

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133270.D
 Acq On : 05 May 2023 18:46
 Operator : CG\JU
 Sample : 02618-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN003

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-BF042123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	475	479	490	rVB	351762	398628	7.06%	1.158%
2	5.275	540	542	543	rBV	85044	75519	1.34%	0.219%
3	5.357	549	556	559	rVB	1451460	2386043	42.25%	6.933%
4	6.363	723	727	730	rBV	1747341	1399255	24.77%	4.066%
5	6.722	785	788	796	rBV	1229385	1054808	18.68%	3.065%
6	7.292	880	885	888	rBV	3577316	3446310	61.02%	10.014%
7	8.010	1003	1007	1010	rBV	1827131	1402345	24.83%	4.075%
8	9.086	1186	1190	1193	rBV	6048374	5647868	100.00%	16.411%
9	9.757	1301	1304	1308	rVB	1769416	1585842	28.08%	4.608%
10	10.474	1422	1426	1434	rVB	1098936	877984	15.55%	2.551%
11	10.551	1434	1439	1442	rBV	3634590	3476723	61.56%	10.102%
12	10.616	1447	1450	1453	rVB	140441	125122	2.22%	0.364%
13	10.780	1474	1478	1481	rBV	173944	161589	2.86%	0.470%
14	11.004	1513	1516	1519	rBV	518502	396841	7.03%	1.153%
15	11.110	1530	1534	1542	rVB3	74322	85136	1.51%	0.247%
16	11.239	1552	1556	1560	rBV	1998283	1617609	28.64%	4.700%
17	11.416	1581	1586	1591	rVB2	155286	182170	3.23%	0.529%
18	11.780	1644	1648	1651	rBV	419888	428700	7.59%	1.246%
19	12.563	1777	1781	1792	rBV3	96595	153621	2.72%	0.446%
20	12.751	1808	1813	1817	rBV	66575	64763	1.15%	0.188%
21	12.833	1821	1827	1830	rBV	5231299	5628042	99.65%	16.353%
22	13.210	1888	1891	1894	rVB	84455	78717	1.39%	0.229%
23	13.733	1977	1980	1990	rBV	177023	296299	5.25%	0.861%
24	13.874	1999	2004	2011	rBV	1542310	1401041	24.81%	4.071%
25	13.968	2014	2020	2030	rBV	662149	745264	13.20%	2.166%
26	14.721	2144	2148	2152	rVB	169764	161817	2.87%	0.470%
27	15.292	2239	2245	2249	rBV	985639	1137238	20.14%	3.304%

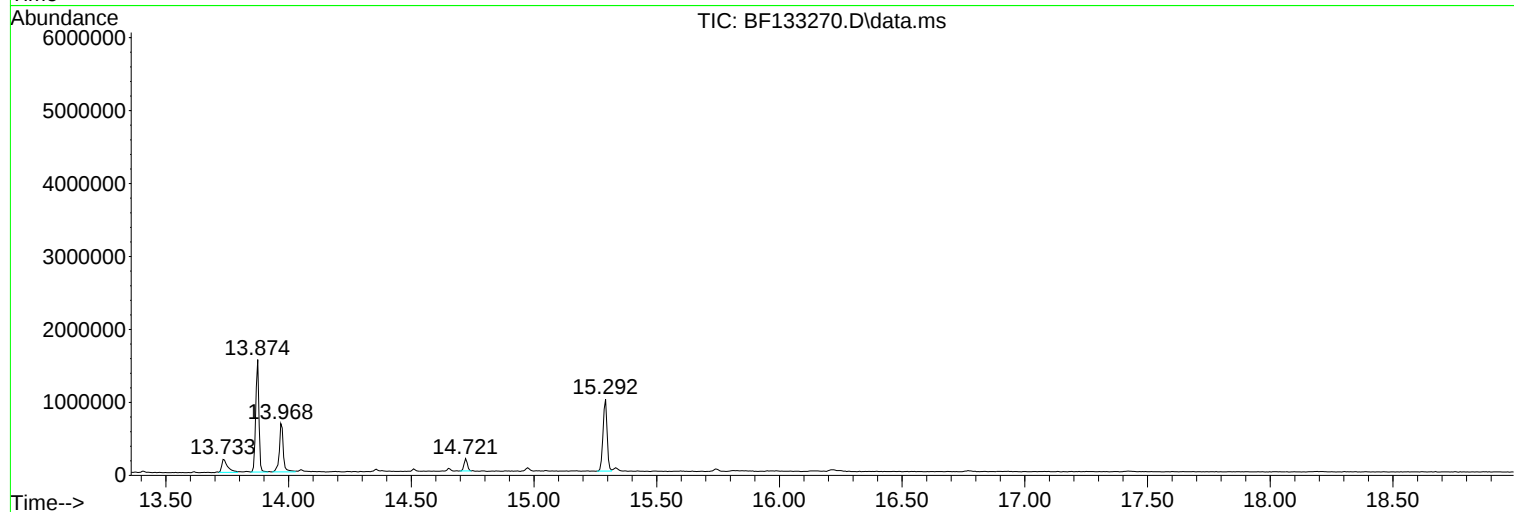
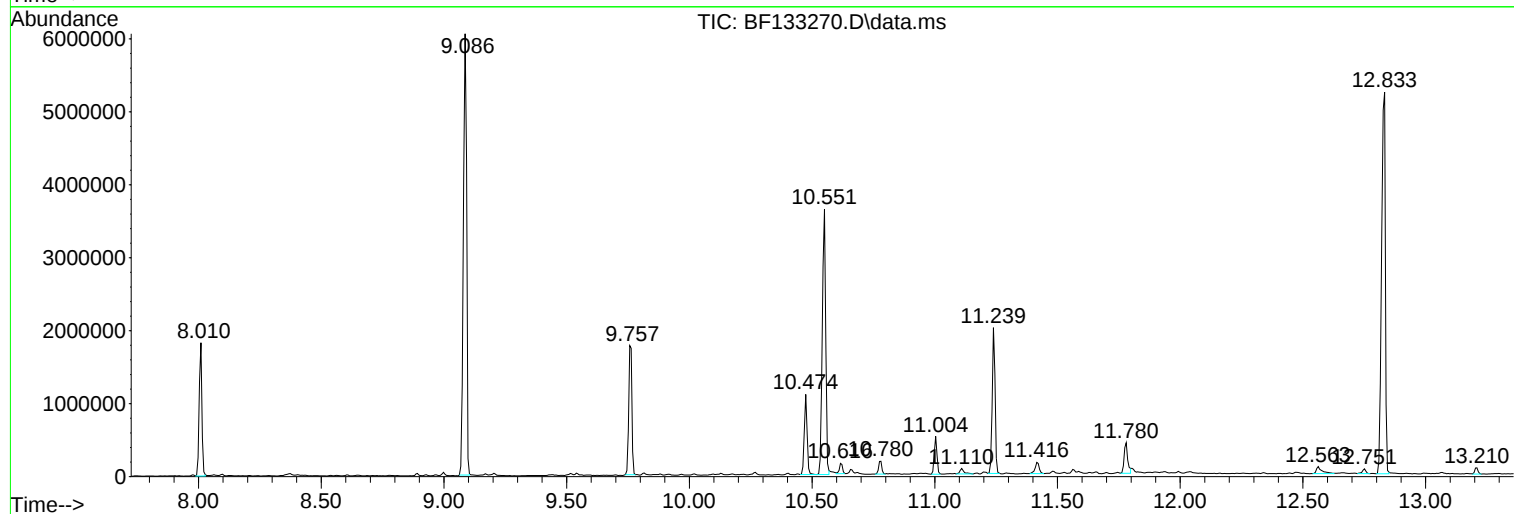
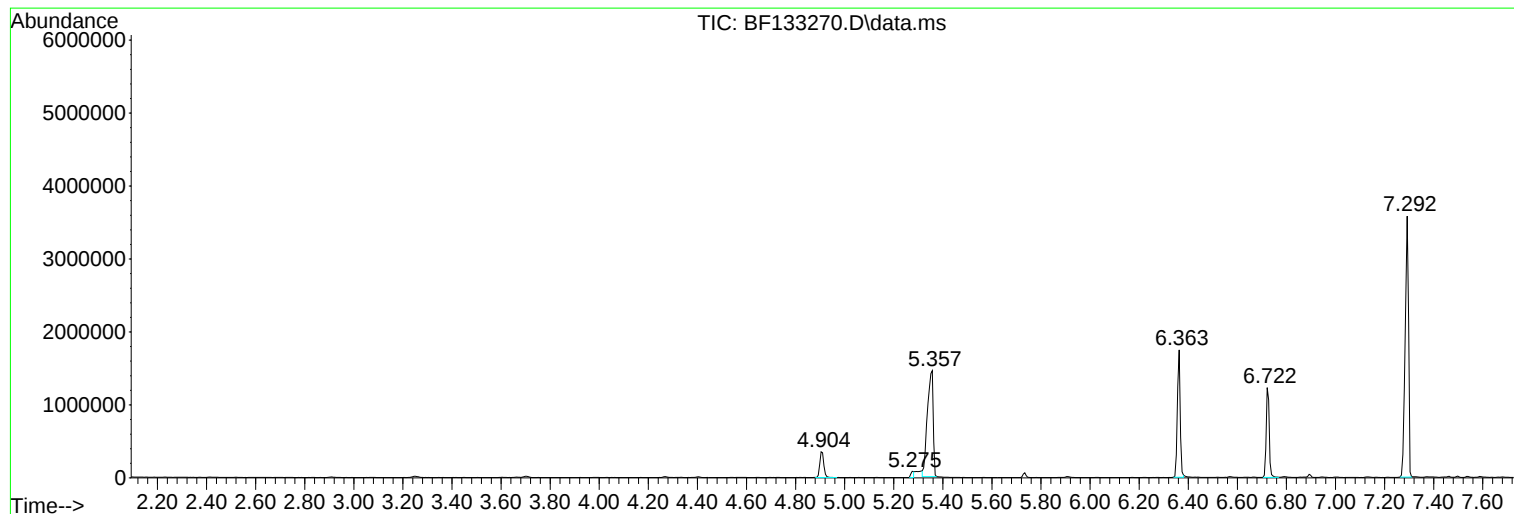
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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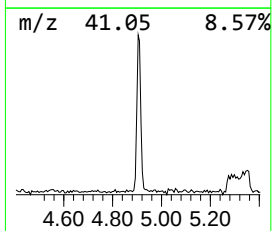
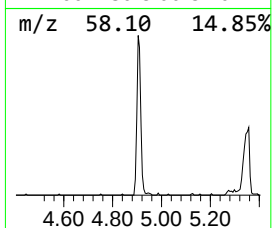
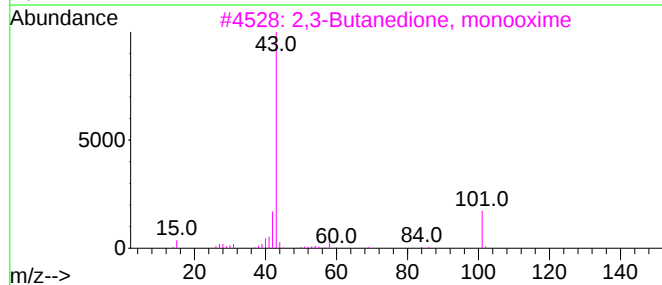
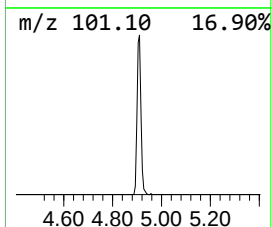
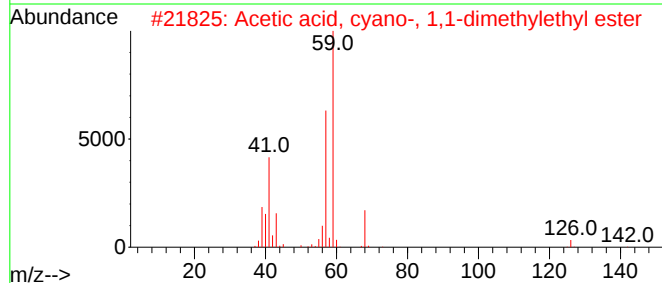
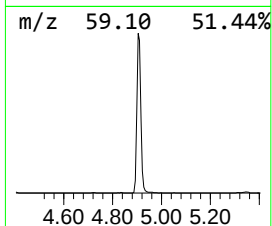
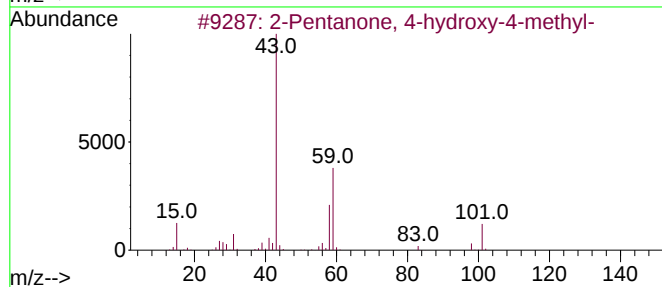
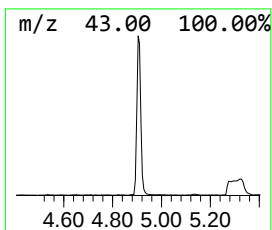
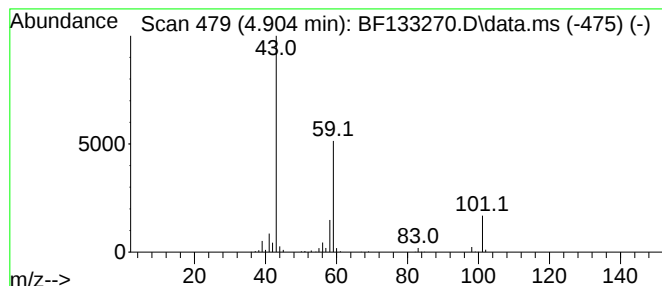
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	7.56 ng	398628	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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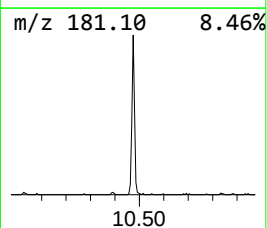
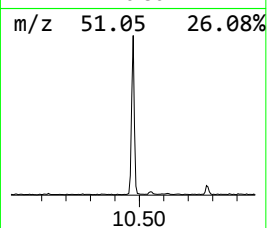
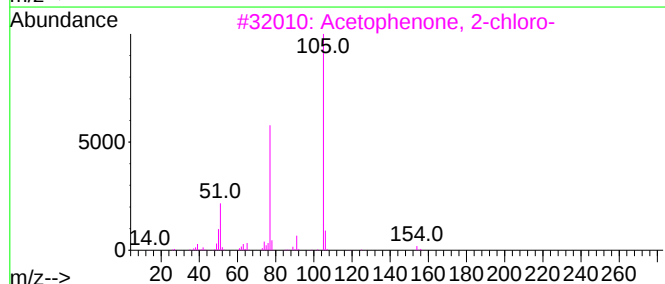
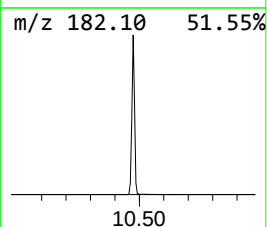
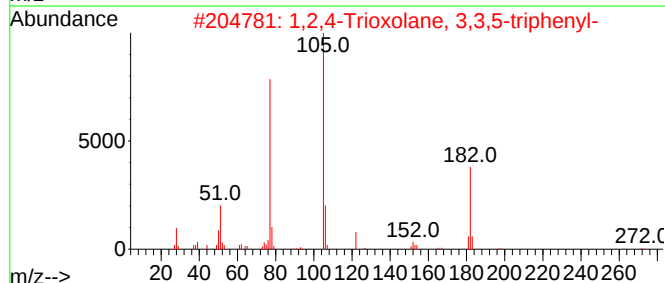
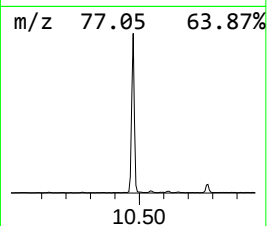
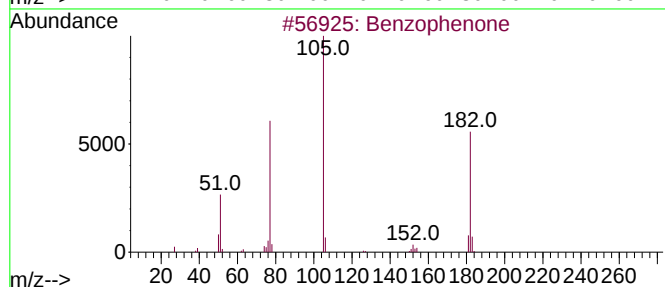
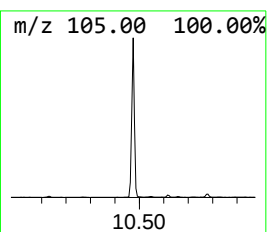
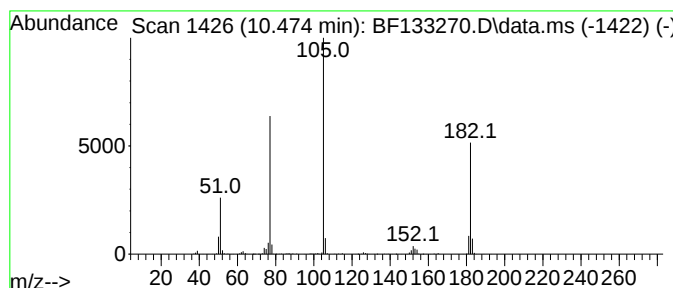
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.474	11.07 ng	877984	Acenaphthene-d10	9.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



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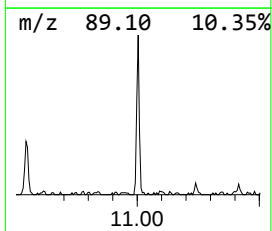
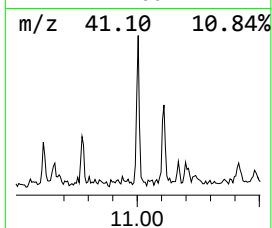
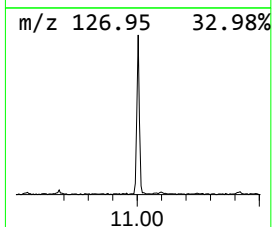
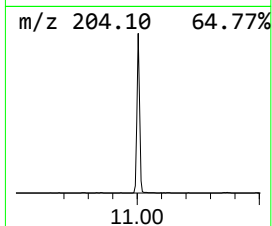
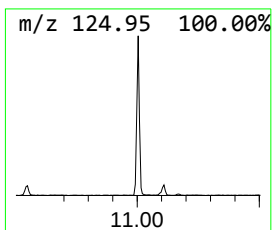
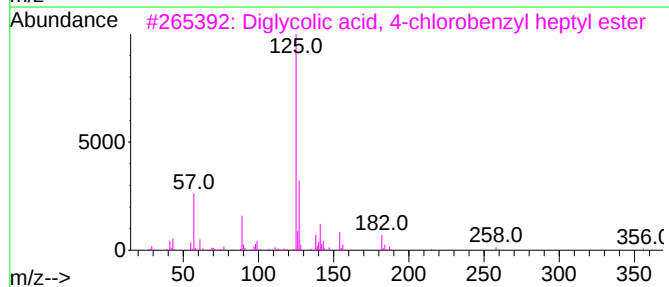
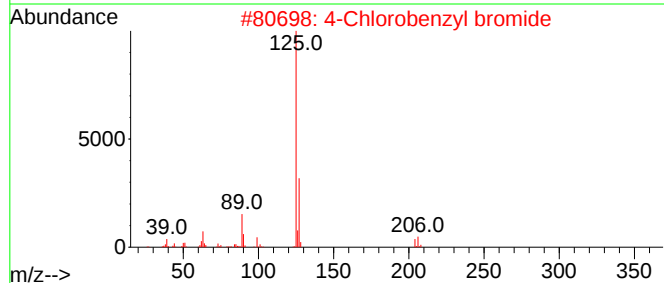
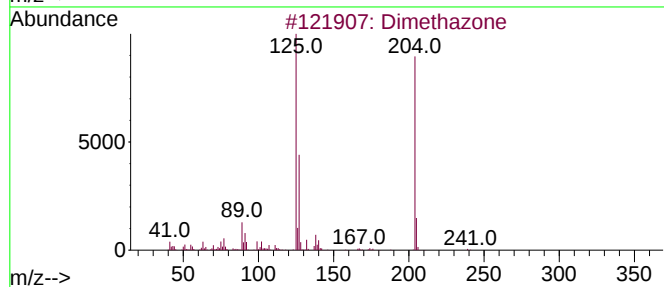
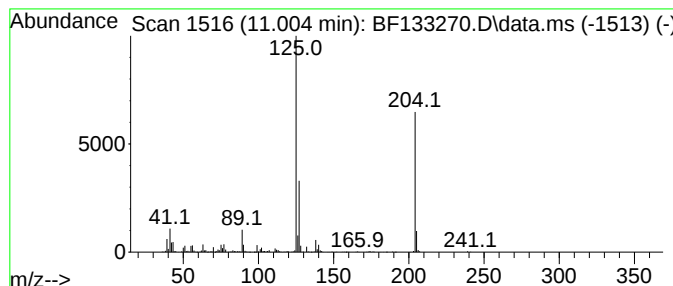
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Peak Number 3 Dimethazone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.004	4.91 ng	396841	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethazone	239	C12H14ClNO2	081777-89-1	96
2			4-Chlorobenzyl bromide	204	C7H6BrCl	000622-95-7	64
3			Diglycolic acid, 4-chlorobenzyl ...	356	C18H25ClO5	1000382-26-0	53
4			Benzene, 1-(bromomethyl)-3-chloro-	204	C7H6BrCl	000766-80-3	52
5			2-[[4-Chlorophenyl)methyl]amino...	241	C13H20ClNO	1000305-39-3	52



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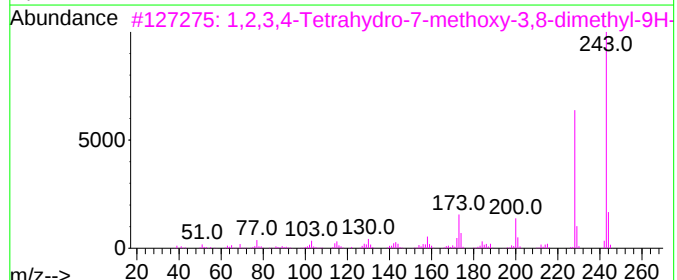
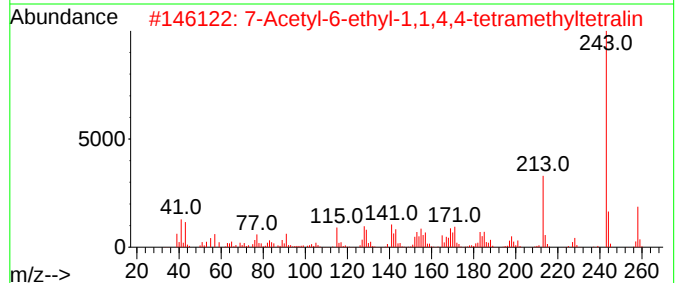
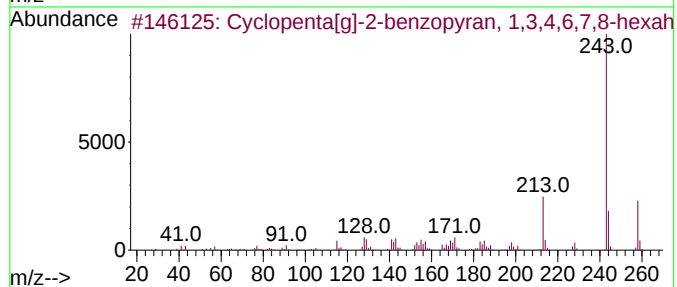
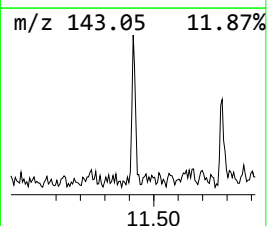
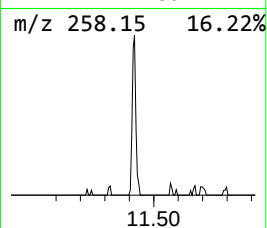
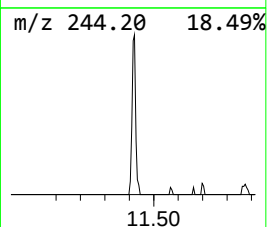
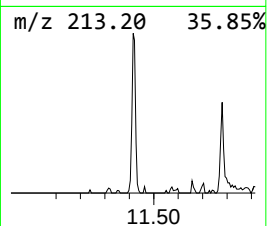
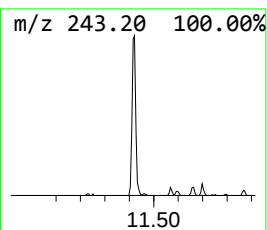
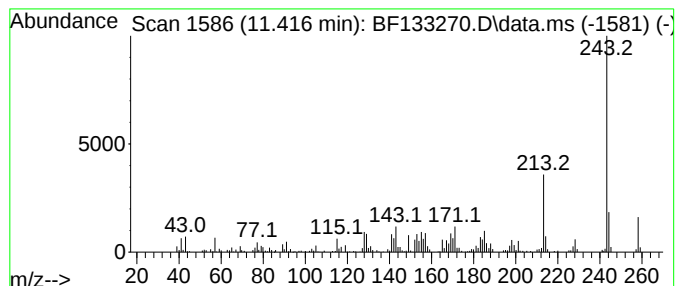
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Peak Number 4 Cyclopenta[g]-2-benzopyran,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.416	2.25 ng	182170	Phenanthrene-d10	11.239	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta[g]-2-benzopyran, 1,3,...	258	C18H26O	001222-05-5	98
2	7-Acetyl-6-ethyl-1,1,4,4-tetrame...	258	C18H26O	000088-29-9	98
3	1,2,3,4-Tetrahydro-7-methoxy-3,8...	243	C15H17NO2	1000281-20-4	53
4	Phenol, 2-amino-4-tricyclo[3.3.1...	243	C16H21NO	1000350-32-7	50
5	5-Amino-1-(2-pyrimidinyl)-1H-pyr...	258	C11H14N6Si	1010479-66-2	50



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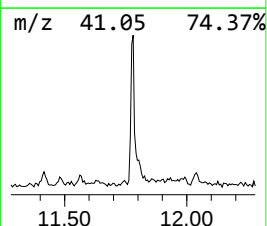
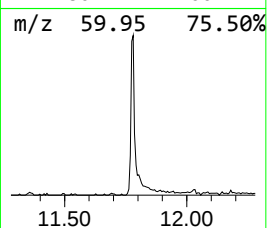
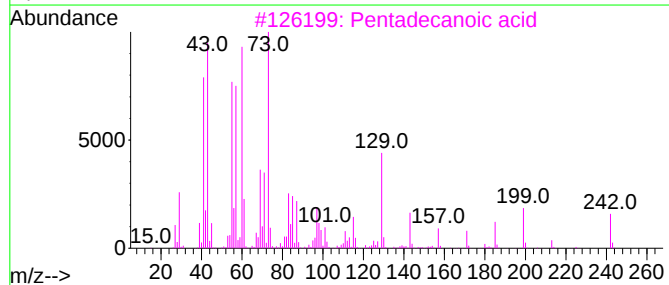
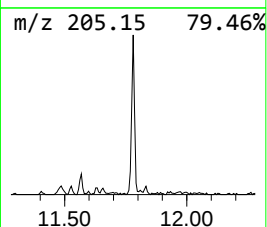
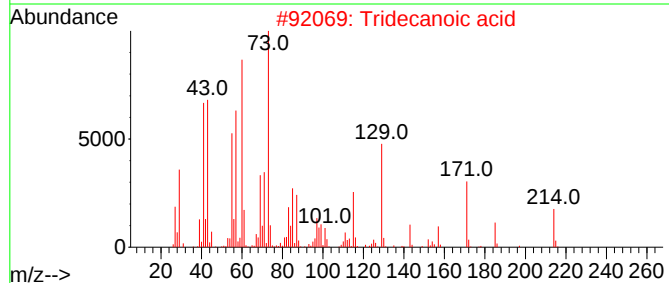
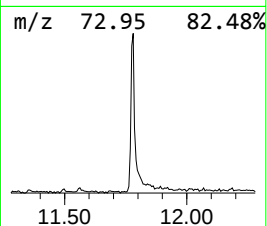
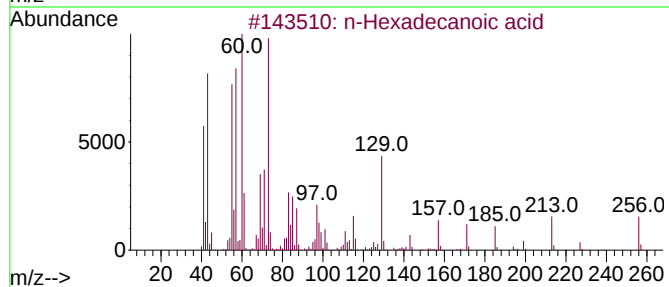
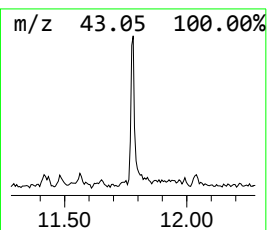
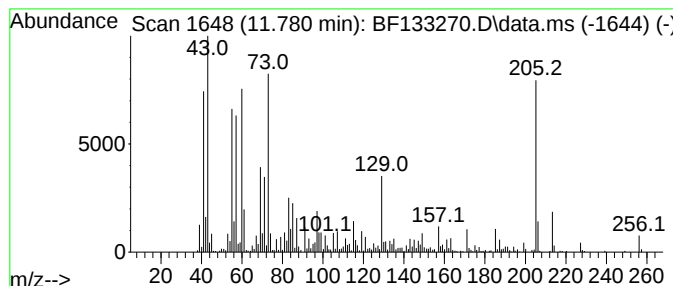
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	5.30 ng	428700	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5			n-Decanoic acid	172	C10H20O2	000334-48-5	46



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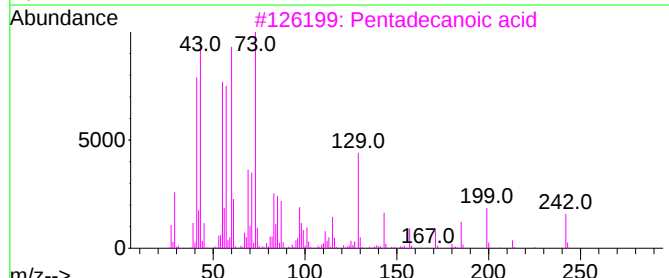
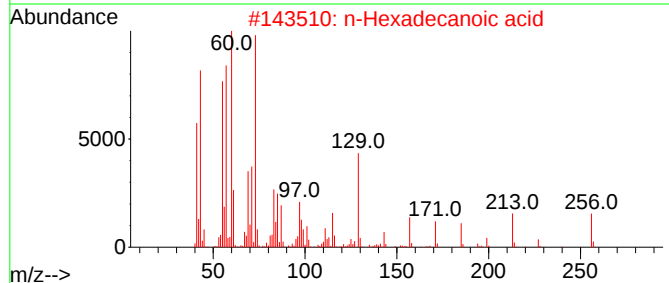
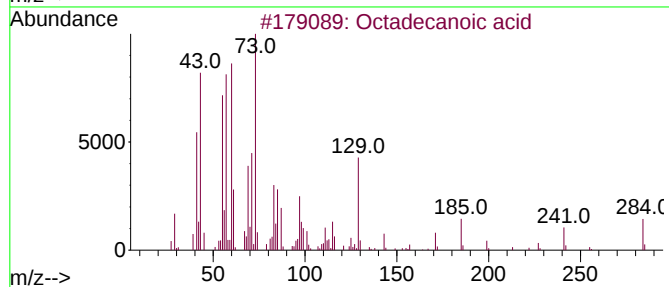
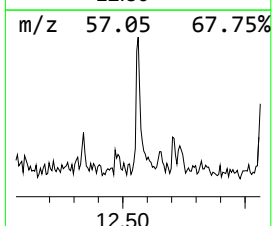
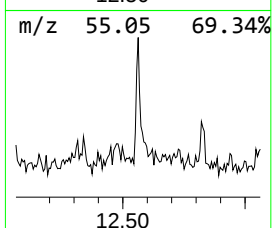
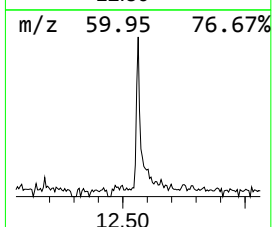
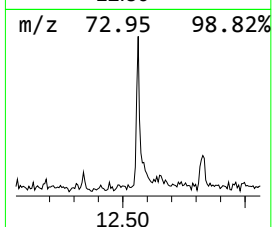
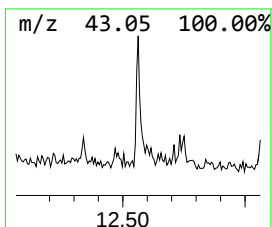
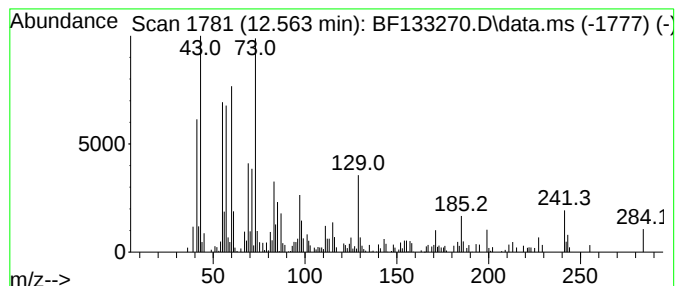
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	2.19 ng	153621	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133270.D
Acq On : 05 May 2023 18:46
Operator : CG\JU
Sample : 02618-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

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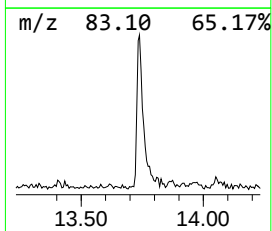
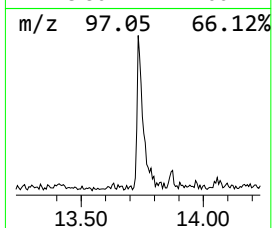
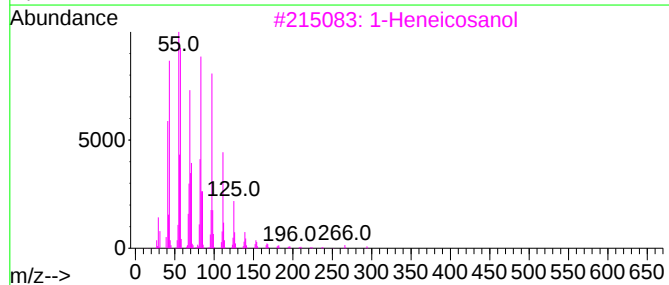
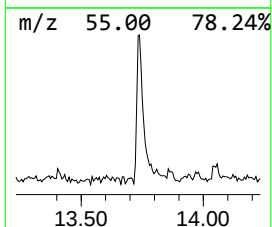
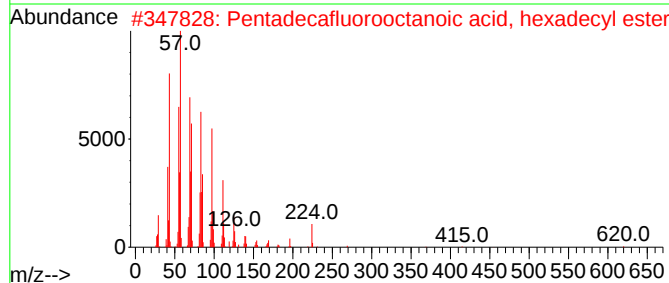
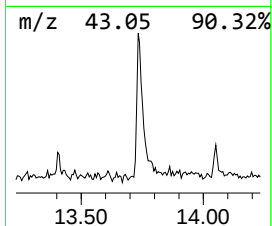
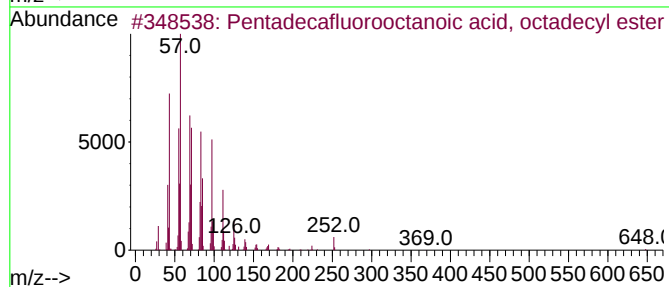
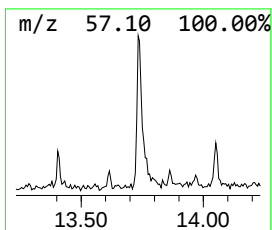
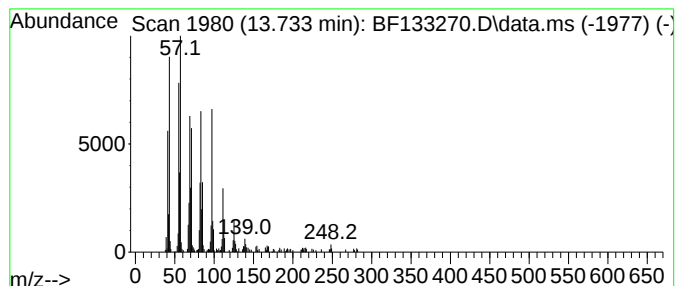
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	4.23 ng	296299	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133270.D
Acq On : 05 May 2023 18:46
Operator : CG\JU
Sample : 02618-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

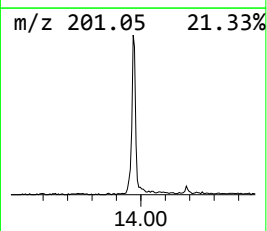
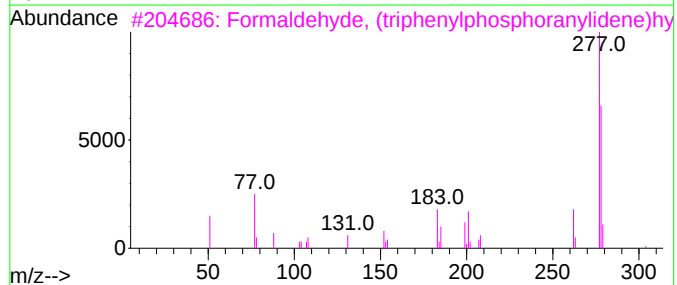
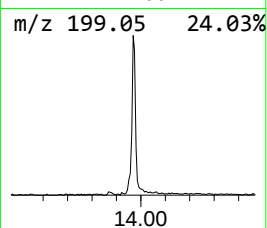
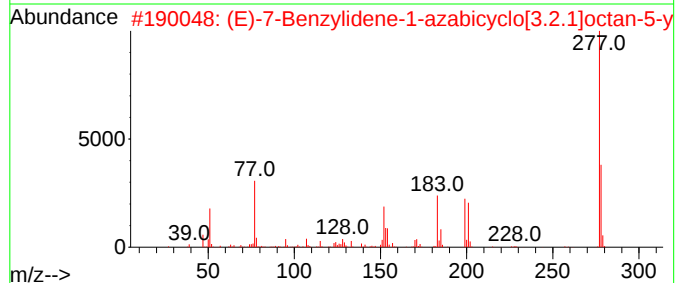
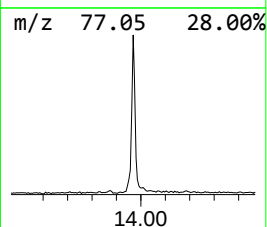
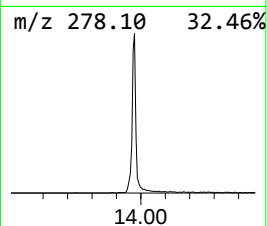
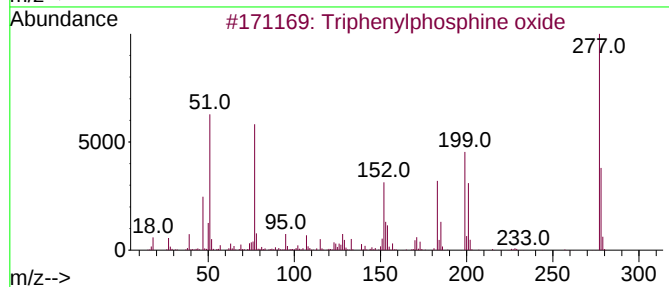
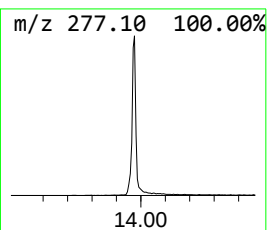
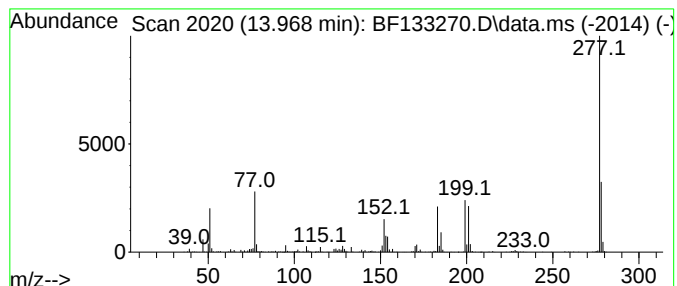
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	10.64 ng	745264	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	87
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	72
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35
5			4-Nitro-4'-methylidiphenylsulfone	277	C13H11N04S	004094-37-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133270.D
Acq On : 05 May 2023 18:46
Operator : CG\JU
Sample : 02618-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

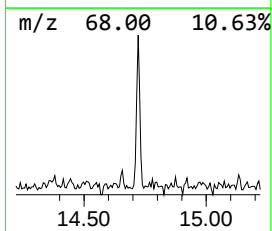
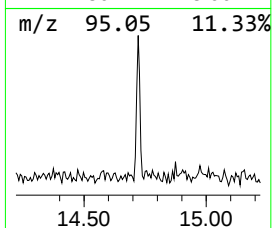
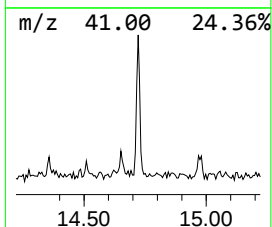
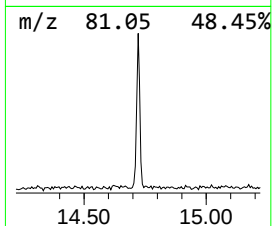
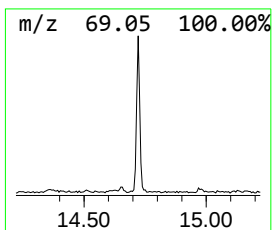
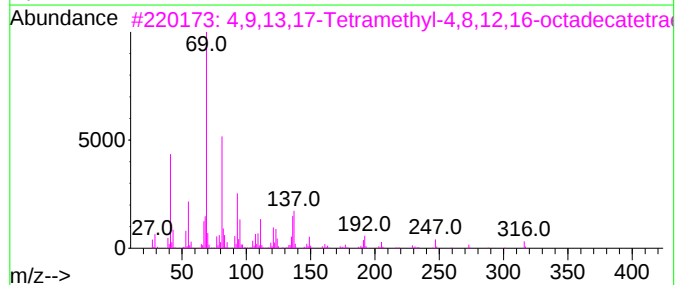
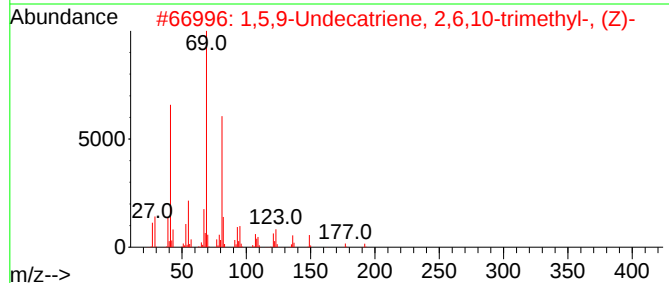
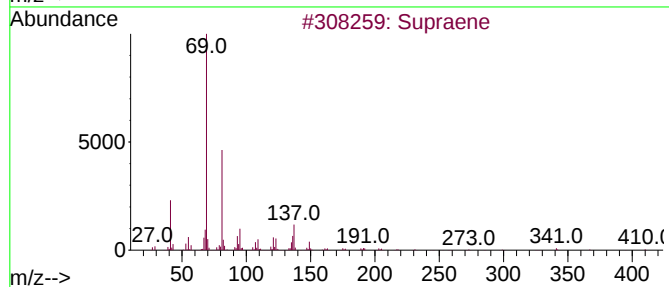
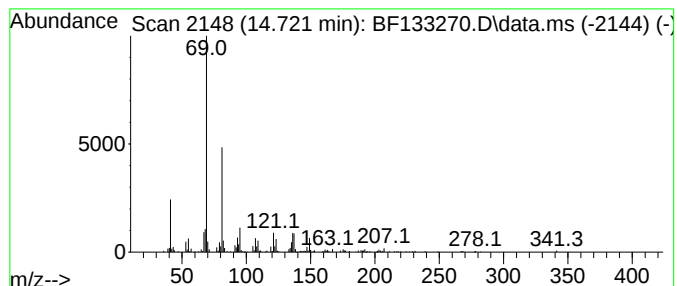
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.85 ng	161817	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	72
5			Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133270.D
Acq On : 05 May 2023 18:46
Operator : CG\JU
Sample : 02618-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.904	7.6	ng	398628	1	6.722	1054810	20.0
Benzophenone	10.474	11.1	ng	877984	3	9.763	1585840	20.0
Dimethazone	11.004	4.9	ng	396841	4	11.239	1617610	20.0
Cyclopenta[g]-2...	11.416	2.3	ng	182170	4	11.239	1617610	20.0
n-Hexadecanoic ...	11.780	5.3	ng	428700	4	11.239	1617610	20.0
Octadecanoic acid	12.563	2.2	ng	153621	5	13.874	1401040	20.0
Pentadecafluoro...	13.733	4.2	ng	296299	5	13.874	1401040	20.0
Triphenylphosph...	13.968	10.6	ng	745264	5	13.874	1401040	20.0
Supraene	14.721	2.9	ng	161817	6	15.292	1137240	20.0