

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
 Data File : BF131927.D
 Acq On : 05 Jan 2023 21:40
 Operator : CG\JU
 Sample : 01027-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1-1-4-2023

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-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131927.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	16	rVB	46861	54964	2.81%	0.342%
2	5.004	491	496	508	rVB	593034	774189	39.55%	4.812%
3	5.416	561	566	569	rBV	2017070	1832469	93.61%	11.390%
4	6.440	735	740	743	rBV	1918732	1886038	96.35%	11.723%
5	6.798	798	801	805	rBV	556375	445346	22.75%	2.768%
6	7.369	893	898	901	rBV	1189731	1230609	62.87%	7.649%
7	8.087	1016	1020	1024	rBV	583331	561490	28.68%	3.490%
8	9.169	1199	1204	1208	rBV	1952680	1957531	100.00%	12.168%
9	9.851	1316	1320	1324	rVB	814509	661767	33.81%	4.113%
10	10.575	1438	1443	1446	rBV	657146	566871	28.96%	3.524%
11	10.645	1451	1455	1459	rBV	1513683	1477871	75.50%	9.186%
12	10.880	1492	1495	1499	rVB	37233	33732	1.72%	0.210%
13	11.345	1570	1574	1577	rBV	848384	707153	36.12%	4.396%
14	11.369	1577	1578	1582	rVB	44115	26818	1.37%	0.167%
15	11.880	1662	1665	1668	rBV2	70383	66680	3.41%	0.414%
16	12.127	1703	1707	1709	rBV	152788	124328	6.35%	0.773%
17	12.563	1778	1781	1785	rVB	90194	75612	3.86%	0.470%
18	12.792	1815	1820	1825	rVB	73194	76815	3.92%	0.477%
19	12.939	1841	1845	1849	rBV	1895443	1760288	89.92%	10.942%
20	13.169	1879	1884	1886	rBV2	25225	28960	1.48%	0.180%
21	13.510	1937	1942	1946	rBV4	19767	24385	1.25%	0.152%
22	13.839	1995	1998	2014	rVB	192736	271673	13.88%	1.689%
23	13.998	2019	2025	2028	rVV	476852	445544	22.76%	2.769%
24	14.021	2028	2029	2034	rVB	24006	21670	1.11%	0.135%
25	14.098	2038	2042	2046	rVB2	20314	25057	1.28%	0.156%
26	14.757	2150	2154	2161	rBV	174891	198349	10.13%	1.233%
27	14.845	2167	2169	2174	rVB	27511	29359	1.50%	0.182%
28	15.110	2211	2214	2219	rVB	23984	25919	1.32%	0.161%
29	15.474	2271	2276	2284	rBV	303204	379106	19.37%	2.356%
30	15.933	2349	2354	2359	rBV4	15783	23703	1.21%	0.147%
31	15.998	2361	2365	2369	rBV6	13908	29332	1.50%	0.182%
32	18.068	2708	2717	2726	rVB8	40174	105073	5.37%	0.653%
33	18.321	2752	2760	2772	rBV10	42494	159016	8.12%	0.988%

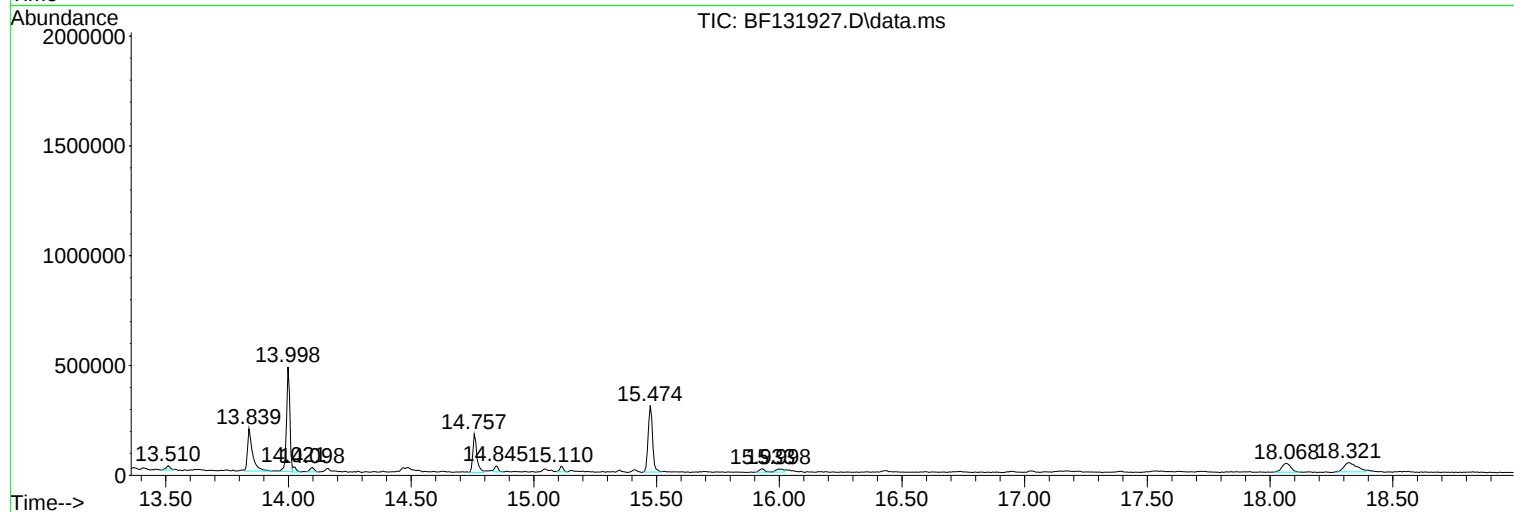
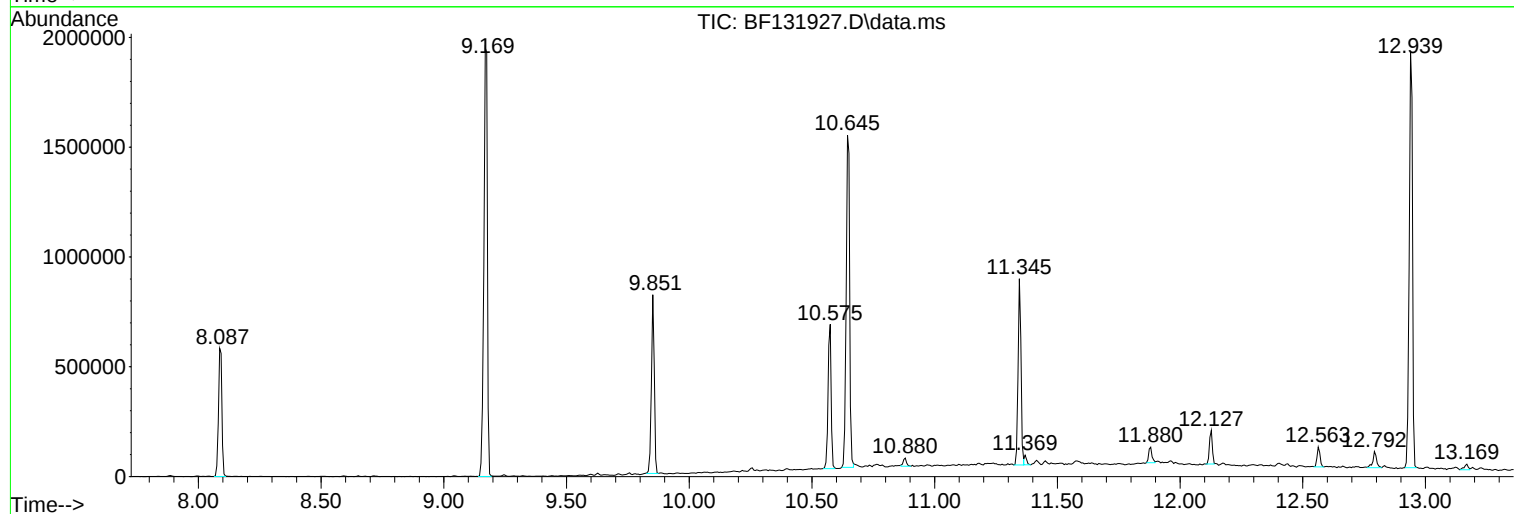
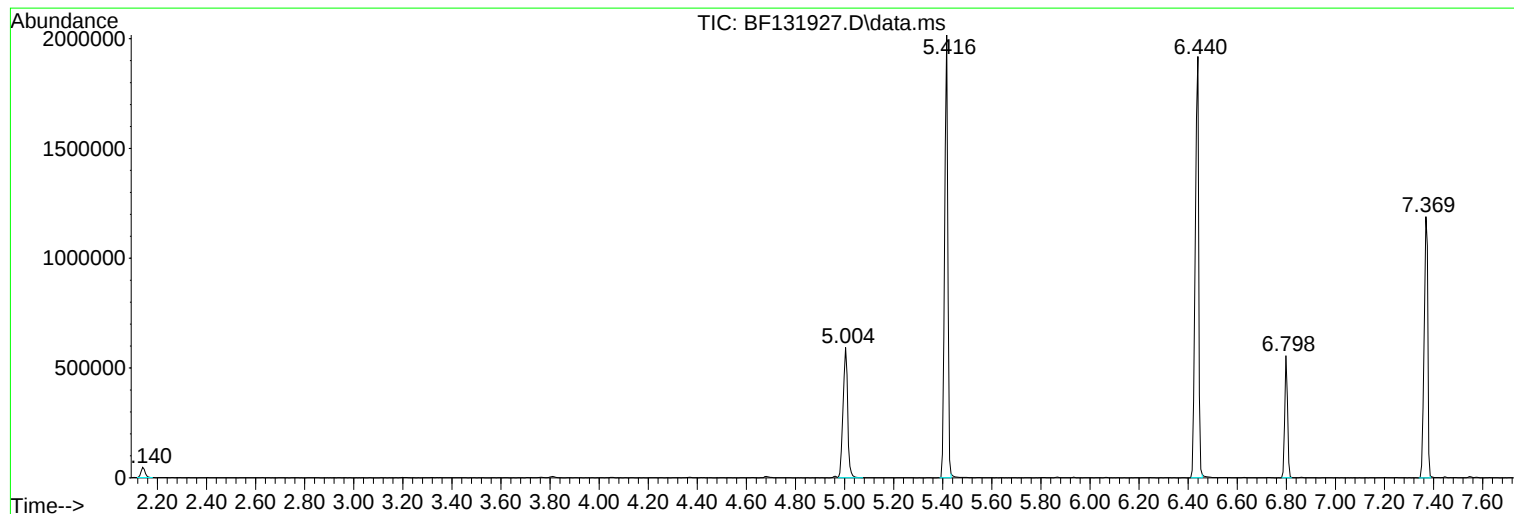
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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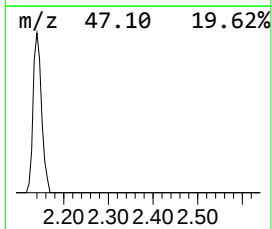
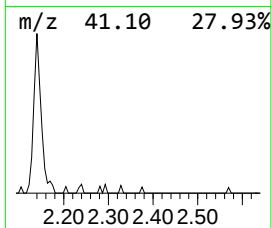
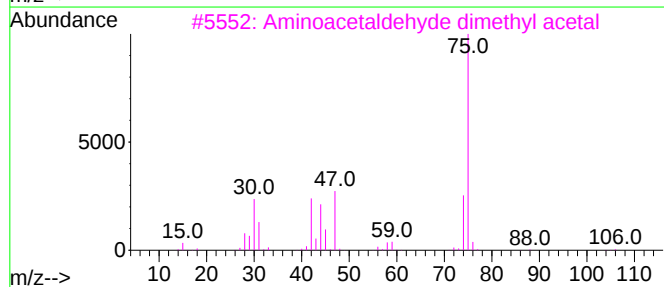
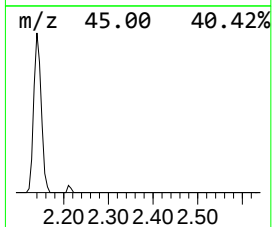
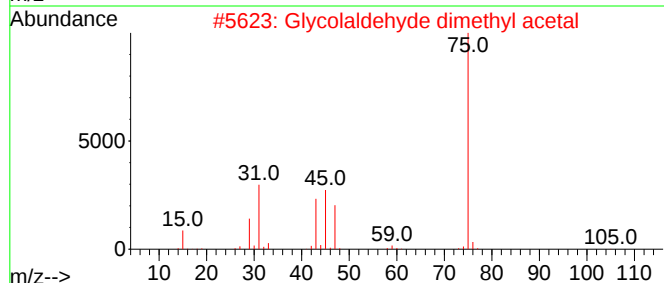
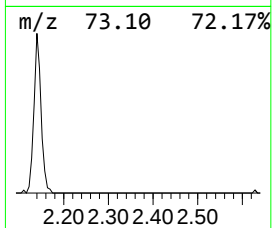
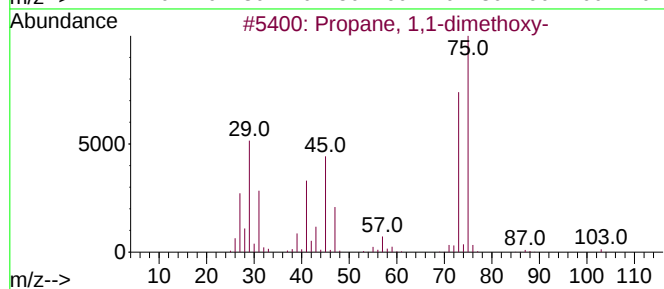
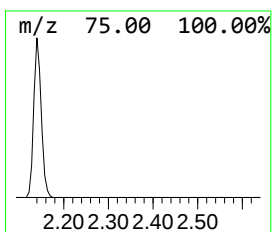
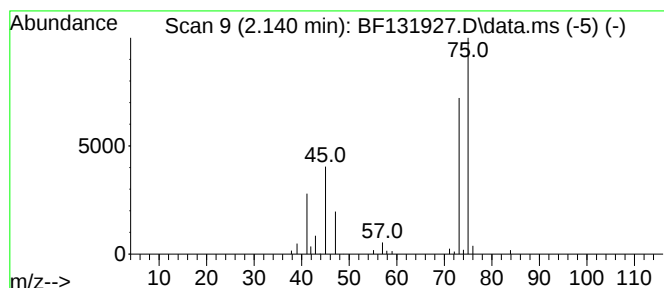
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	2.47 ng	54964	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
3			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			Glycine	75	C2H5NO2	000056-40-6	5



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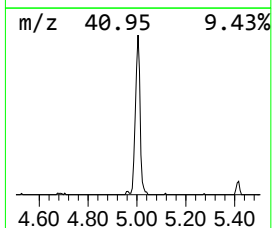
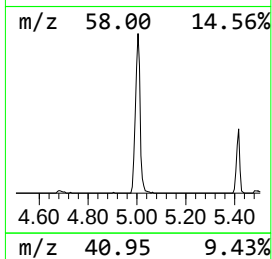
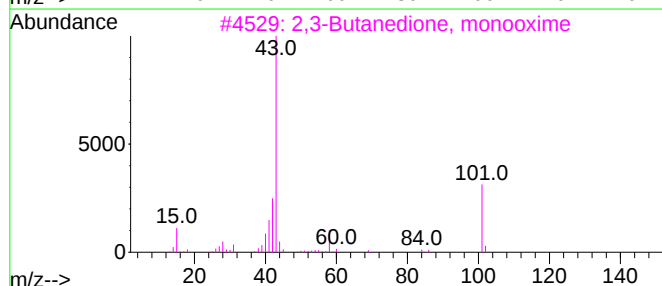
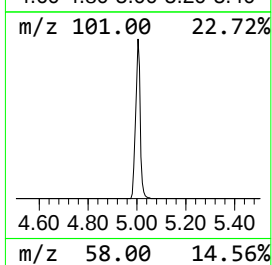
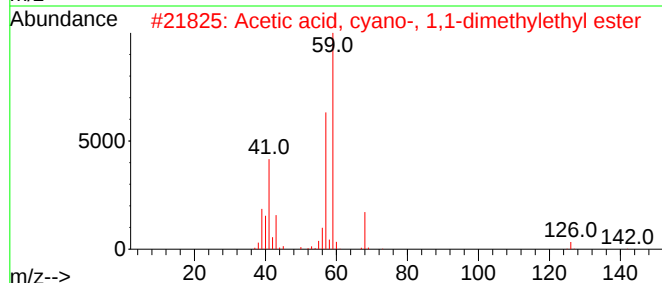
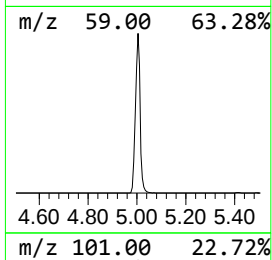
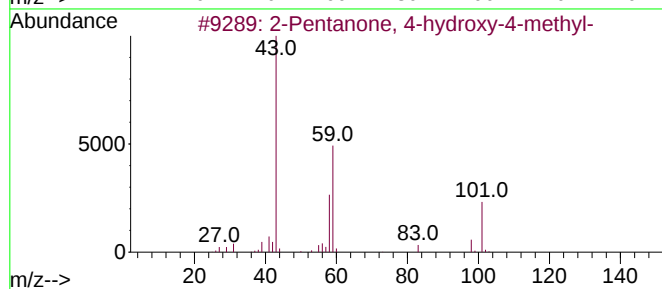
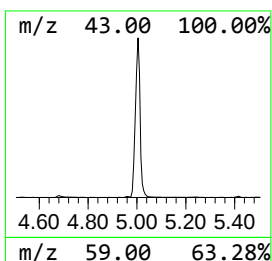
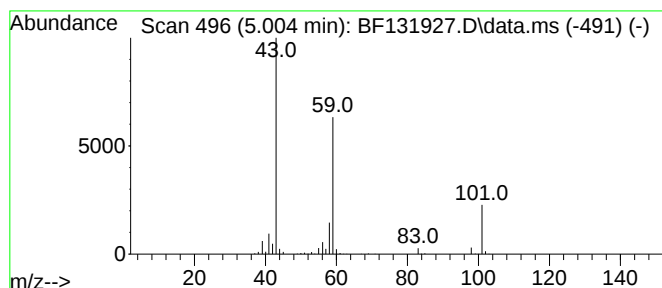
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	34.77 ng	774189	1,4-Dichlorobenzene-d4	6.798

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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	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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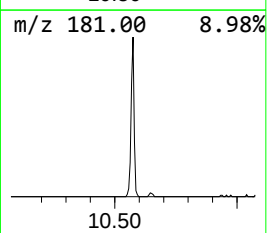
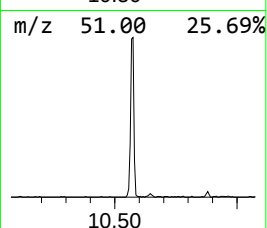
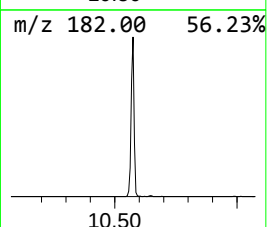
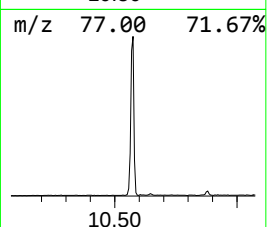
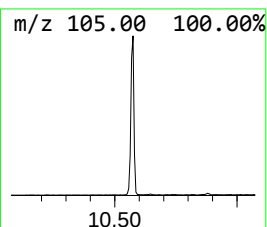
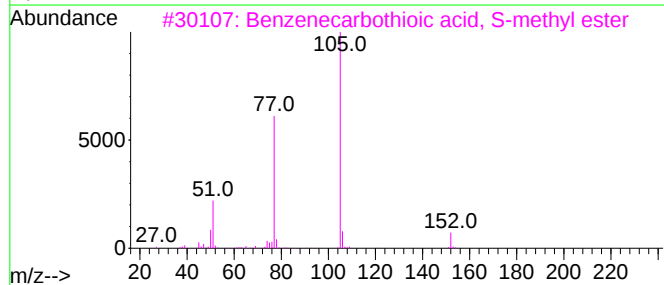
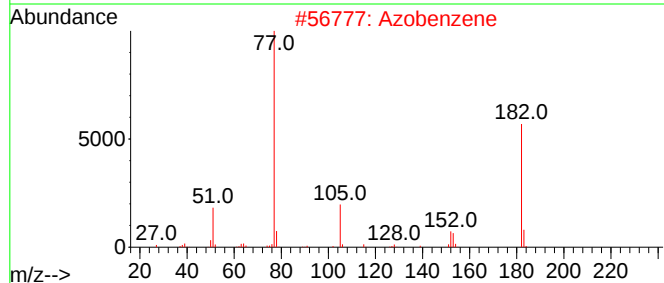
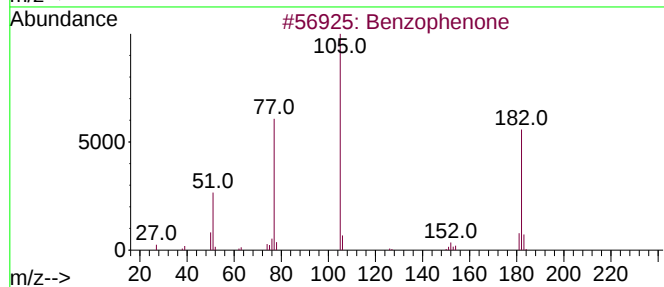
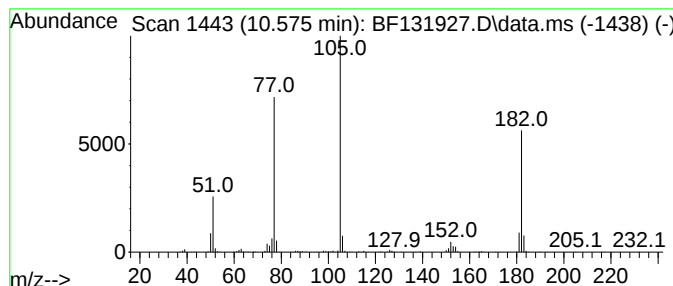
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.575	17.13 ng	566871	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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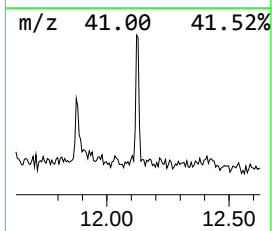
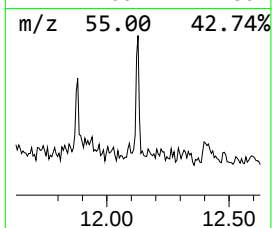
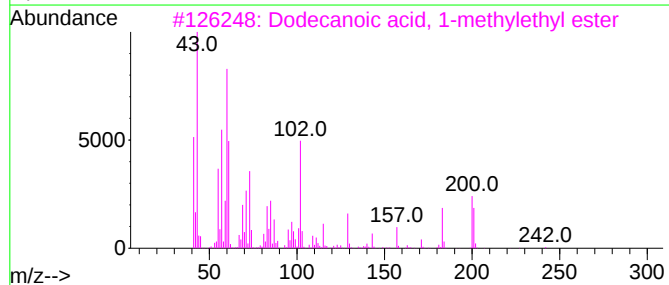
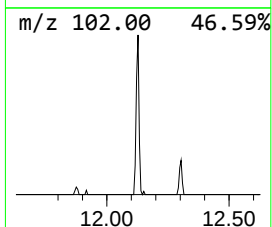
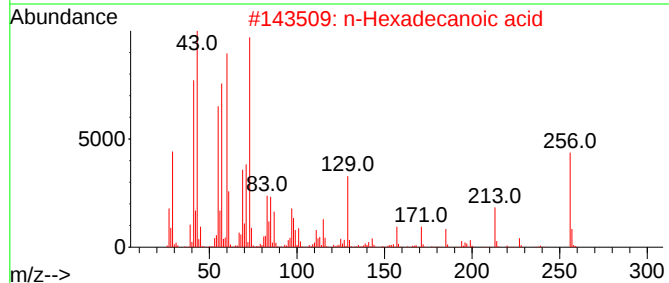
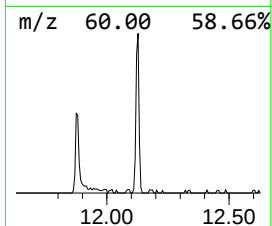
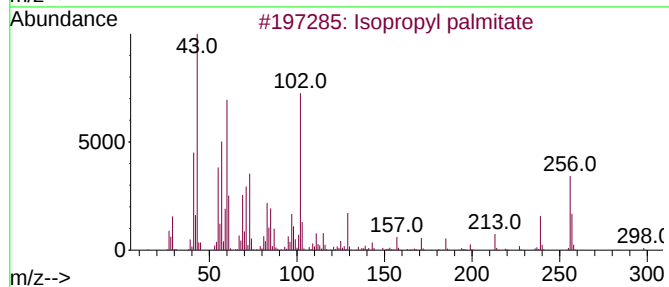
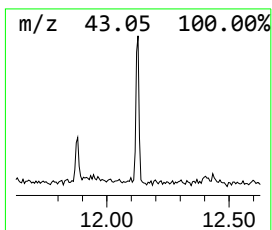
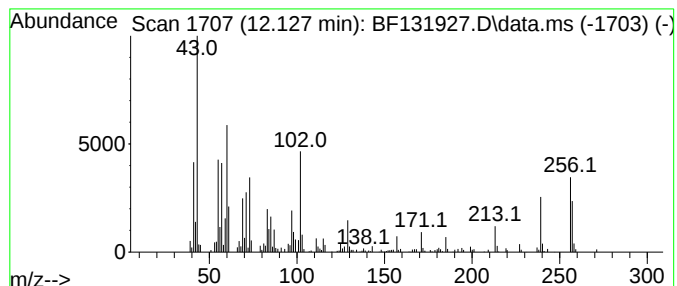
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Peak Number 4 Isopropyl palmitate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.127	3.52 ng	124328	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	38
4			4-Methylcyclohexylamine, N,N-bis...	197	C11H19NO2	1000454-13-3	27
5			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	27



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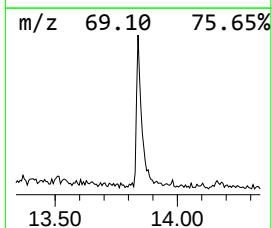
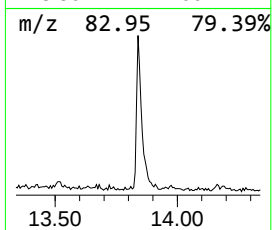
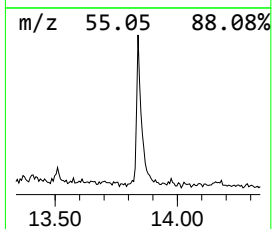
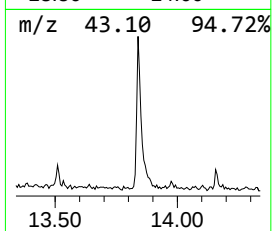
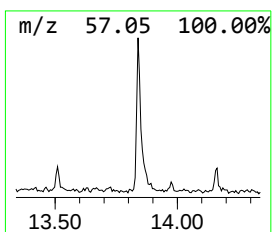
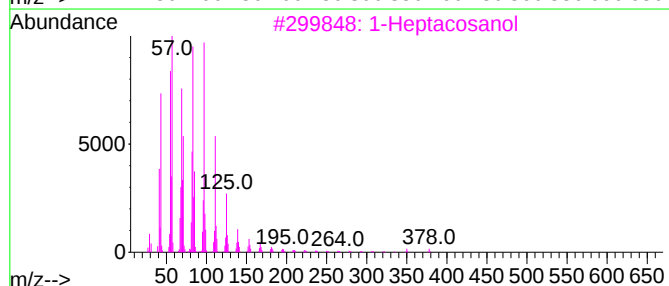
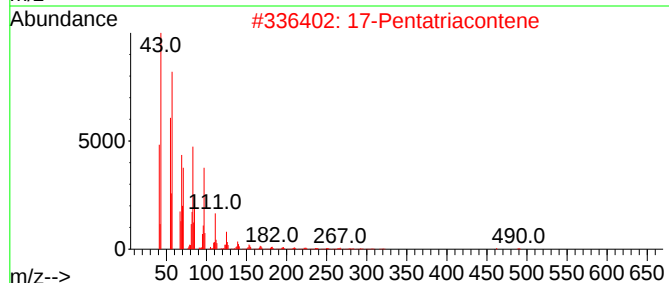
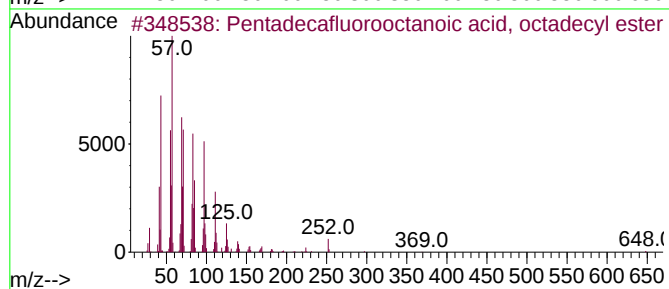
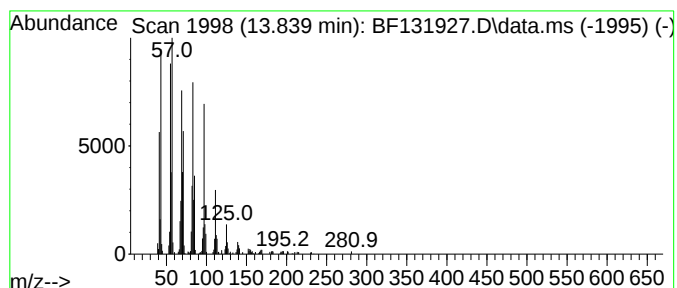
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Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	12.20 ng	271673	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5			1-Tetracosene	336	C24H48	010192-32-2	91



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Sample : 01027-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1-1-4-2023

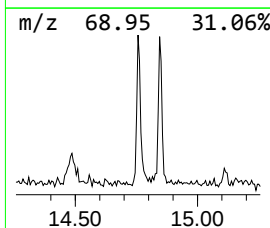
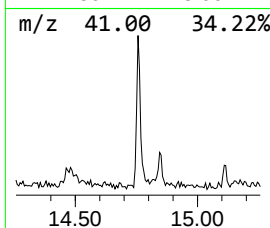
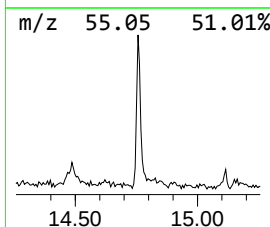
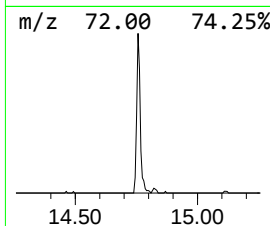
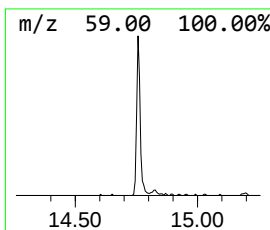
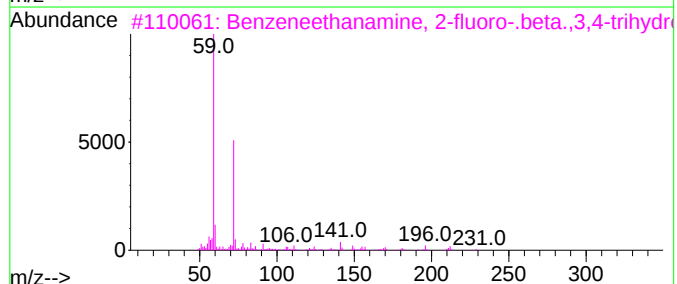
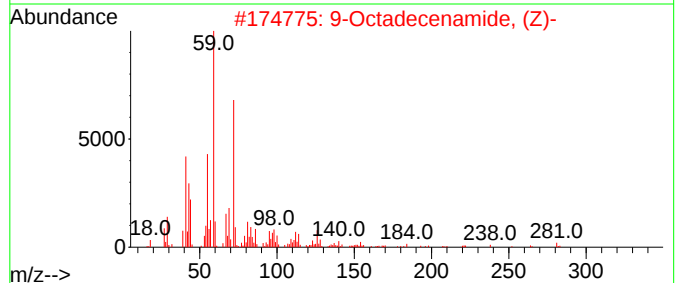
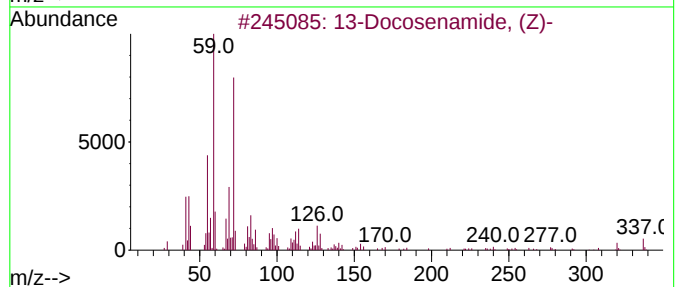
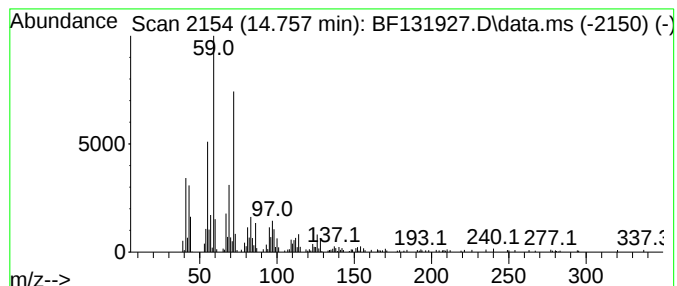
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	10.46 ng	198349	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	47
4			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131927.D
Acq On : 05 Jan 2023 21:40
Operator : CG\JU
Sample : 01027-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1-1-4-2023

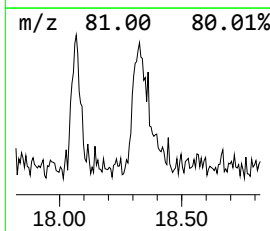
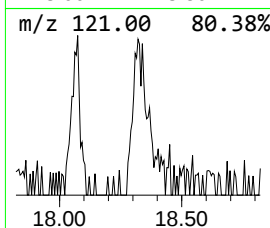
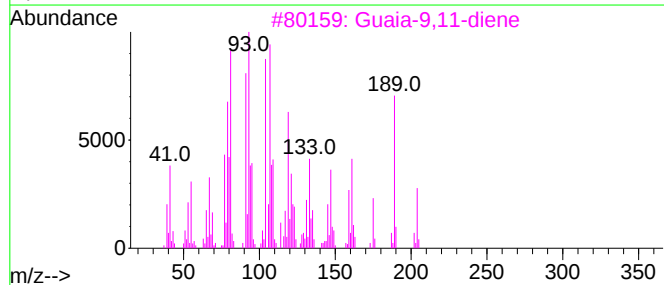
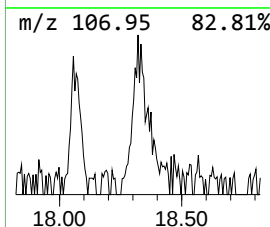
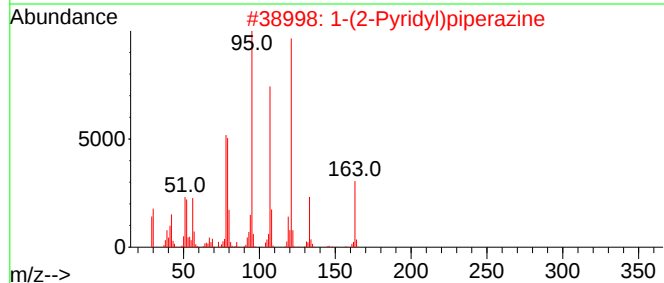
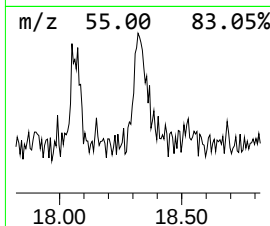
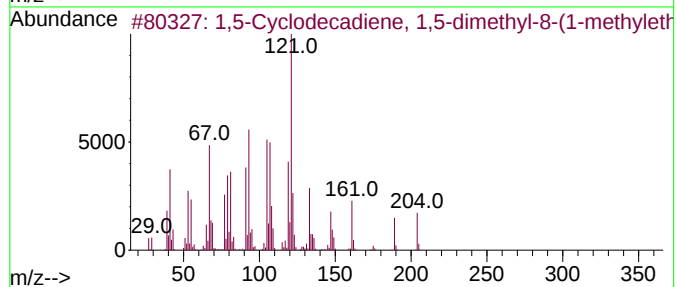
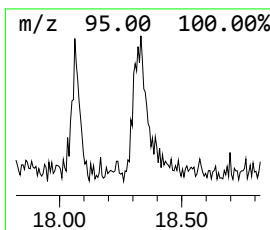
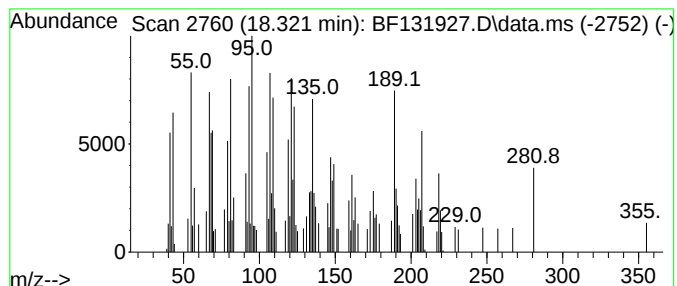
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,5-Cyclodecadiene, 1,5-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.321	8.39 ng	159016	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	53		
2	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	46		
3	Guaia-9,11-diene	204	C15H24	1000374-19-8	43		
4	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	38		
5	15.alpha.-Hydroxyculmorin	254	C15H26O3	144447-99-4	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131927.D
Acq On : 05 Jan 2023 21:40
Operator : CG\JU
Sample : 01027-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1-1-4-2023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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
Propane, 1,1-di...	2.140	2.5	ng	54964	1	6.798	445346	20.0
2-Pentanone, 4-...	5.004	34.8	ng	774189	1	6.798	445346	20.0
Benzophenone	10.575	17.1	ng	566871	3	9.851	661767	20.0
Isopropyl palmi...	12.127	3.5	ng	124328	4	11.345	707153	20.0
Pentadecafluoro...	13.839	12.2	ng	271673	5	13.998	445544	20.0
13-Docosenamide...	14.757	10.5	ng	198349	6	15.474	379106	20.0
1,1,6-trimethyl...	18.068	5.5	ng	105073	6	15.474	379106	20.0
1,5-Cyclodecadi...	18.321	8.4	ng	159016	6	15.474	379106	20.0