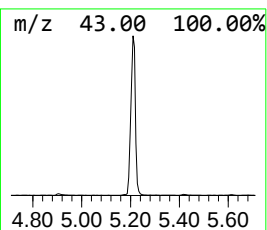
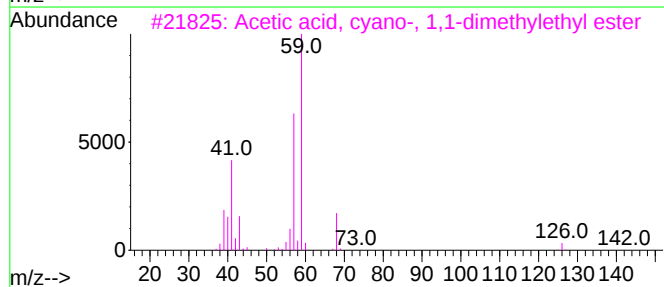
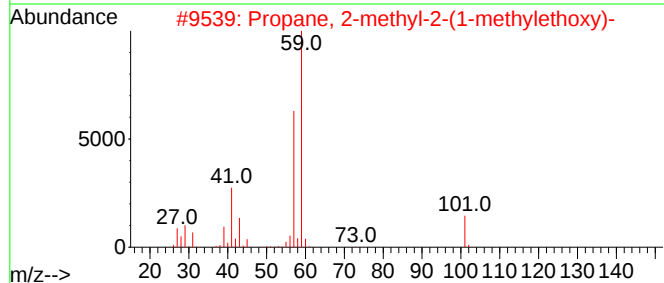
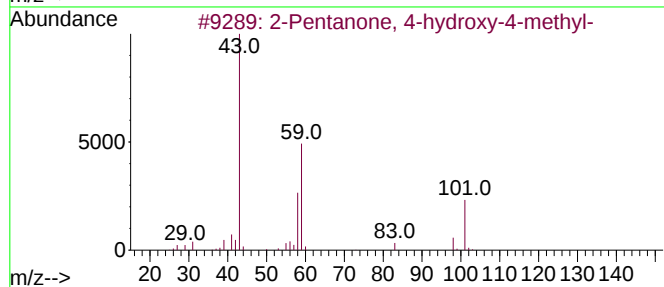
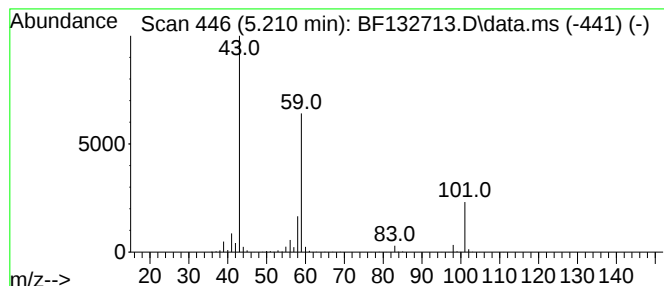
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	35.14 ng	1941240	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	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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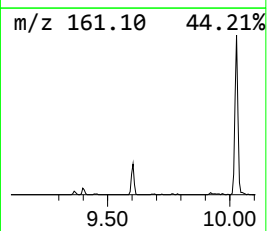
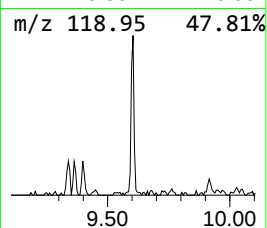
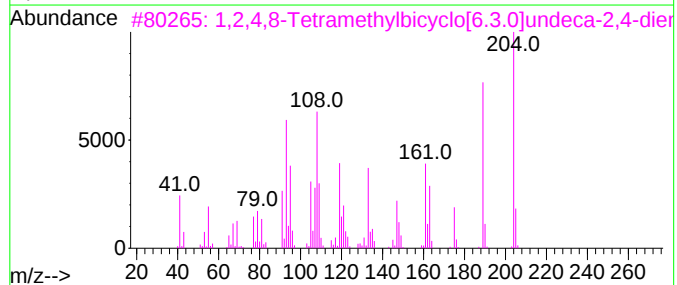
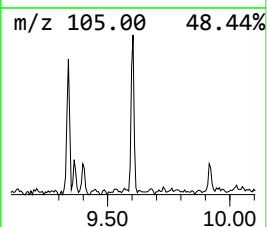
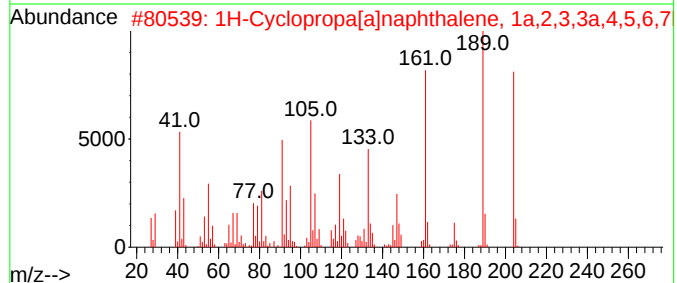
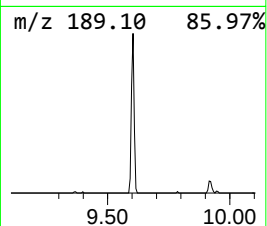
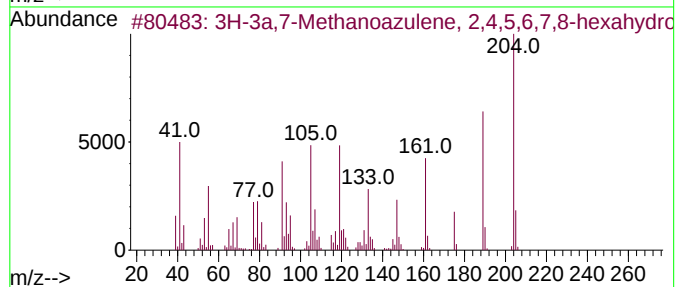
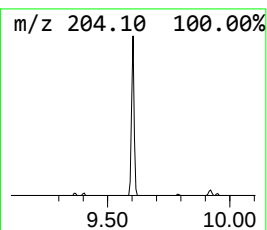
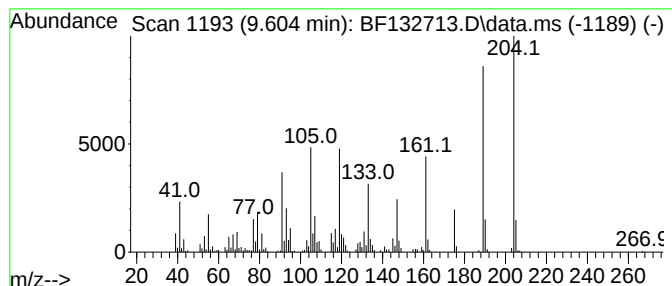
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Peak Number 2 3H-3a,7-Methanoazulene, 2,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	2.21 ng	182462	Acenaphthene-d10	10.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	96
2			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	93
3			1,2,4,8-Tetramethylbicyclo[6.3.0]...	204	C15H24	137235-51-9	87
4			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	76
5			2H-1,3-Oxazine, 2-[(2,6-dimethyl...	204	C12H16N2O	054708-09-7	76



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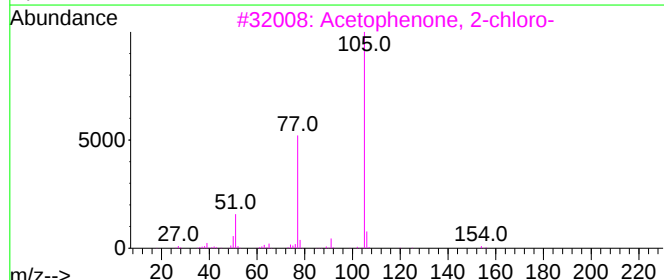
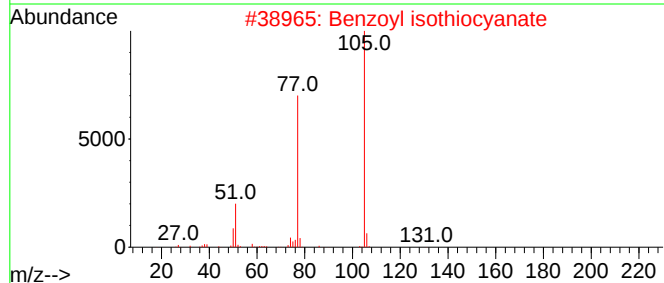
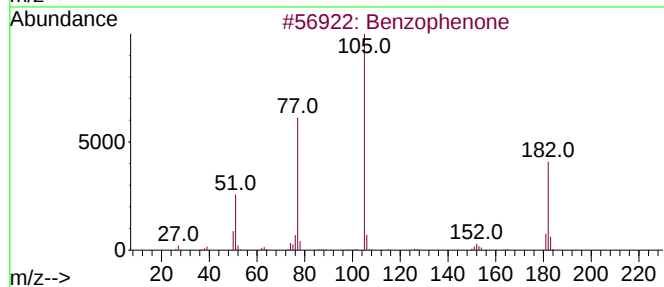
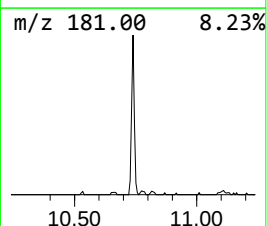
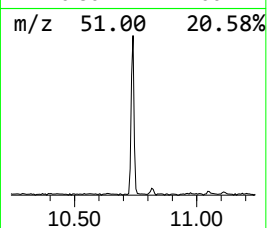
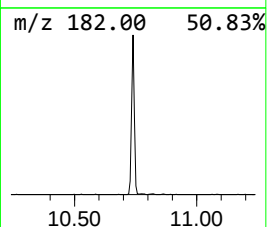
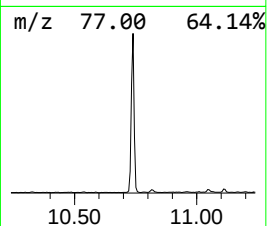
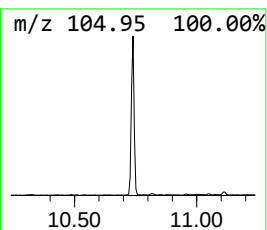
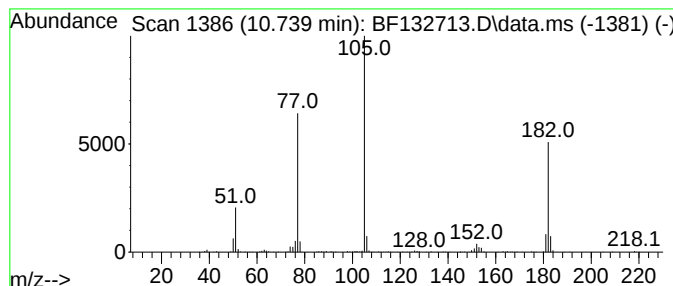
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	6.02 ng	496697	Acenaphthene-d10	10.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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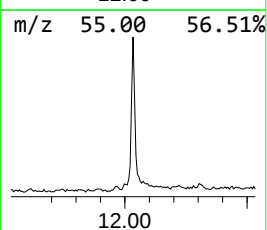
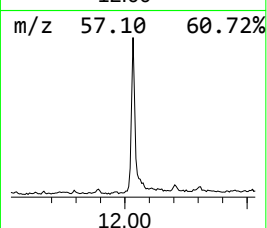
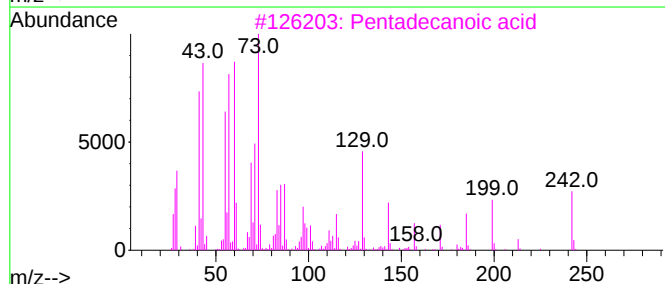
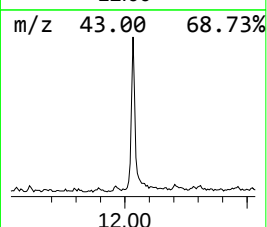
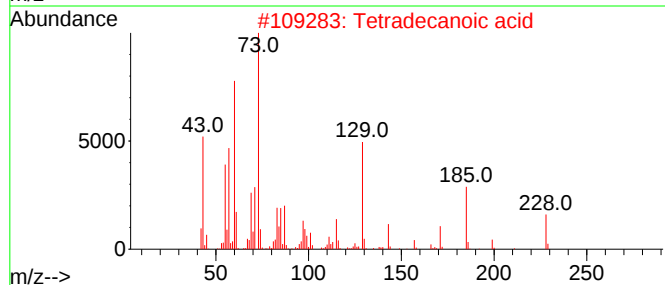
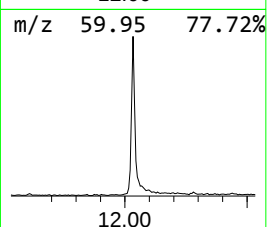
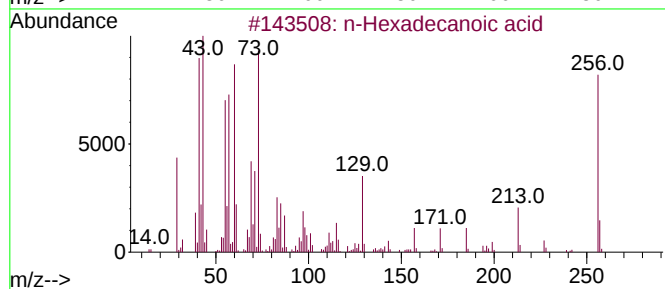
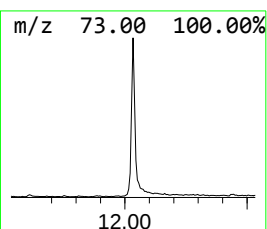
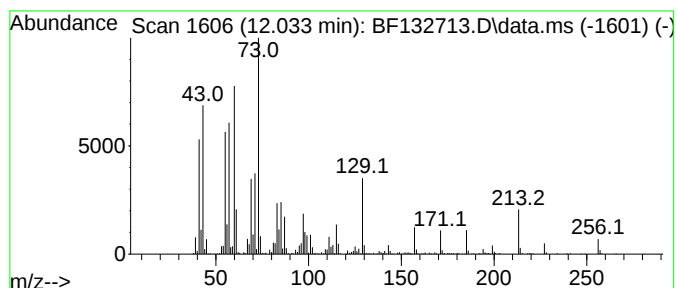
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	11.80 ng	930955	Phenanthrene-d10	11.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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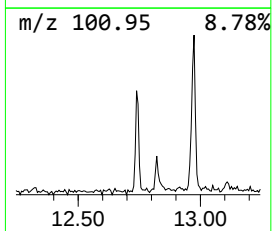
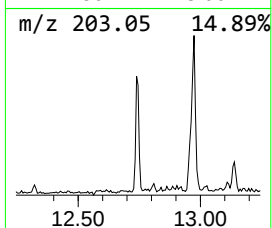
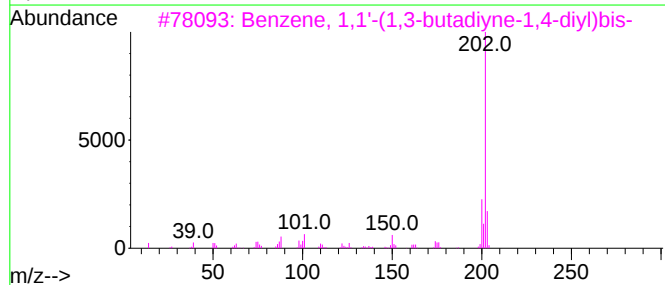
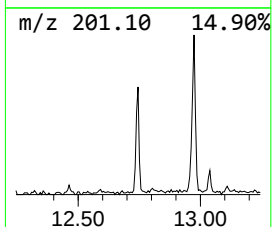
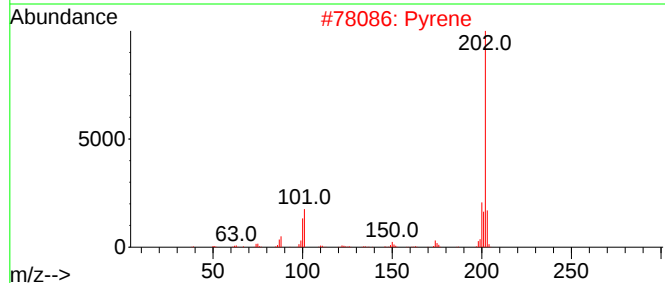
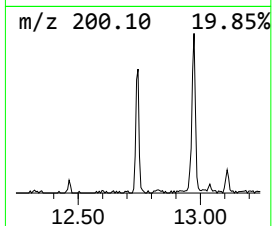
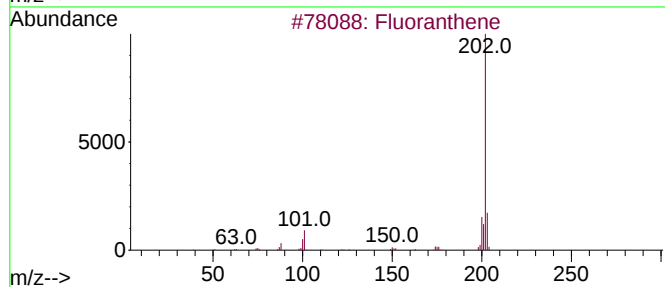
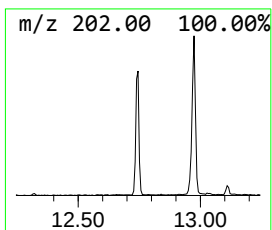
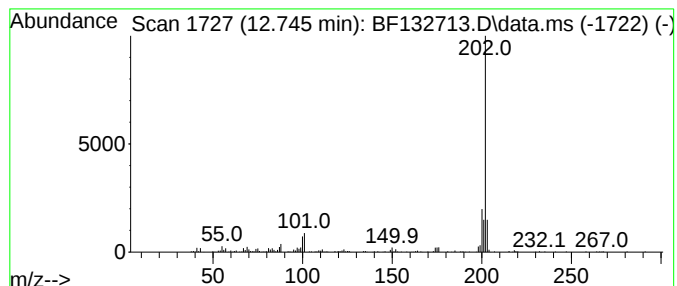
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Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.745	3.04 ng	240115	Phenanthrene-d10	11.522	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	94
2	Pyrene	202	C16H10	000129-00-0	90
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	68
4	1-Leucyl-1-leucine, N,N'-dimethy...	528	C29H56N2O6	1000328-59-7	50
5	1-Leucine, N-methyl-N-(2-methoxy...	499	C29H57NO5	1000328-55-2	50



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SS-01-20230306

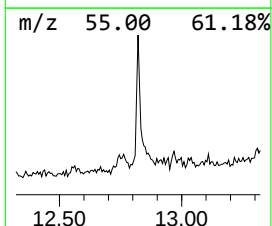
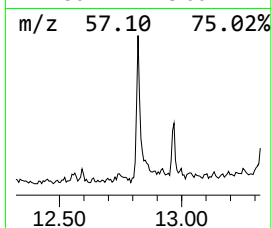
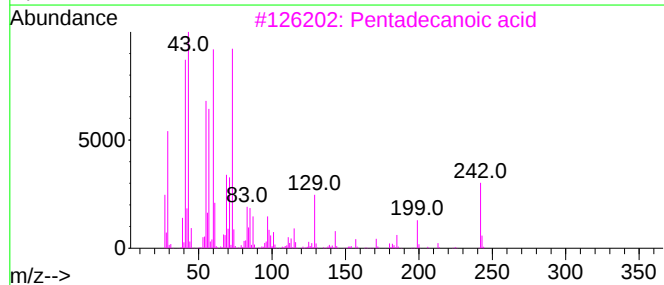
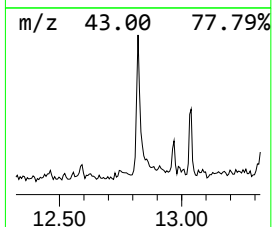
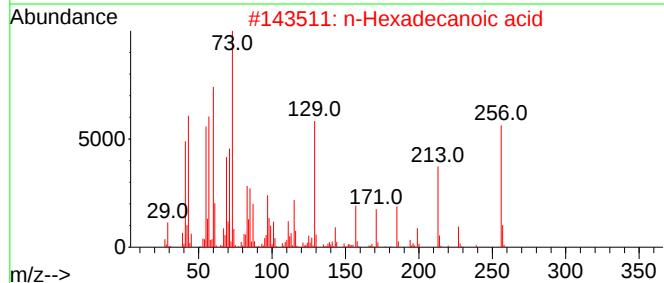
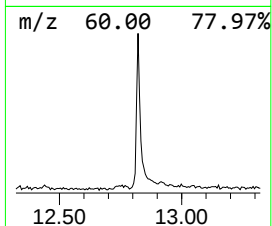
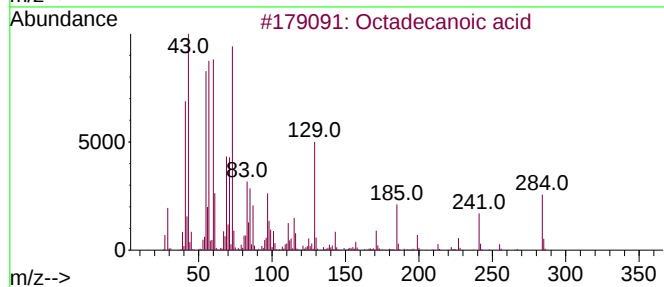
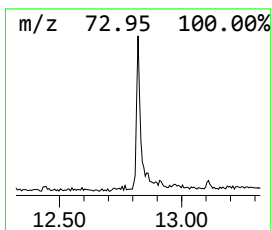
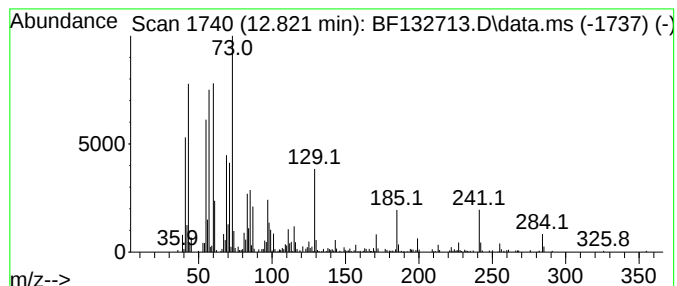
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.821	4.87 ng	384028	Phenanthrene-d10	11.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Heneicosanoic acid	326	C21H42O2	002363-71-5	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132713.D
Acq On : 09 Mar 2023 12:24
Operator : CG\JU
Sample : 01829-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

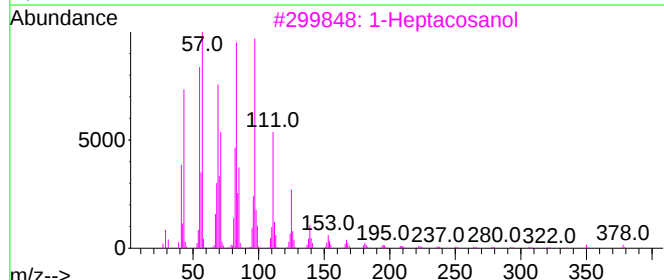
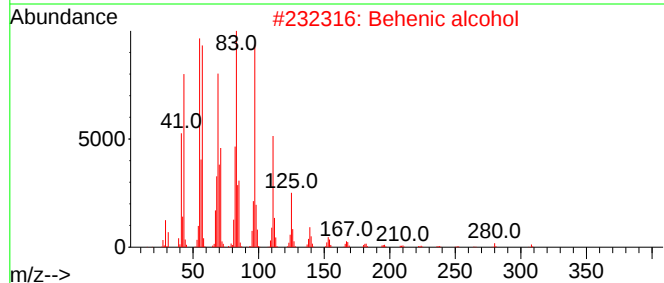
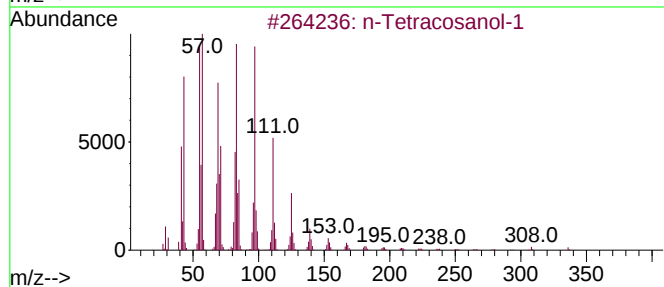
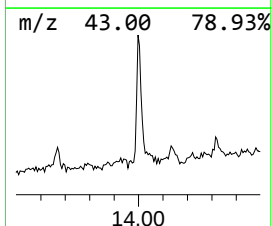
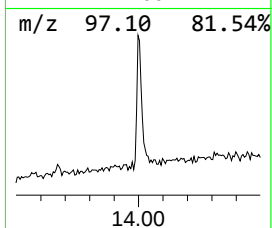
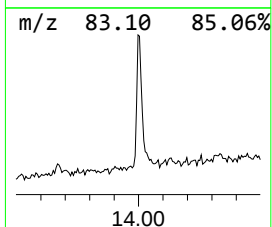
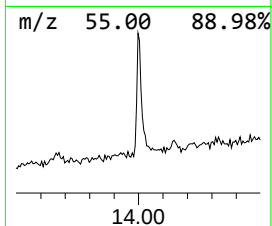
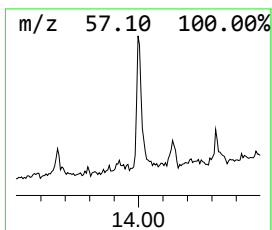
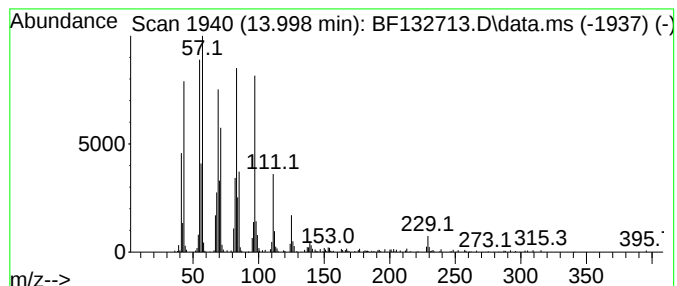
Instrument :
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ClientSampleId :
SS-01-20230306

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 7 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.998	7.38 ng	433869	Chrysene-d12	14.180	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132713.D
Acq On : 09 Mar 2023 12:24
Operator : CG\JU
Sample : 01829-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-01-20230306

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
2-Pentanone, 4-...	5.210	35.1	ng	1941240	1	6.981	1104900	20.0
3H-3a,7-Methano...	9.604	2.2	ng	182462	3	10.028	1651390	20.0
Benzophenone	10.739	6.0	ng	496697	3	10.028	1651390	20.0
n-Hexadecanoic ...	12.033	11.8	ng	930955	4	11.522	1578320	20.0
Benzene, 1,1'-(...	12.745	3.0	ng	240115	4	11.522	1578320	20.0
Octadecanoic acid	12.821	4.9	ng	384028	4	11.522	1578320	20.0
n-Tetracosanol-1	13.998	7.4	ng	433869	5	14.180	1176080	20.0