

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
 Data File : BF132551.D
 Acq On : 27 Feb 2023 14:22
 Operator : CG\JU
 Sample : 01665-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-231

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: BF132551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.237	403	408	417	rVB	1369080	1590397	48.92%	5.500%
2	5.631	470	475	478	rBV	3069487	2815610	86.61%	9.736%
3	6.019	537	541	545	rBV	45754	40176	1.24%	0.139%
4	6.625	640	644	647	rBV	3006433	2842039	87.42%	9.828%
5	7.001	705	708	711	rBV	1227378	932702	28.69%	3.225%
6	7.566	799	804	807	rBV	2227368	1878291	57.78%	6.495%
7	8.289	923	927	930	rBV	1423463	1203780	37.03%	4.163%
8	9.366	1105	1110	1113	rBV	3492123	3250925	100.00%	11.242%
9	10.048	1222	1226	1230	rBV	1695716	1374516	42.28%	4.753%
10	10.766	1344	1348	1351	rBV	1311501	1101565	33.88%	3.809%
11	10.842	1357	1361	1364	rBV	2523952	2185835	67.24%	7.559%
12	11.071	1397	1400	1404	rVB	119279	94360	2.90%	0.326%
13	11.542	1477	1480	1483	rBV	1584598	1435158	44.15%	4.963%
14	11.566	1483	1484	1488	rVB	268316	184724	5.68%	0.639%
15	11.619	1488	1493	1496	rBV	63721	72337	2.23%	0.250%
16	12.054	1563	1567	1576	rBV3	358988	441231	13.57%	1.526%
17	12.160	1582	1585	1588	rBV	65728	71300	2.19%	0.247%
18	12.683	1671	1674	1679	rBV	28245	33938	1.04%	0.117%
19	12.766	1684	1688	1691	rBV	479964	436291	13.42%	1.509%
20	12.842	1696	1701	1707	rBV3	54494	78874	2.43%	0.273%
21	12.995	1724	1727	1733	rVB	430413	378365	11.64%	1.308%
22	13.136	1744	1751	1754	rBV	3009334	2752772	84.68%	9.519%
23	13.207	1760	1763	1768	rVB2	26161	41350	1.27%	0.143%
24	13.324	1780	1783	1785	rVB	54604	46484	1.43%	0.161%
25	13.430	1797	1801	1803	rBV2	32180	36073	1.11%	0.125%
26	13.948	1885	1889	1892	rBV2	30528	42699	1.31%	0.148%
27	14.024	1899	1902	1915	rVB3	154914	303511	9.34%	1.050%
28	14.201	1927	1932	1935	rBV2	1063844	1081382	33.26%	3.739%
29	14.224	1935	1936	1942	rVB	200296	142181	4.37%	0.492%
30	14.589	1993	1998	2000	rBV	36227	46025	1.42%	0.159%
31	15.283	2112	2116	2120	rBV	192132	315136	9.69%	1.090%
32	15.401	2133	2136	2144	rVB	42155	65472	2.01%	0.226%
33	15.618	2169	2173	2178	rVB	126521	165813	5.10%	0.573%
34	15.683	2180	2184	2189	rVB	153927	195339	6.01%	0.675%
35	15.754	2190	2196	2200	rBV2	741887	1001230	30.80%	3.462%
36	17.342	2461	2466	2476	rVB2	64627	145173	4.47%	0.502%

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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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.830	2544	2549	2557	rVB2	46674	95625	2.94%	0.331%
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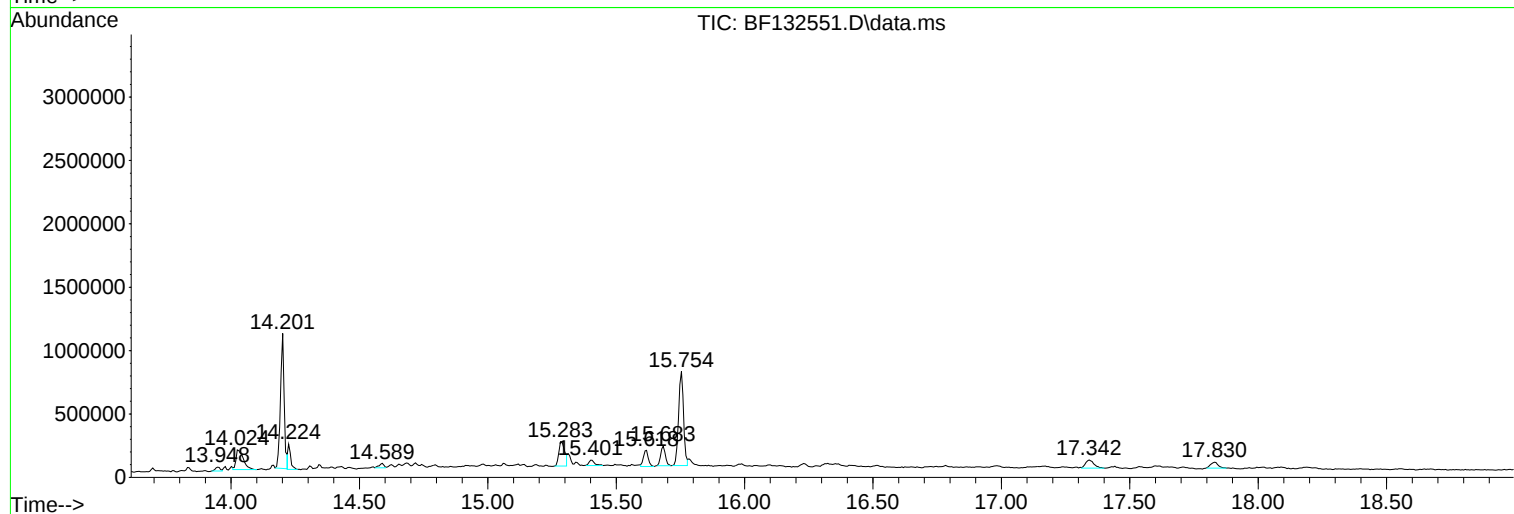
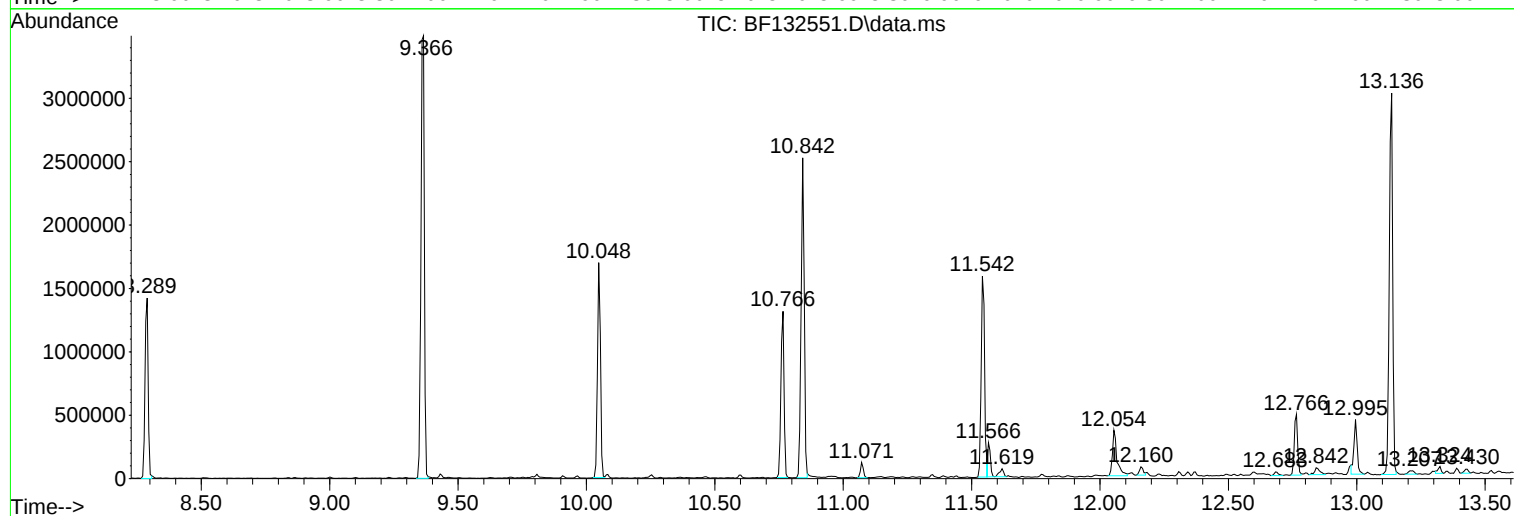
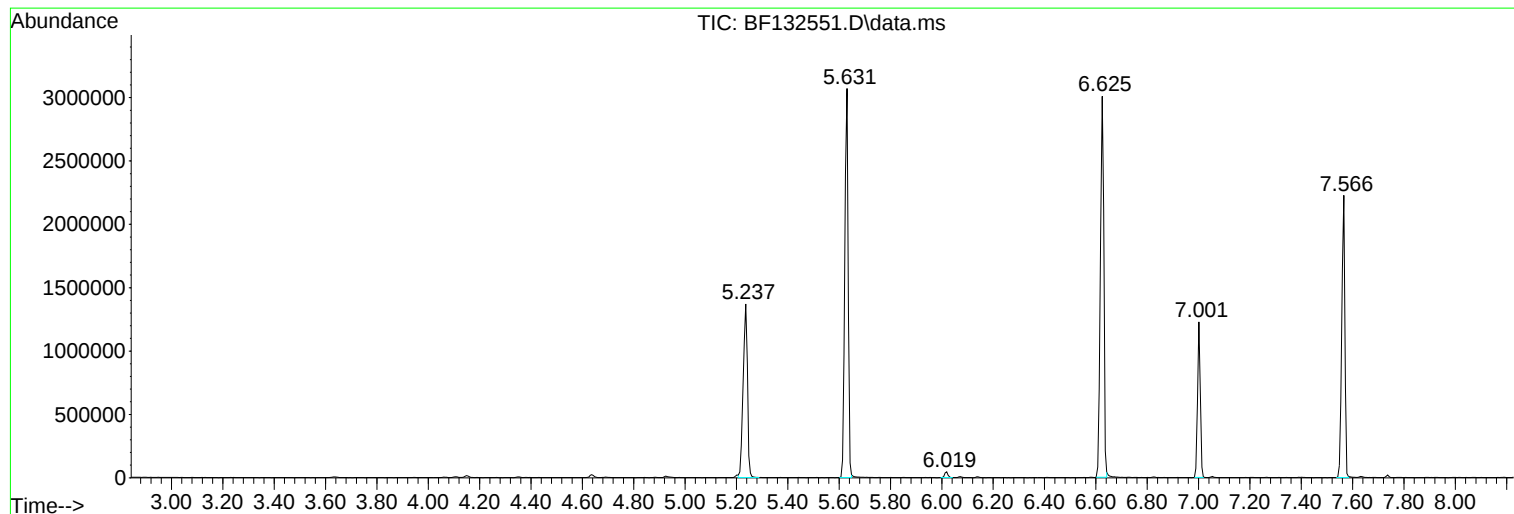
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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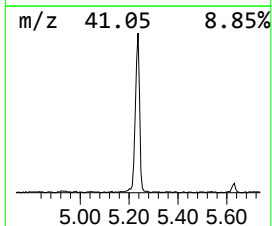
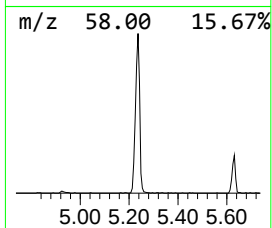
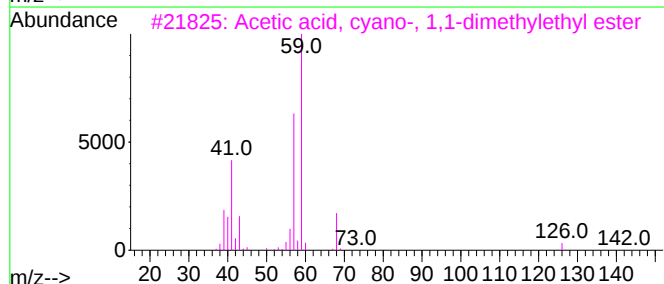
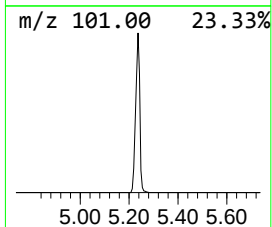
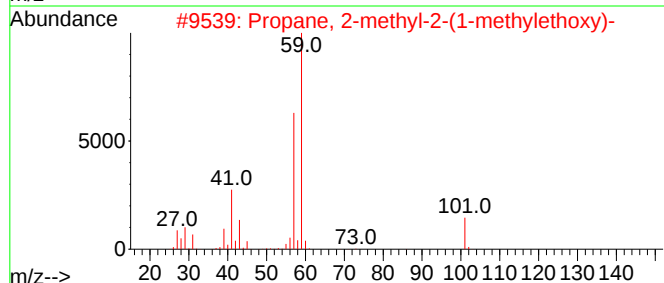
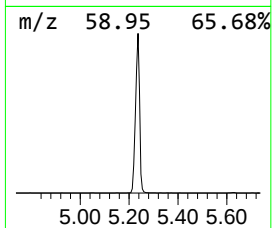
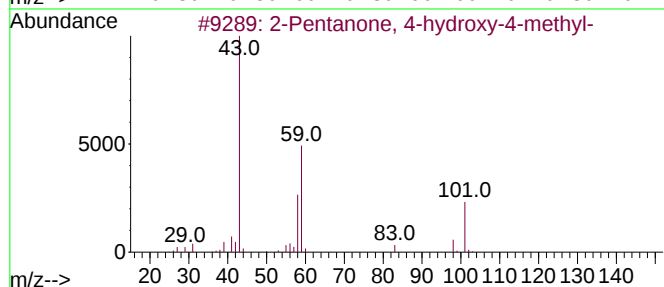
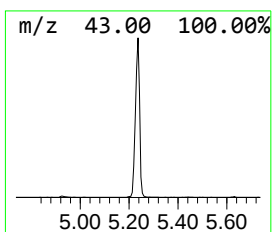
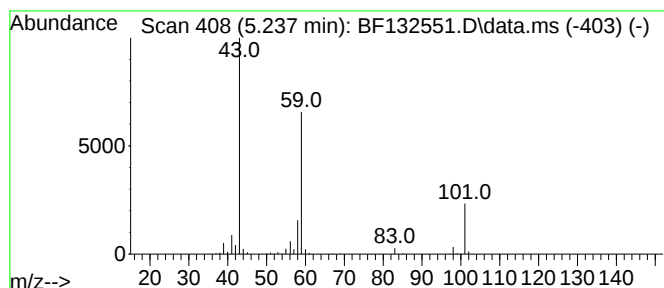
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.237	34.10 ng	1590400	1,4-Dichlorobenzene-d4	7.001

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	53		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	Guanidine	59	CH5N3	000113-00-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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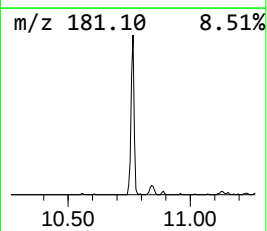
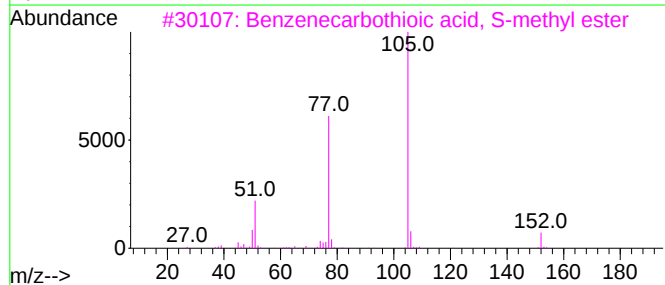
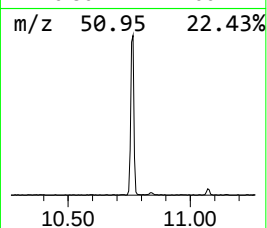
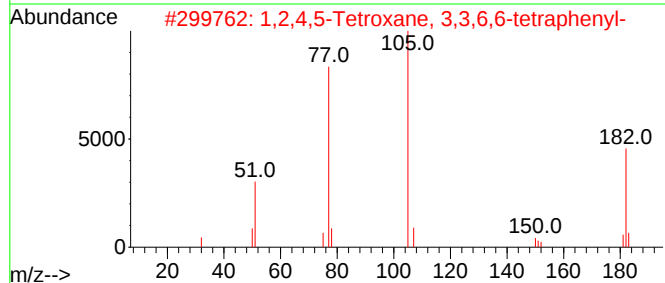
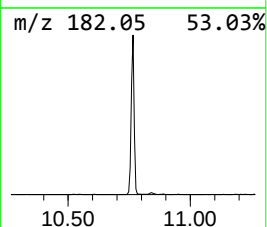
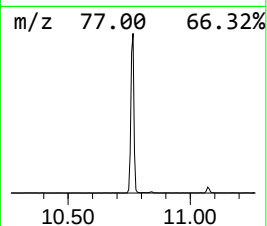
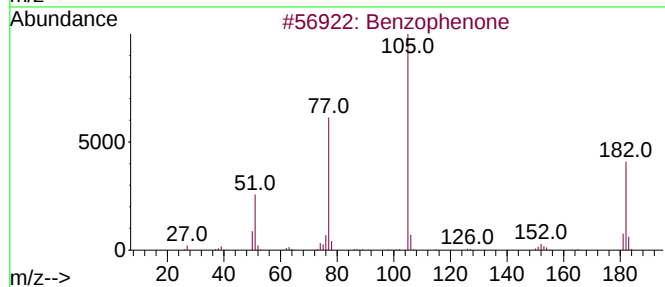
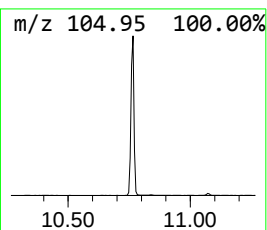
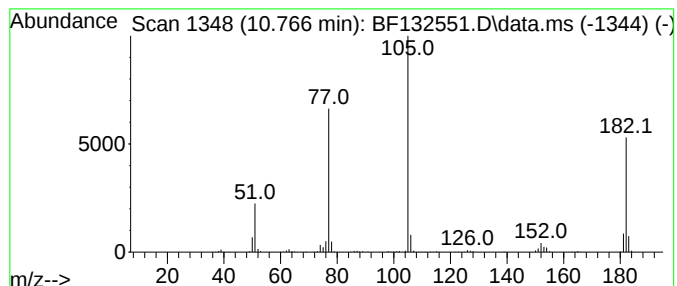
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.766	16.03 ng	1101570	Acenaphthene-d10	10.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49



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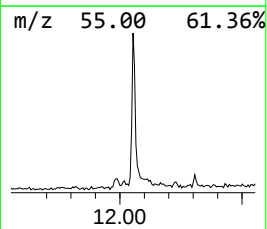
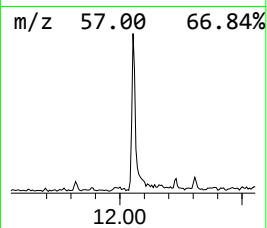
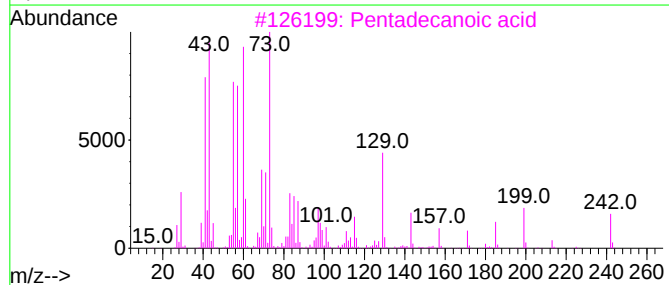
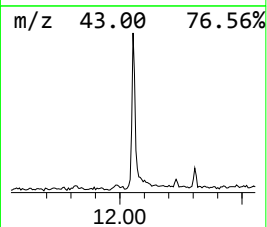
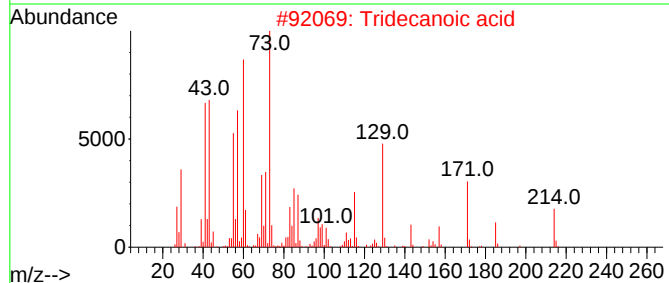
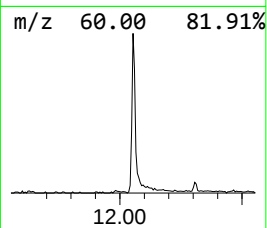
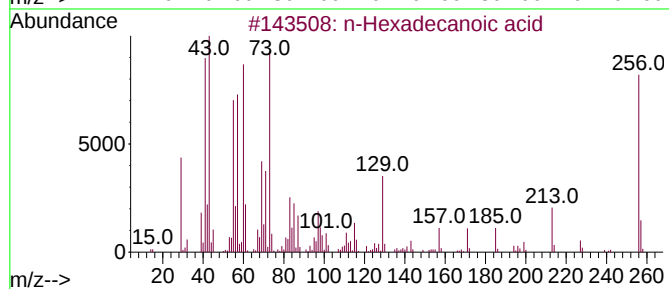
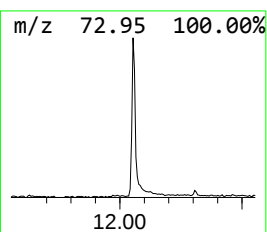
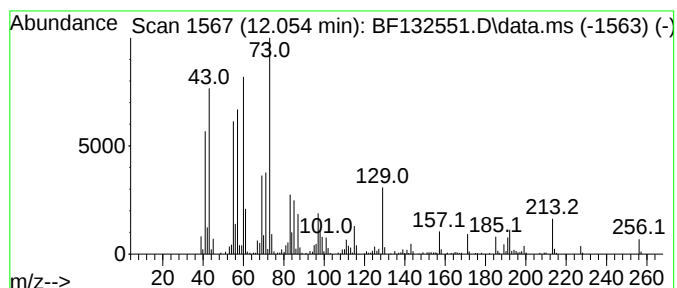
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.054	6.15 ng	441231	Phenanthrene-d10	11.542

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Nonanoic acid	158	C9H18O2	000112-05-0	58



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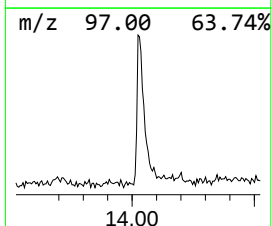
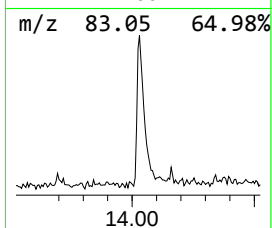
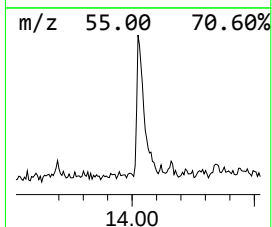
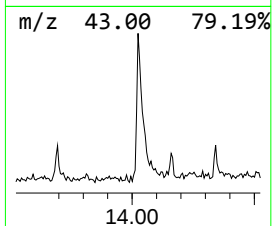
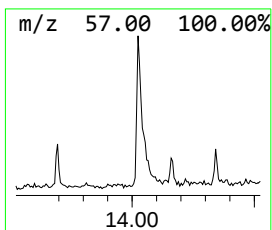
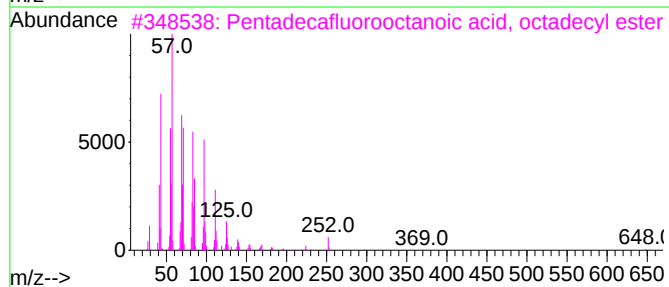
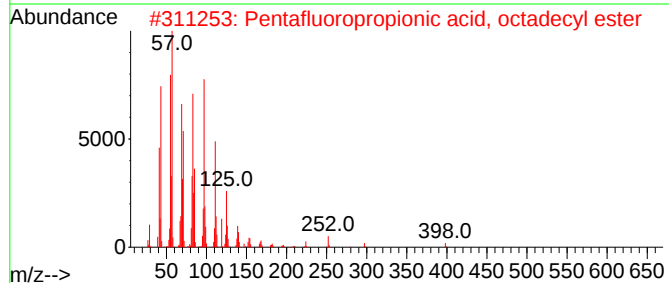
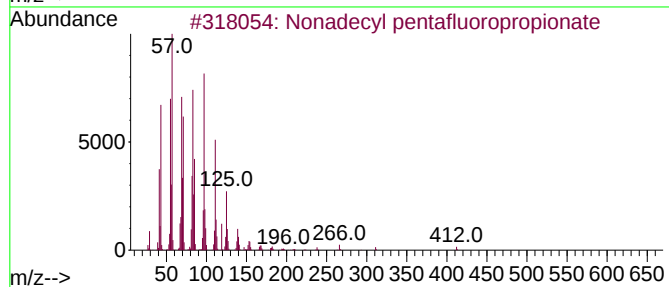
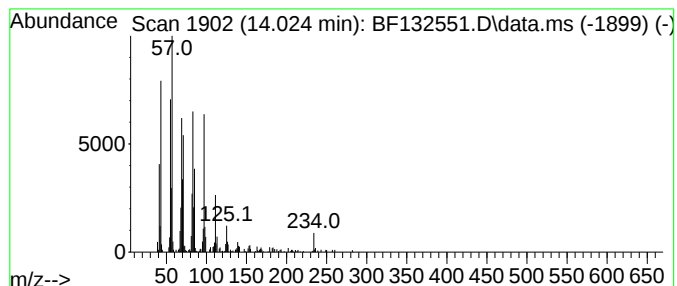
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Nonadecyl pentafluoropropio... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.024	5.61 ng	303511	Chrysene-d12	14.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	90
3			Pentadecafluorooctanoic acid, octadecyl ester	666	C26H37F15O2	1000406-04-8	90
4			Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	87
5			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	87



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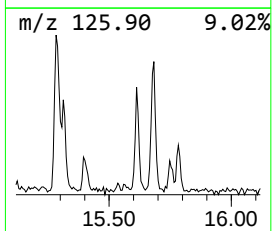
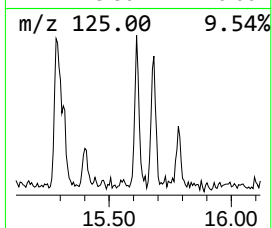
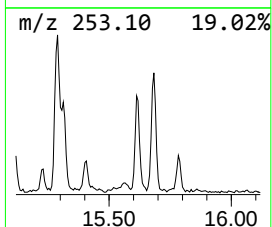
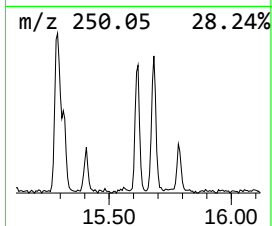
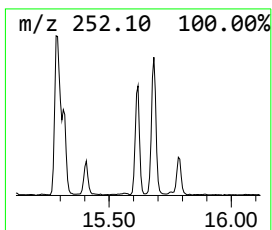
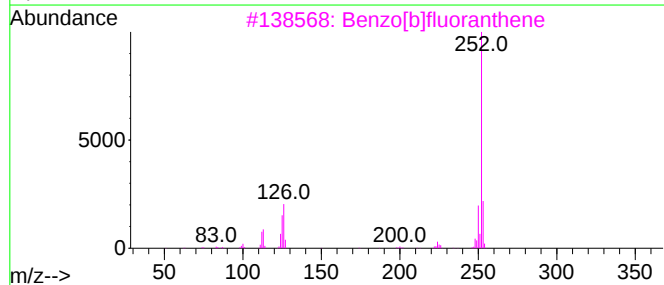
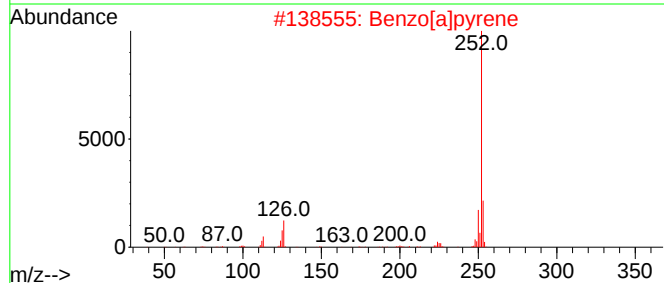
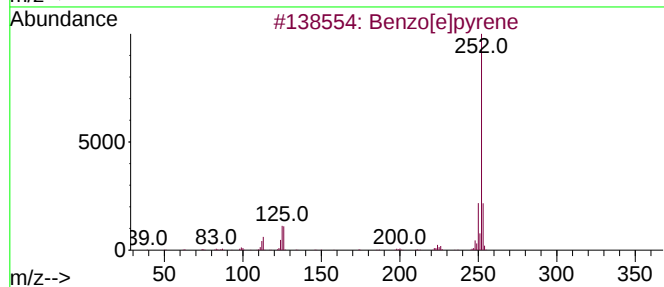
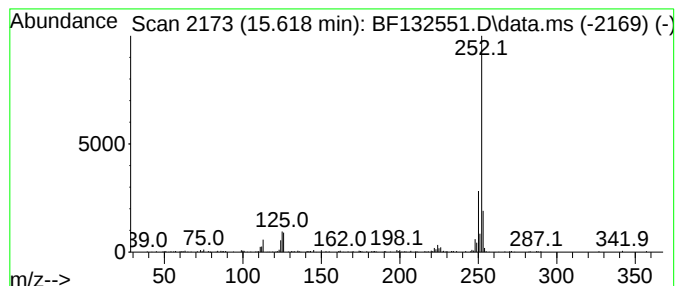
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.618	3.31 ng	165813	Perylene-d12	15.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Benzo[a]pyrene	252	C20H12	000050-32-8	91
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132551.D
Acq On : 27 Feb 2023 14:22
Operator : CG\JU
Sample : 01665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-231

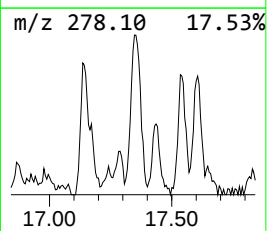
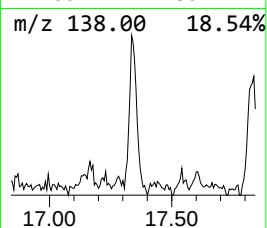
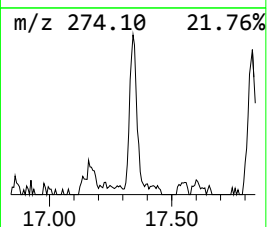
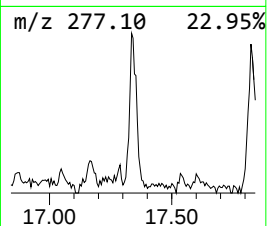
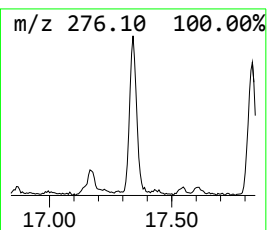
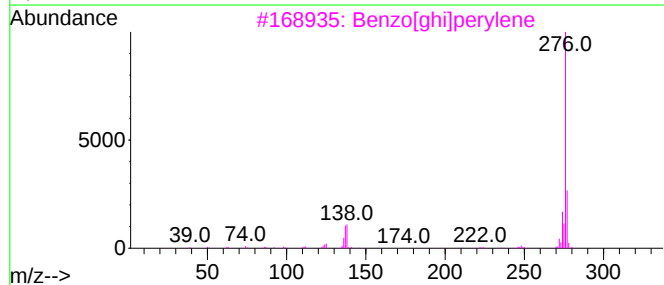
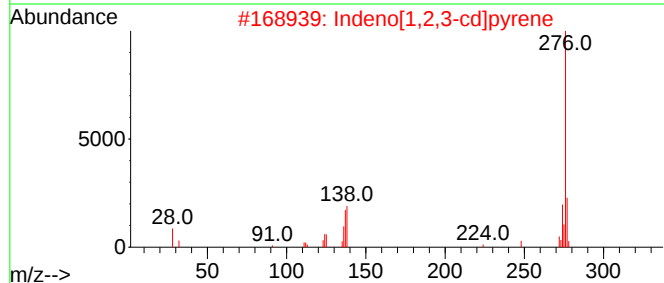
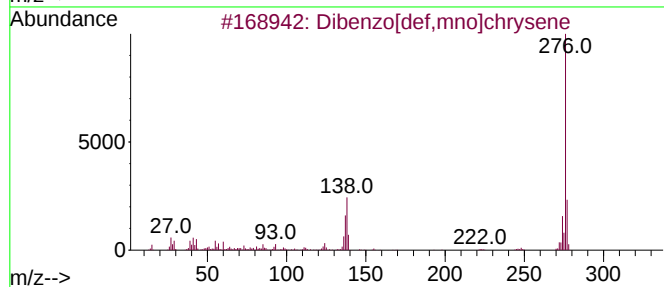
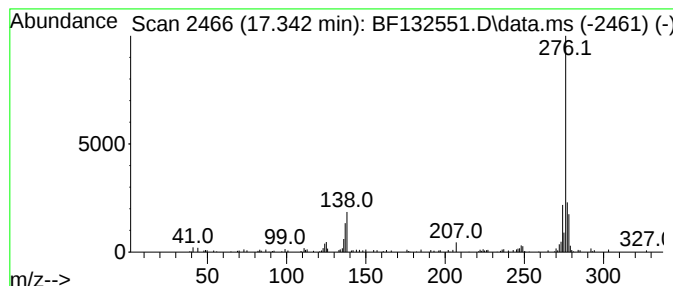
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.342	2.90 ng	145173	Perylene-d12	15.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	96
2			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	94
3			Benzo[ghi]perylene	276	C22H12	000191-24-2	93
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	90
5			12H-Benzothieno[2,3-d]pyrido[1,2...	276	C14H16N2S2	102254-63-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132551.D
Acq On : 27 Feb 2023 14:22
Operator : CG\JU
Sample : 01665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-231

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-...	5.237	34.1	ng	1590400	1	7.001	932702	20.0
Benzophenone	10.766	16.0	ng	1101570	3	10.048	1374520	20.0
n-Hexadecanoic ...	12.054	6.2	ng	441231	4	11.542	1435160	20.0
Nonadecyl penta...	14.024	5.6	ng	303511	5	14.201	1081380	20.0
Benzo[e]pyrene	15.618	3.3	ng	165813	6	15.754	1001230	20.0
Dibenzo[def,mno...	17.342	2.9	ng	145173	6	15.754	1001230	20.0