

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
 Data File : BF133336.D
 Acq On : 10 May 2023 18:03
 Operator : CG\JU
 Sample : 02719-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01_0-2_20230509

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: BF133336.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.699	100	104	114	rVB	38616	56265	1.30%	0.164%
2	4.257	365	369	377	rBV	159919	195039	4.52%	0.567%
3	4.904	474	479	487	rBV	1162579	1475388	34.17%	4.292%
4	5.334	548	552	564	rBV	3902741	3757393	87.03%	10.930%
5	5.728	615	619	624	rBV	118453	108052	2.50%	0.314%
6	6.010	664	667	672	rBV	61635	60897	1.41%	0.177%
7	6.363	722	727	730	rBV	3963594	3713782	86.02%	10.803%
8	6.722	784	788	791	rBV	1440847	1271928	29.46%	3.700%
9	7.287	879	884	887	rBV	2770422	2396197	55.50%	6.970%
10	8.004	1002	1006	1009	rBV	2237533	1726085	39.98%	5.021%
11	9.081	1185	1189	1192	rBV	5269703	4317432	100.00%	12.559%
12	9.757	1300	1304	1307	rBV	2369199	1964500	45.50%	5.714%
13	10.469	1421	1425	1429	rBV	311858	255799	5.92%	0.744%
14	10.545	1434	1438	1450	rBV	2055855	1821093	42.18%	5.297%
15	11.239	1552	1556	1558	rBV	2246388	1935447	44.83%	5.630%
16	11.263	1558	1560	1563	rVV	310404	251688	5.83%	0.732%
17	11.310	1563	1568	1572	rVB	80135	84123	1.95%	0.245%
18	11.769	1643	1646	1651	rBV2	90485	118454	2.74%	0.345%
19	11.851	1657	1660	1662	rBV2	63566	67136	1.55%	0.195%
20	12.445	1756	1761	1765	rBV	577785	513465	11.89%	1.494%
21	12.563	1775	1781	1785	rBV4	62402	120762	2.80%	0.351%
22	12.674	1794	1800	1803	rBV	509851	499172	11.56%	1.452%
23	12.721	1803	1808	1817	rVB4	74179	143440	3.32%	0.417%
24	12.827	1821	1826	1829	rVV	3757601	3685143	85.35%	10.720%
25	13.110	1870	1874	1877	rBV	50088	56338	1.30%	0.164%
26	13.404	1917	1924	1927	rBV3	44842	59742	1.38%	0.174%
27	13.621	1957	1961	1964	rBV2	37679	51078	1.18%	0.149%
28	13.768	1981	1986	1996	rVB7	53583	153015	3.54%	0.445%
29	13.874	1999	2004	2006	rBV2	1239574	1286511	29.80%	3.742%
30	13.898	2006	2008	2011	rVB	166426	132170	3.06%	0.384%
31	14.886	2172	2176	2179	rBV	169730	244293	5.66%	0.711%
32	15.174	2221	2225	2230	rVB	99768	126514	2.93%	0.368%
33	15.227	2231	2234	2240	rVB	140513	172145	3.99%	0.501%
34	15.292	2240	2245	2249	rBV	1068015	1252916	29.02%	3.645%
35	15.739	2318	2321	2326	rVB2	39419	51453	1.19%	0.150%
36	16.662	2474	2478	2490	rVB2	72386	153293	3.55%	0.446%

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

37	17.074	2545	2548	2557	rVB	50203	99368	2.30%	0.289%
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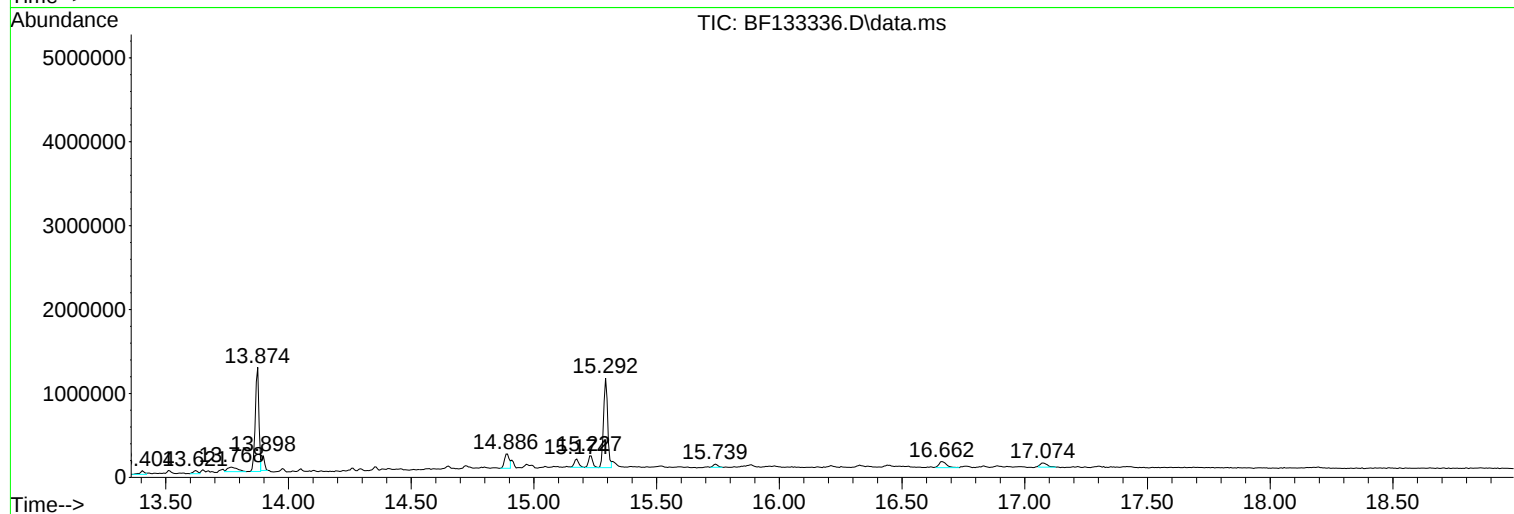
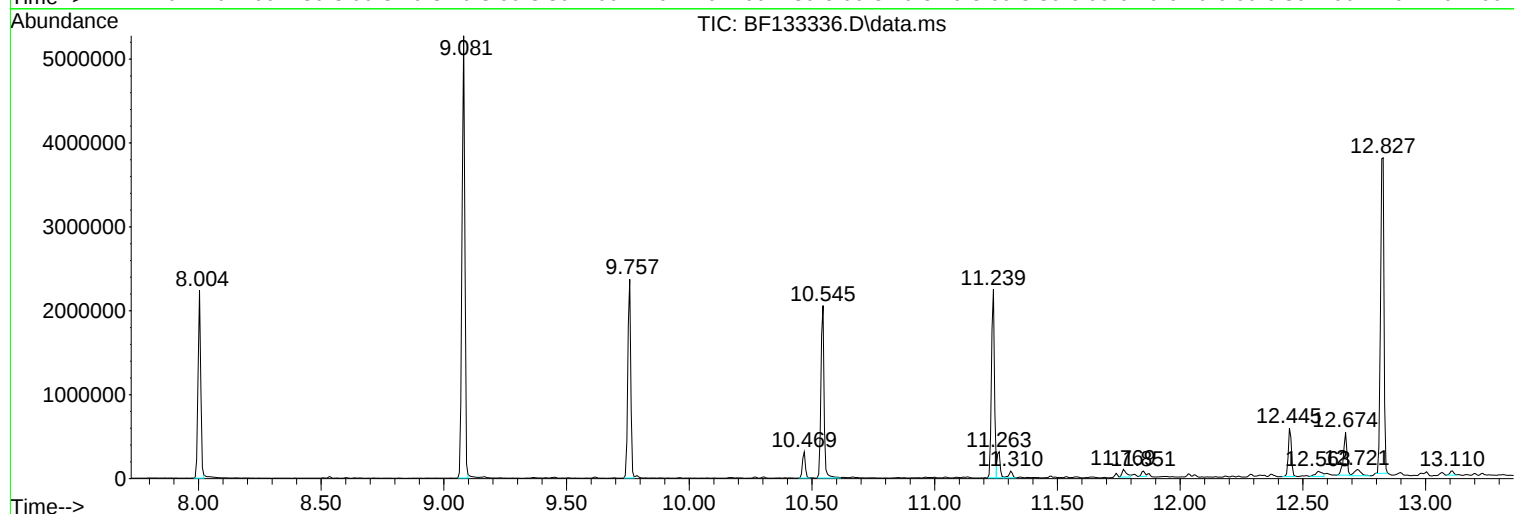
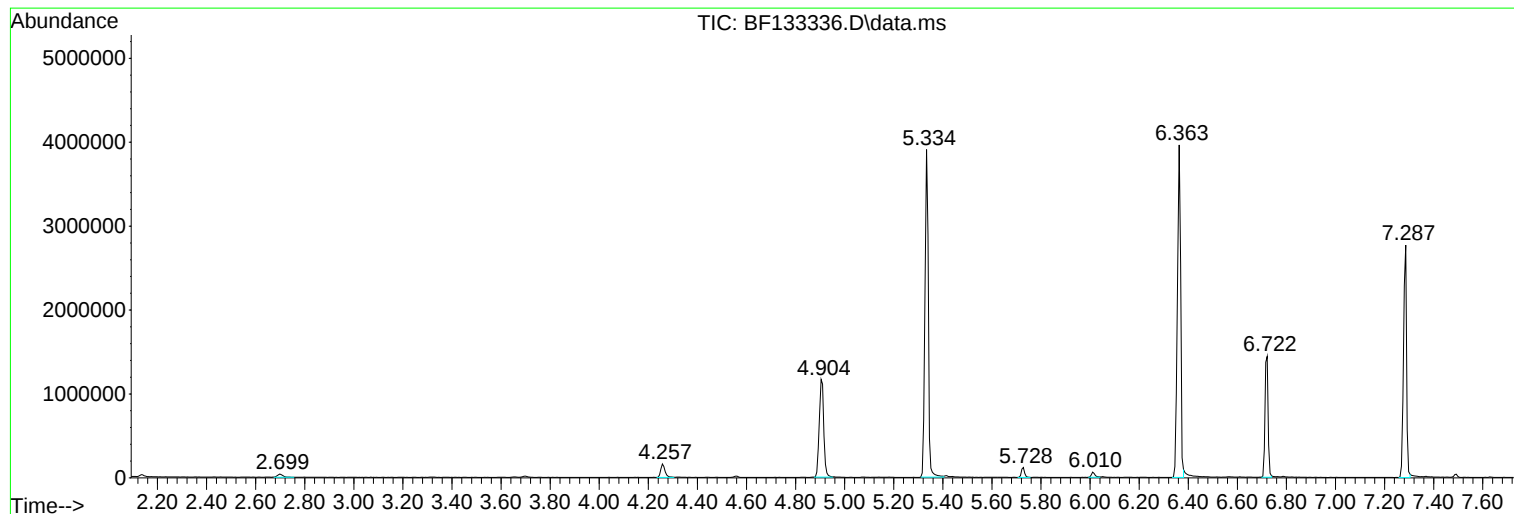
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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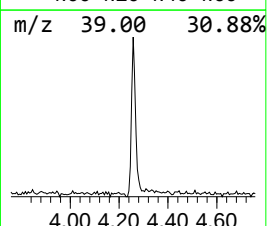
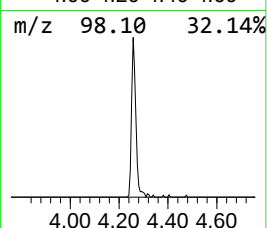
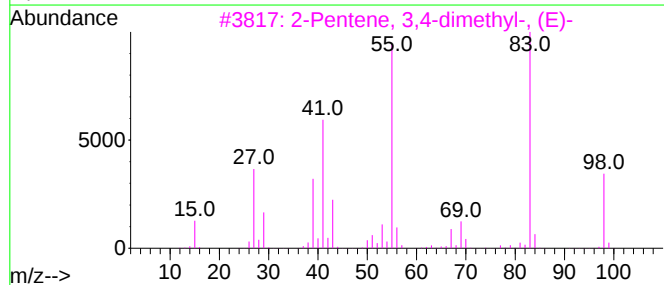
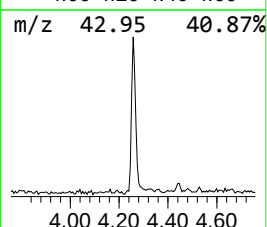
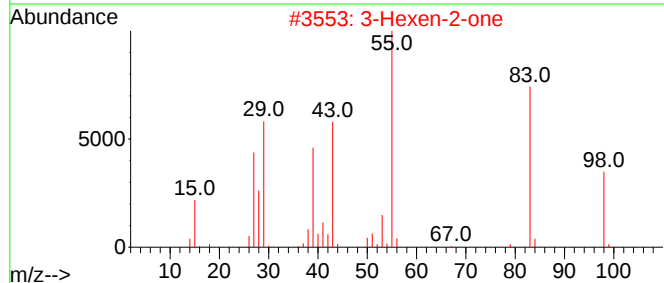
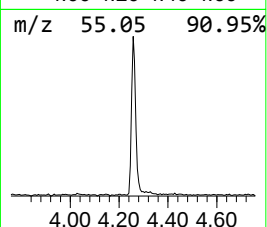
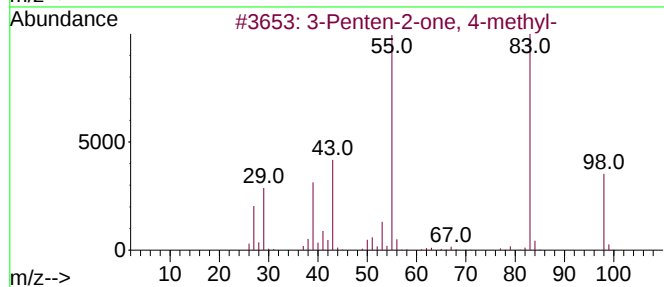
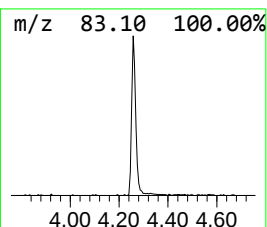
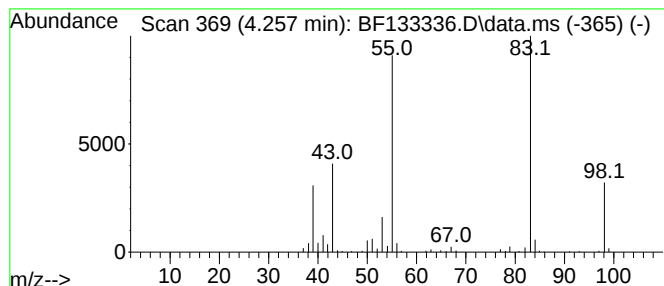
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.257	3.07 ng	195039	1,4-Dichlorobenzene-d4	6.722

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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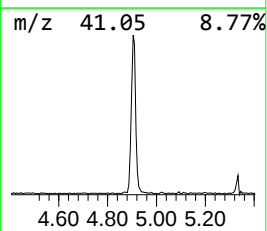
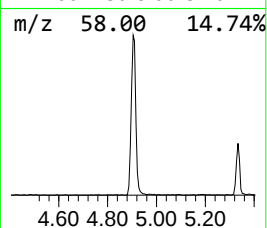
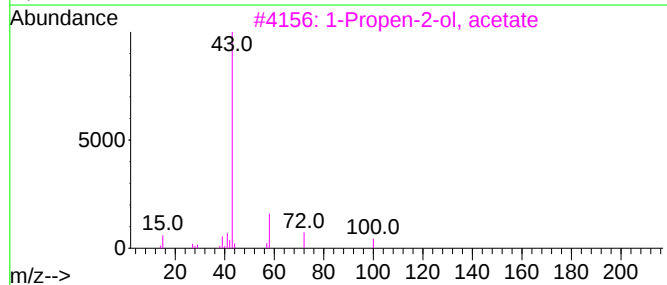
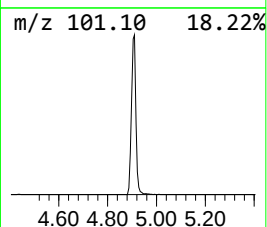
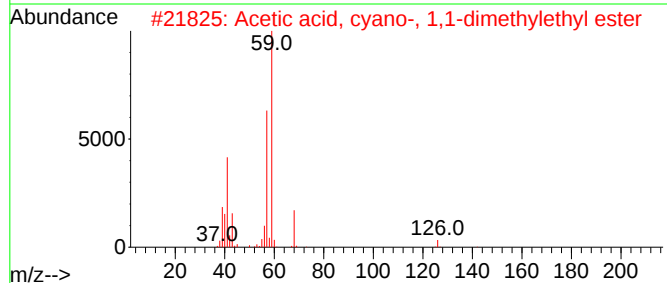
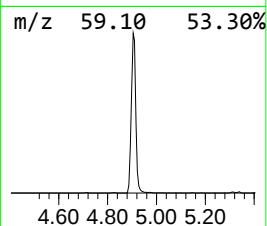
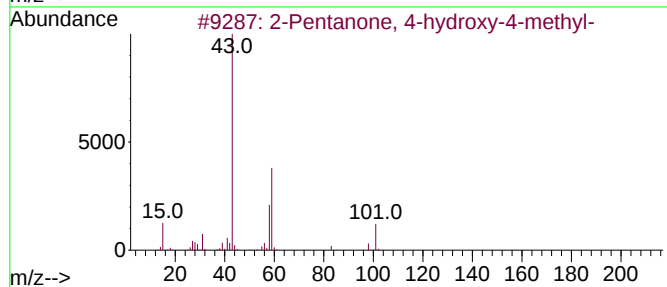
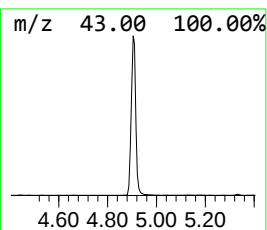
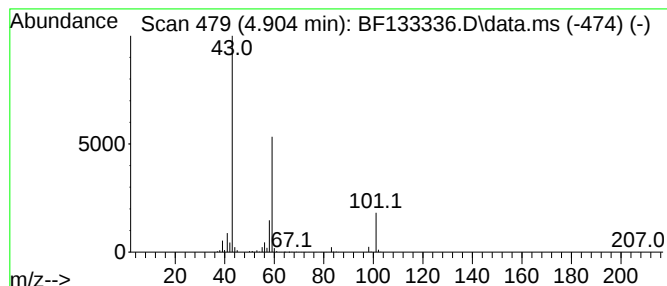
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.904	23.20 ng	1475390	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	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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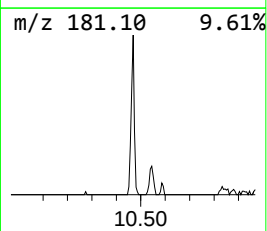
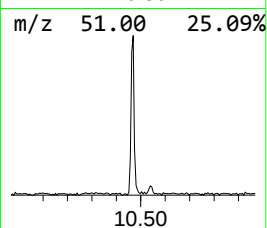
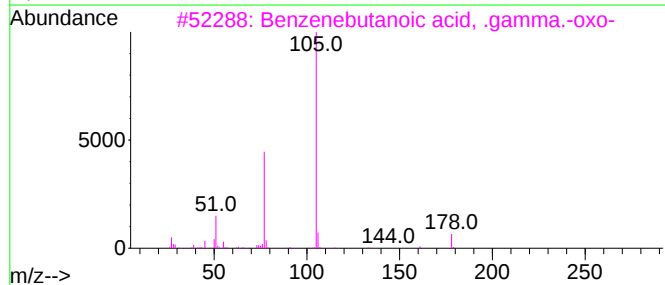
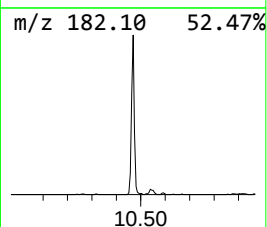
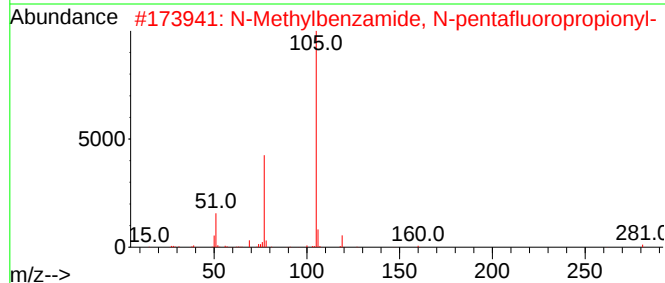
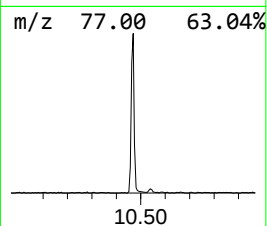
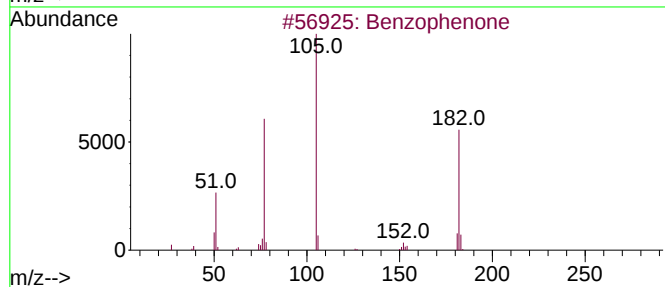
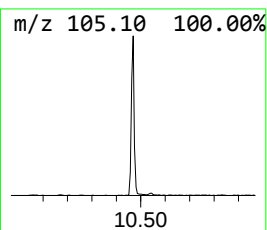
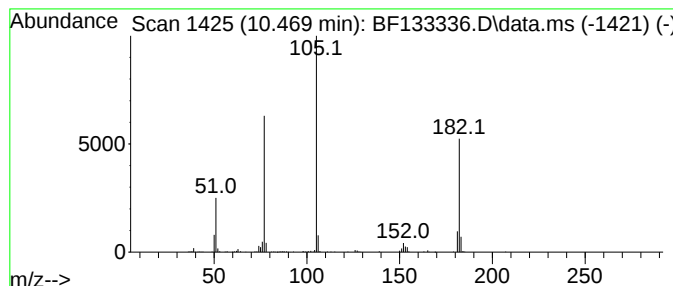
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.60 ng	255799	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



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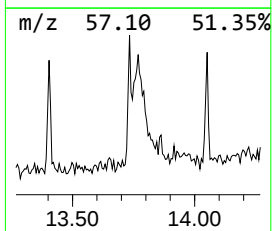
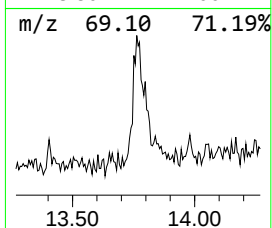
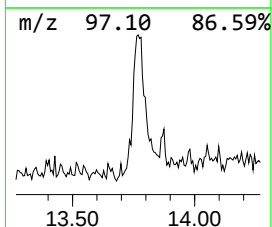
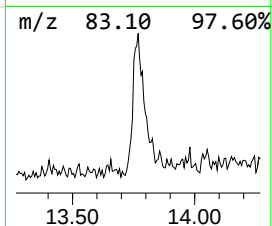
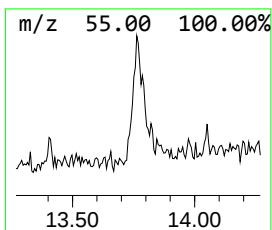
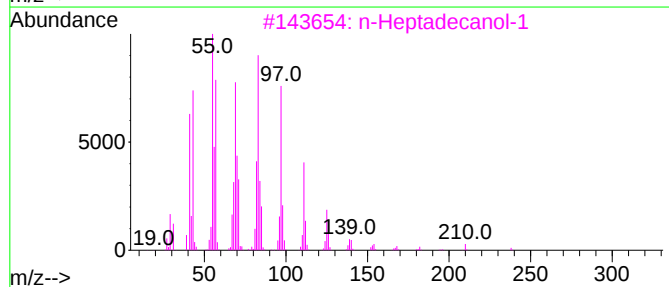
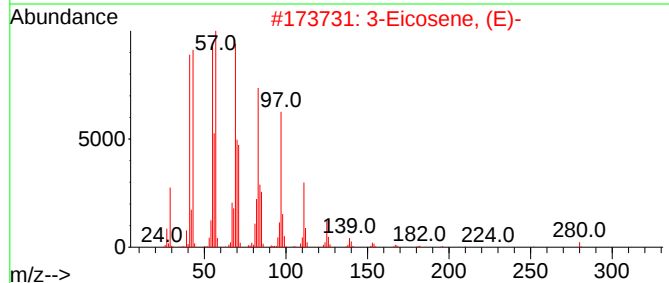
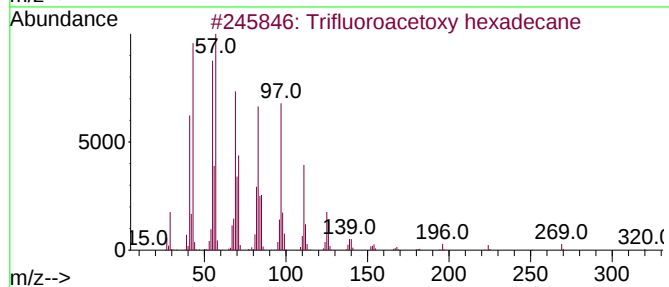
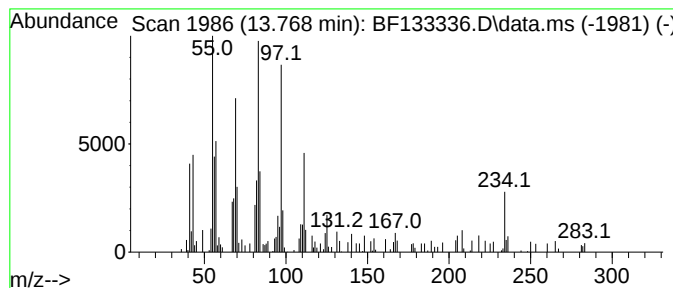
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	2.38 ng	153015	Chrysene-d12	13.874

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	53
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	52
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	46
4		1-Tetradecanol	214	C14H30O	000112-72-1	46
5		4-Isopropylidicyclohexylmethane	222	C16H30	054965-61-6	43



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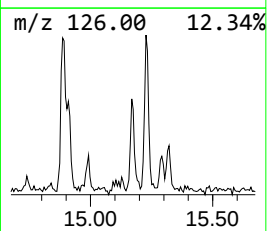
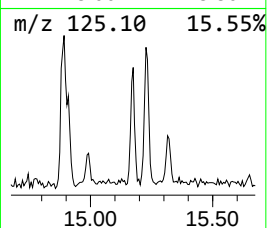
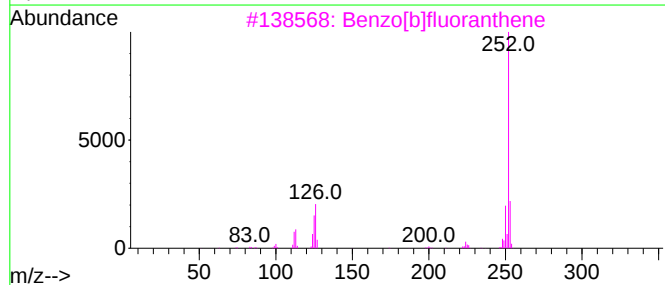
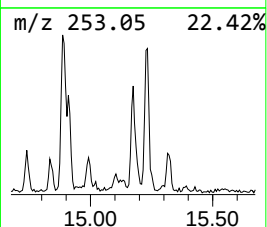
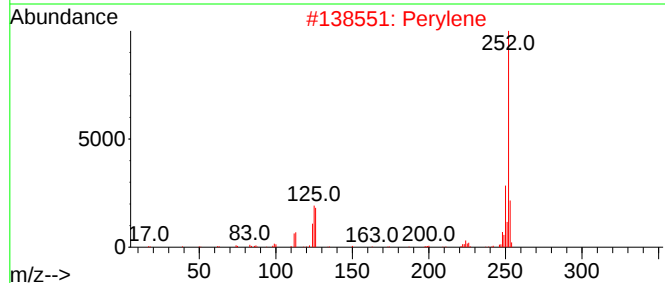
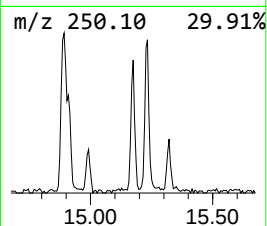
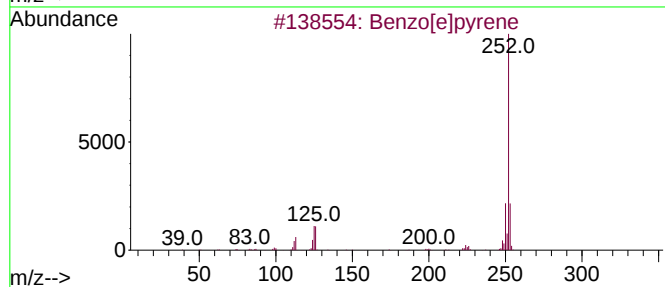
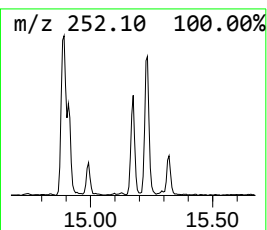
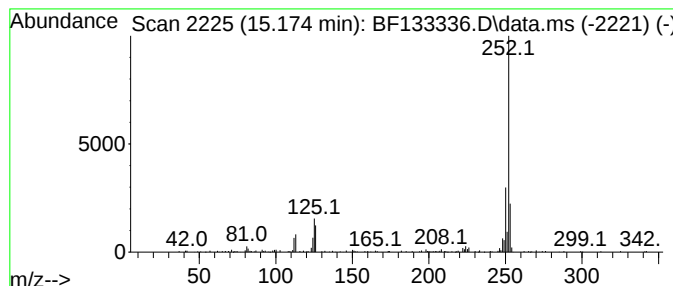
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.02 ng	126514	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Perylene	252	C20H12	000198-55-0	91
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5			Benzo[a]pyrene	252	C20H12	000050-32-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133336.D
Acq On : 10 May 2023 18:03
Operator : CG\JU
Sample : 02719-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01_0-2_20230509

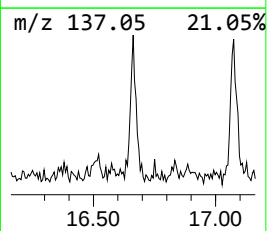
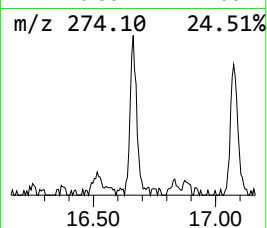
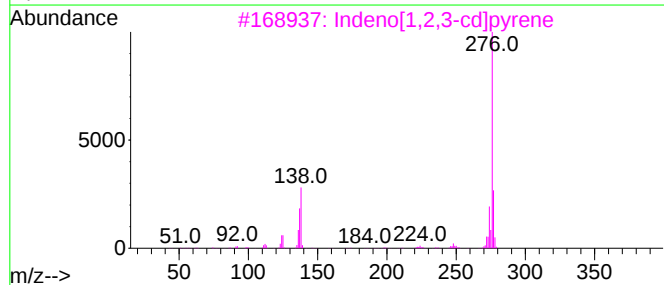
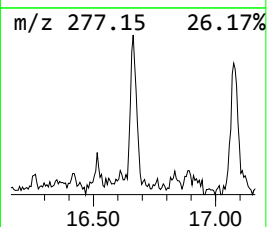
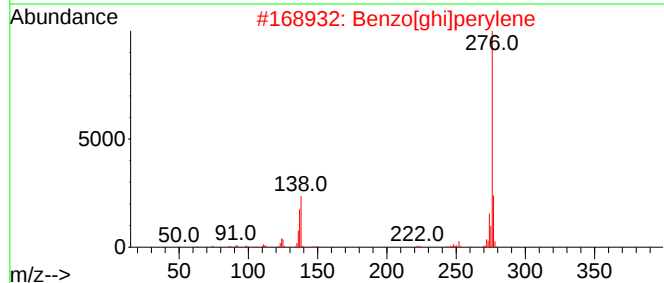
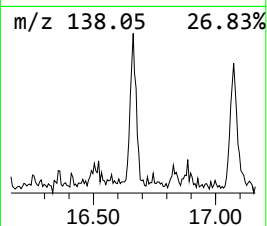
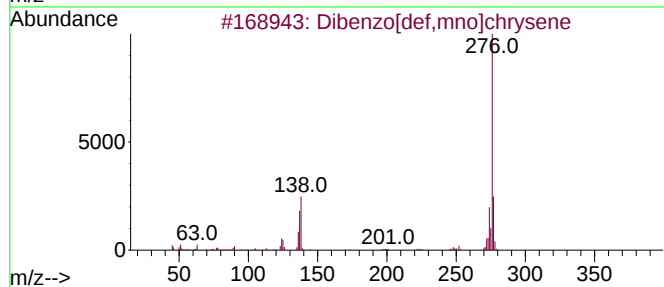
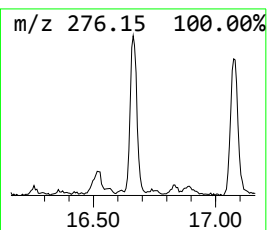
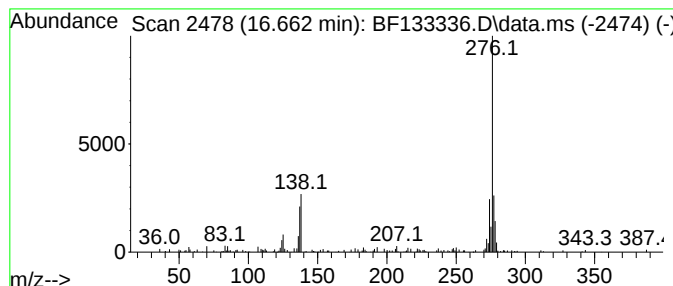
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.662	2.45 ng	153293	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	96
2			Benzo[ghi]perylene	276	C22H12	000191-24-2	96
3			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	91
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	90
5			2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133336.D
Acq On : 10 May 2023 18:03
Operator : CG\JU
Sample : 02719-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01_0-2_20230509

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
3-Penten-2-one,...	4.257	3.1	ng	195039	1	6.722	1271930	20.0
2-Pentanone, 4-...	4.904	23.2	ng	1475390	1	6.722	1271930	20.0
Benzophenone	10.469	2.6	ng	255799	3	9.757	1964500	20.0
Trifluoroacetox...	13.769	2.4	ng	153015	5	13.874	1286510	20.0
Benzo[e]pyrene	15.174	2.0	ng	126514	6	15.292	1252920	20.0
Dibenzo[def,mno...	16.662	2.5	ng	153293	6	15.292	1252920	20.0