

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
 Data File : BF133872.D
 Acq On : 21 Jun 2023 15:48
 Operator : CG\JU
 Sample : 03289-20
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-4.0-6.0

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133872.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	4	9	15	rVB	146705	182316	6.34%	0.997%
2	2.258	23	29	36	rBV3	18128	33715	1.17%	0.184%
3	5.093	507	511	520	rBV	410024	454969	15.82%	2.487%
4	5.493	575	579	592	rBV	2078304	1901342	66.10%	10.395%
5	6.499	745	750	753	rBV	2206203	2258513	78.52%	12.347%
6	6.857	808	811	815	rBV	842200	679896	23.64%	3.717%
7	7.422	902	907	910	rBV	1603533	1372914	47.73%	7.506%
8	8.140	1025	1029	1032	rBV	1080714	857145	29.80%	4.686%
9	9.216	1208	1212	1215	rBV	3539230	2876366	100.00%	15.725%
10	9.898	1324	1328	1331	rBV	1031226	850471	29.57%	4.649%
11	10.616	1446	1450	1453	rBV	197183	175456	6.10%	0.959%
12	10.692	1458	1463	1466	rBV	1693527	1663042	57.82%	9.092%
13	11.392	1578	1582	1585	rBV	749534	687234	23.89%	3.757%
14	11.922	1668	1672	1684	rBV2	201776	236277	8.21%	1.292%
15	12.610	1786	1789	1794	rBV	36514	39825	1.38%	0.218%
16	12.710	1803	1806	1817	rBV2	40908	56859	1.98%	0.311%
17	12.839	1823	1828	1833	rVB	32701	35888	1.25%	0.196%
18	12.986	1849	1853	1857	rBV	2659133	2466859	85.76%	13.486%
19	13.898	2004	2008	2018	rBV2	88273	158420	5.51%	0.866%
20	14.045	2029	2033	2037	rBV	633563	633241	22.02%	3.462%
21	14.145	2047	2050	2054	rBV	32678	39941	1.39%	0.218%
22	14.916	2178	2181	2187	rVB	123177	128861	4.48%	0.704%
23	15.557	2285	2290	2295	rBV	390540	502199	17.46%	2.745%

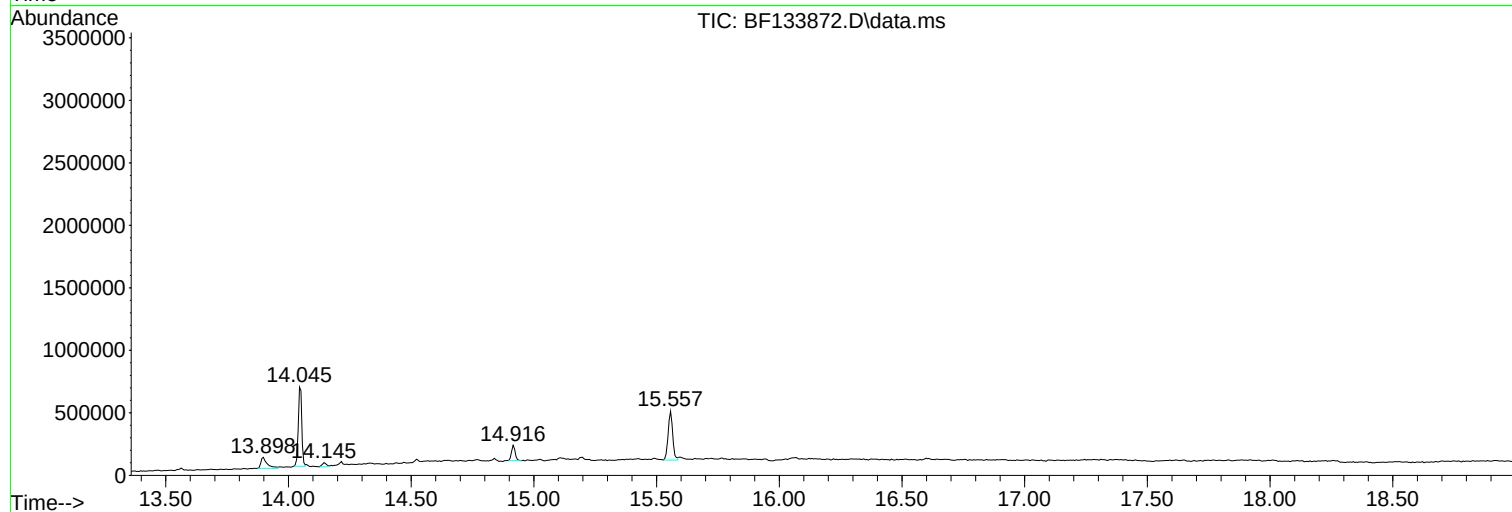
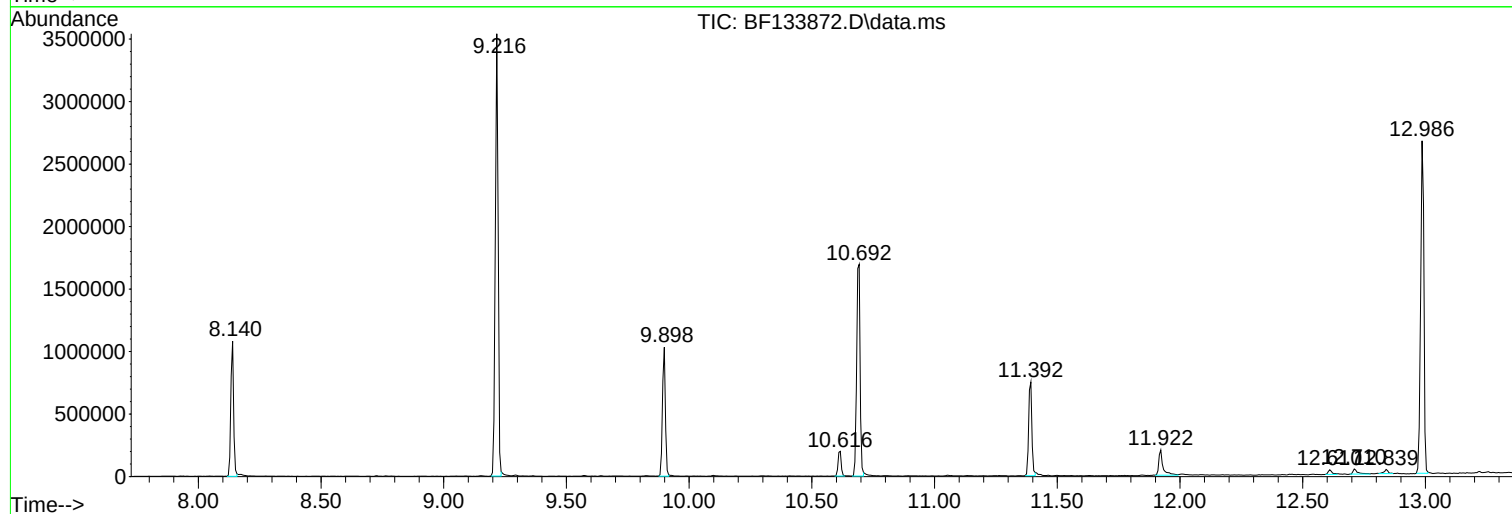
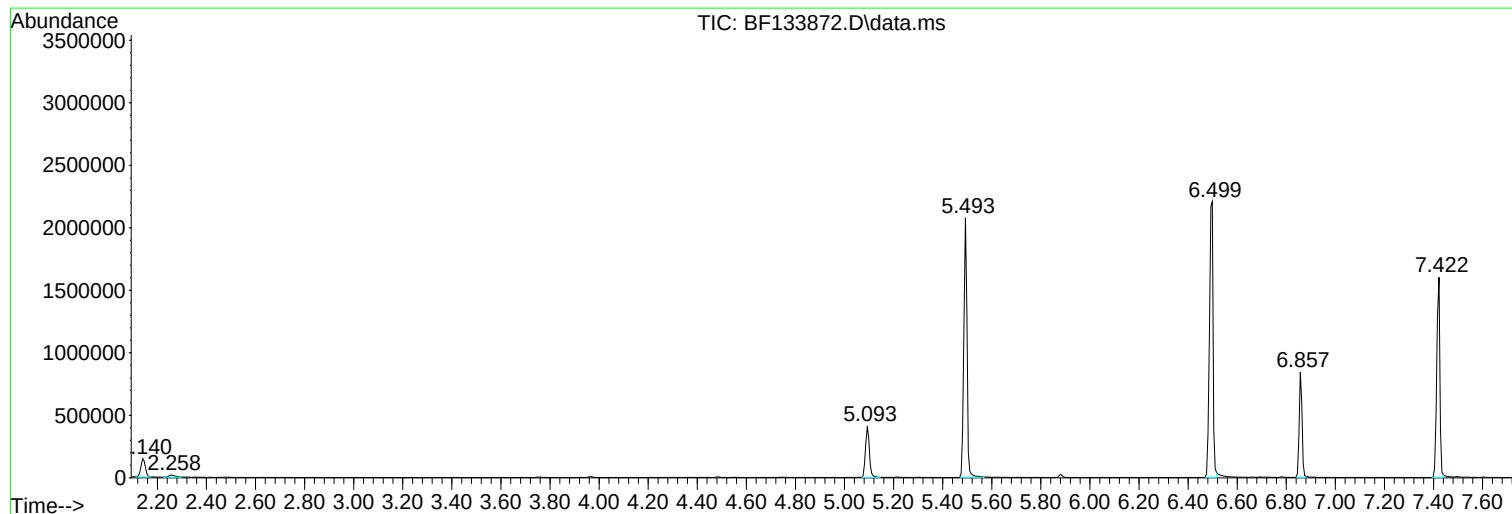
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ClientSampleId :
SB-07-4.0-6.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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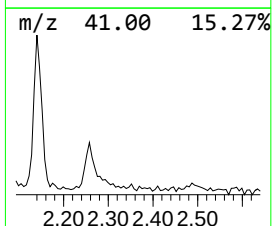
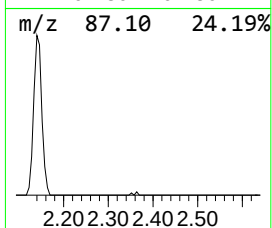
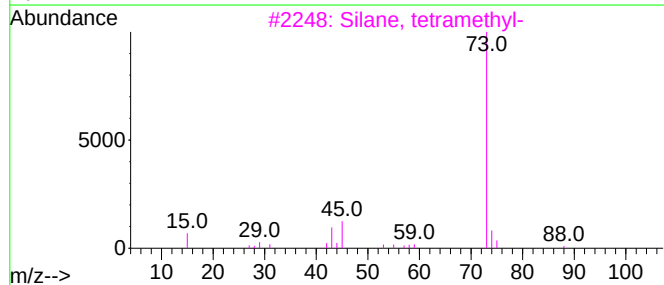
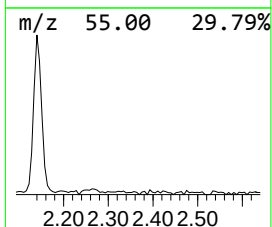
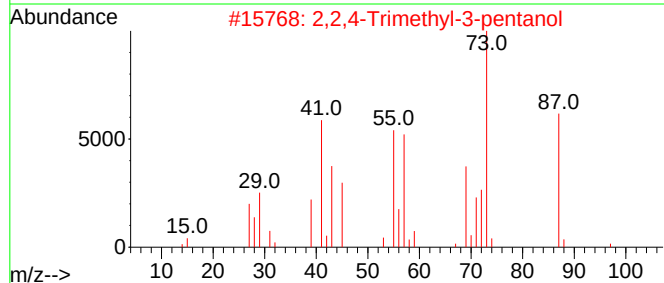
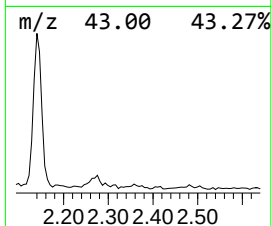
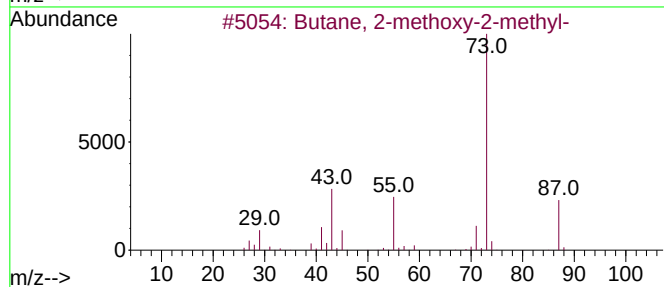
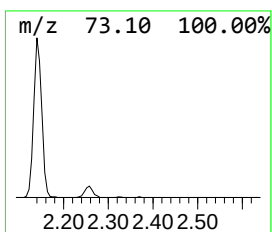
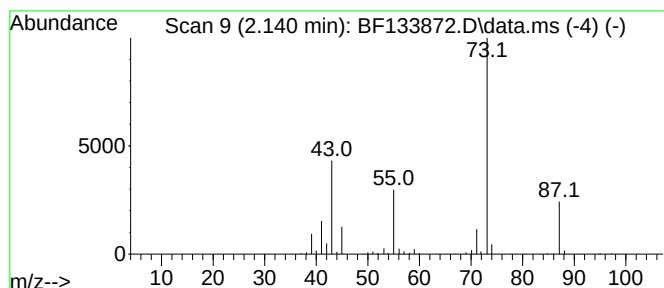
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	5.36 ng	182316	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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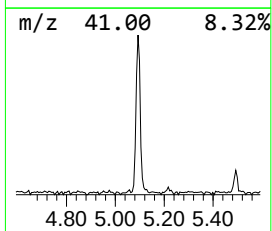
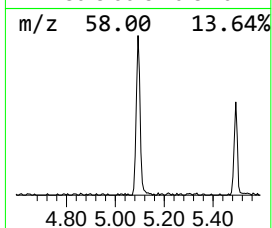
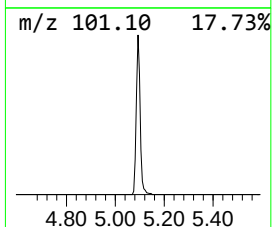
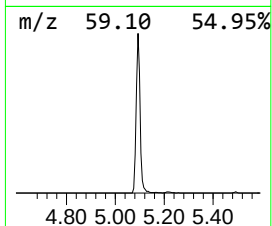
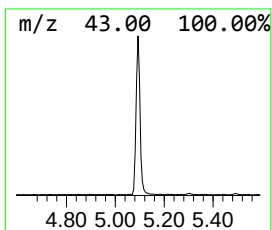
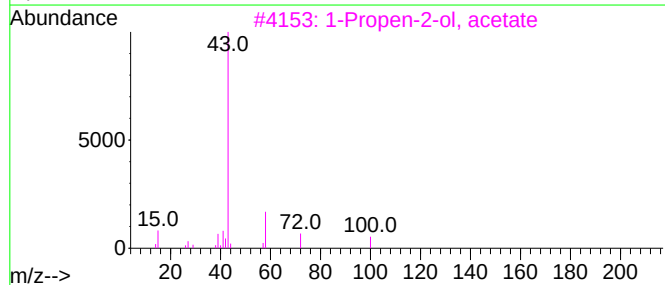
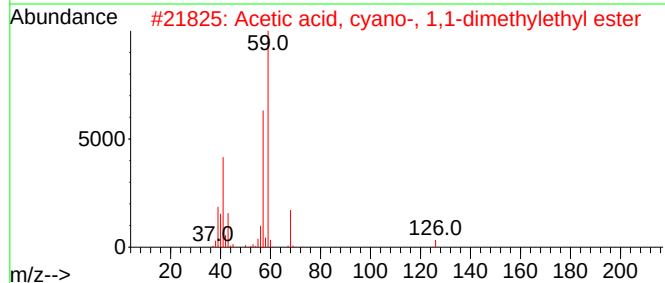
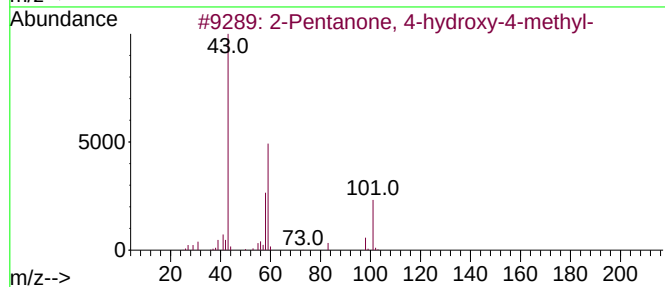
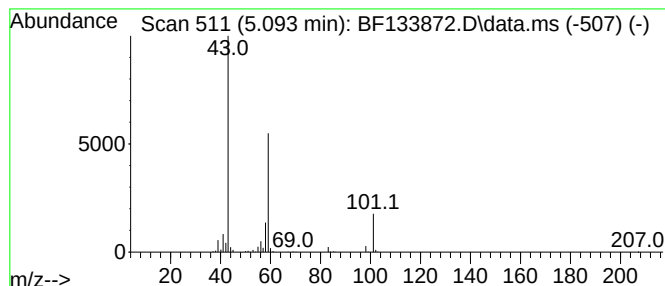
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	13.38 ng	454969	1,4-Dichlorobenzene-d4	6.857

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			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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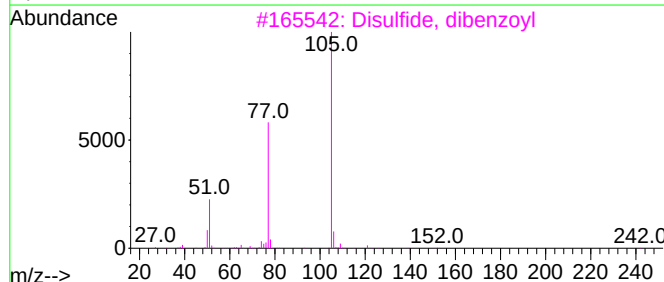
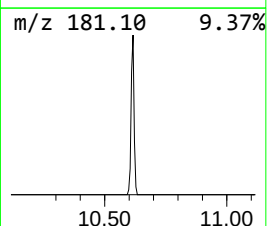
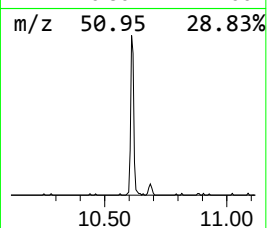
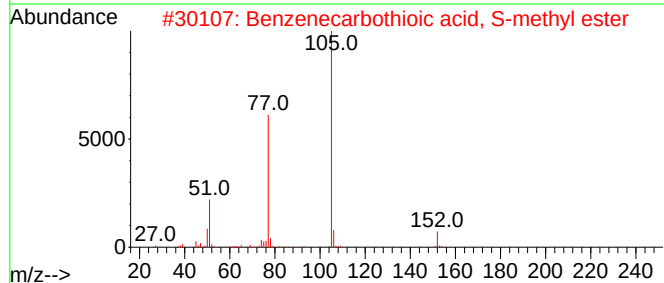
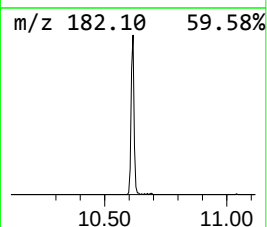
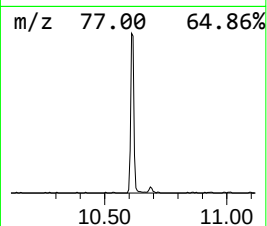
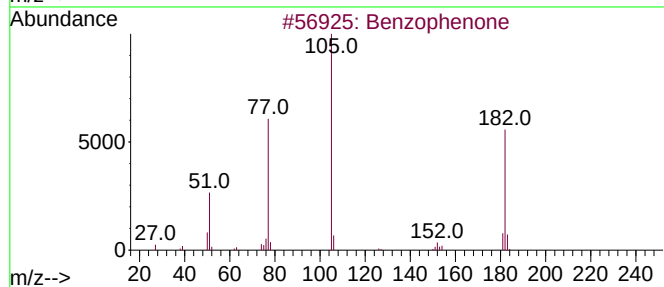
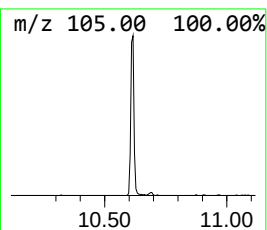
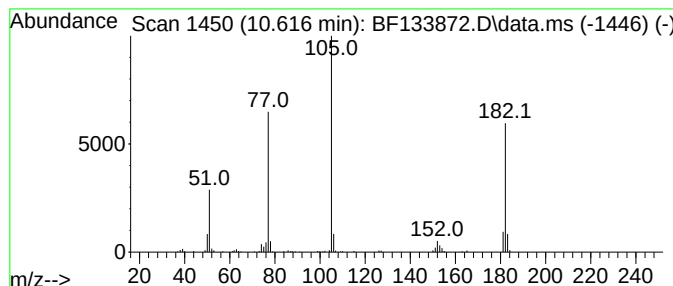
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	4.13 ng	175456	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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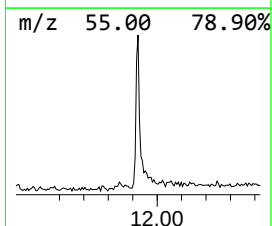
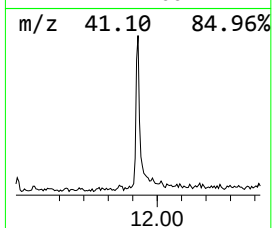
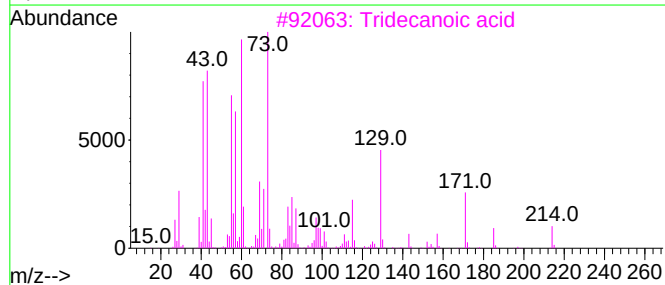
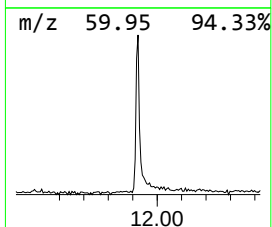
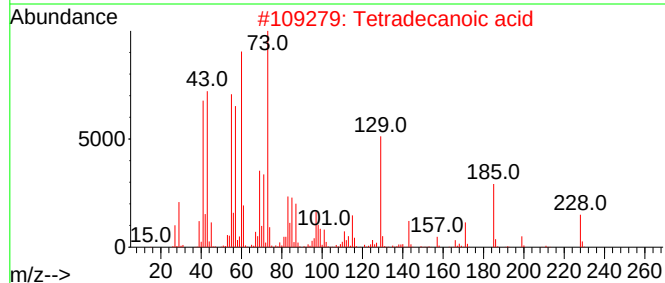
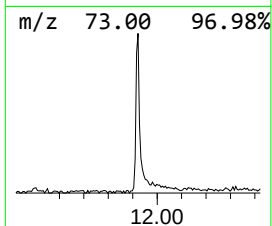
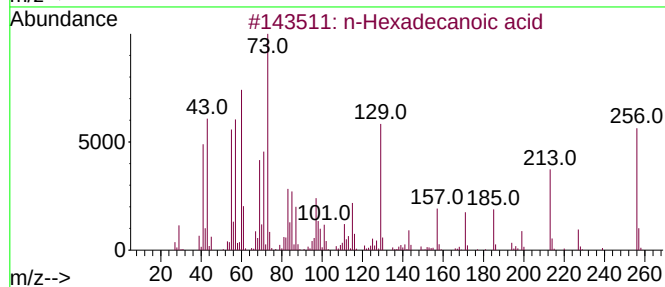
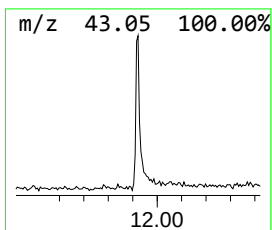
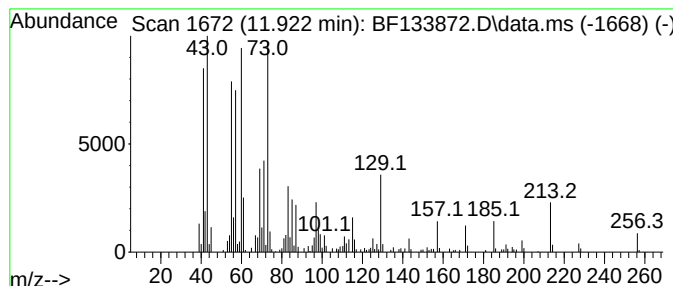
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.88 ng	236277	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3			Tridecanoic acid	214	C13H26O2	000638-53-9	60
4			Dodecanoic acid	200	C12H24O2	000143-07-7	58
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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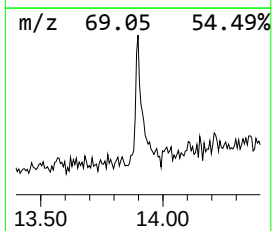
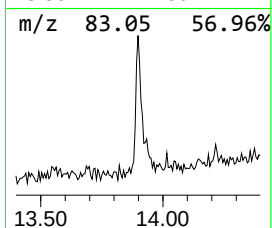
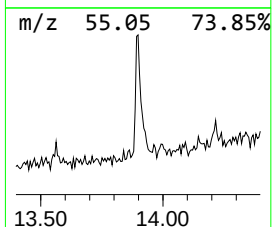
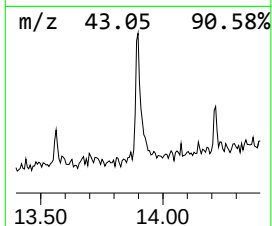
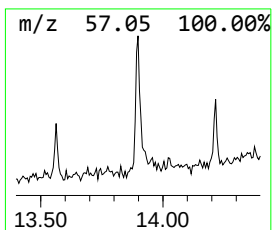
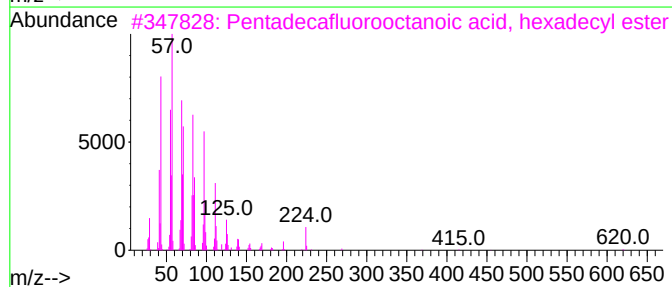
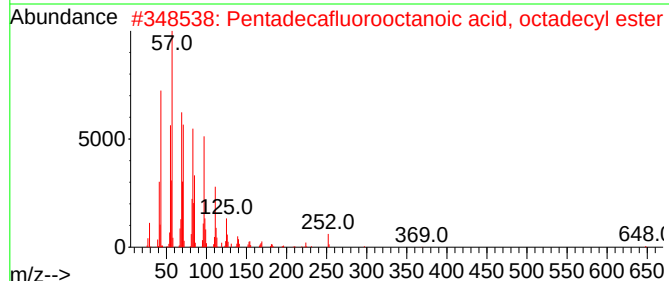
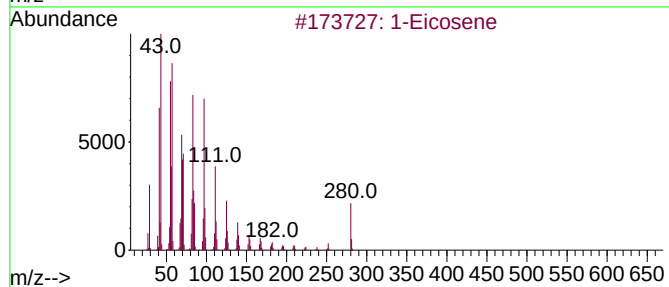
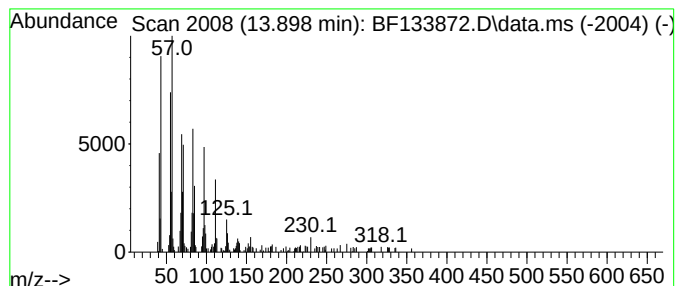
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Eicosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.00 ng	158420	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Eicosene	280	C20H40	003452-07-1	96
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



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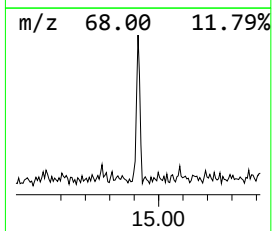
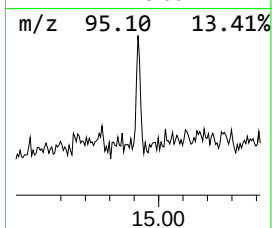
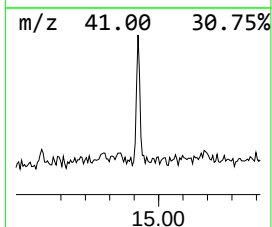
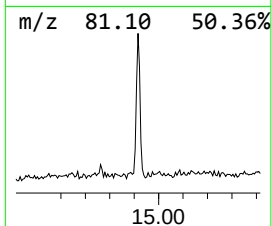
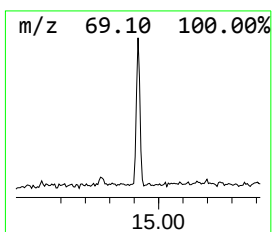
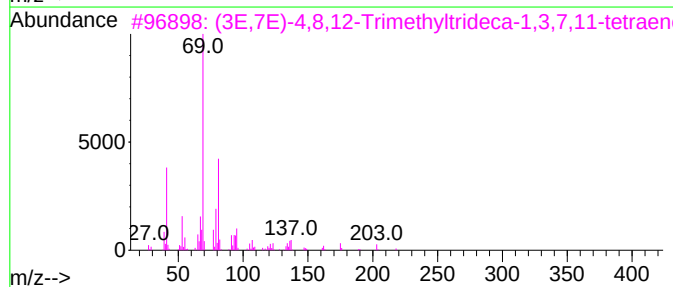
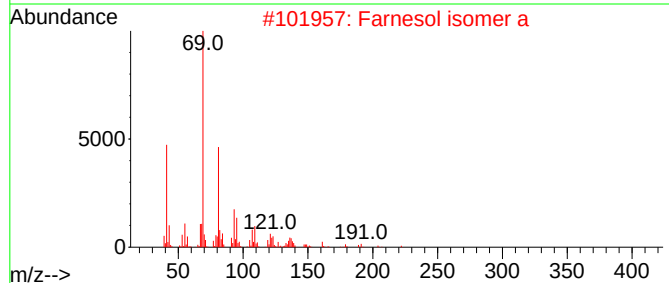
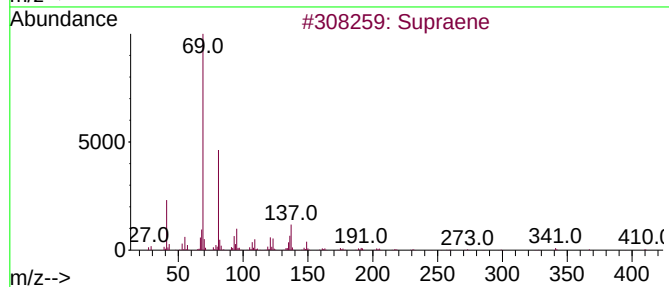
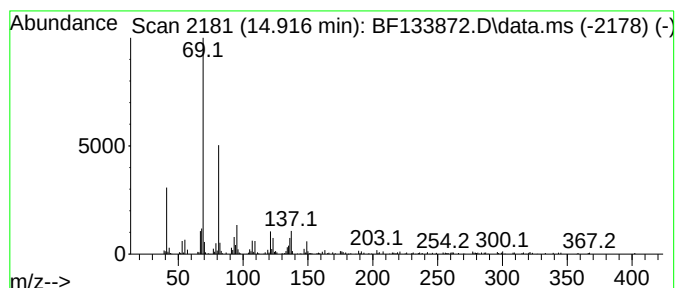
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	5.13 ng	128861	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Farnesol isomer a	222	C15H26O	1000108-92-4	72
3			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	64
4			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59
5			3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133872.D
Acq On : 21 Jun 2023 15:48
Operator : CG\JU
Sample : 03289-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-4.0-6.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
Butane, 2-metho...	2.140	5.4	ng	182316	1	6.857	679896	20.0
2-Pentanone, 4-...	5.093	13.4	ng	454969	1	6.857	679896	20.0
Benzophenone	10.616	4.1	ng	175456	3	9.898	850471	20.0
n-Hexadecanoic ...	11.922	6.9	ng	236277	4	11.392	687234	20.0
1-Eicosene	13.898	5.0	ng	158420	5	14.045	633241	20.0
Supraene	14.916	5.1	ng	128861	6	15.557	502199	20.0