

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
 Data File : BF132328.D
 Acq On : 03 Feb 2023 18:35
 Operator : CG\JU
 Sample : 01416-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-01-SB01

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132328.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.301	414	419	427	rVB	1093537	1454084	31.04%	3.772%
2	5.684	479	484	487	rBV	3359772	3334628	71.18%	8.651%
3	6.672	646	652	655	rBV	3074793	3412707	72.84%	8.853%
4	7.054	714	717	721	rVB	1415638	1172294	25.02%	3.041%
5	7.619	807	813	816	rBV	2495322	2425257	51.77%	6.292%
6	8.342	932	936	939	rBV	2003102	1637644	34.95%	4.248%
7	9.419	1114	1119	1122	rBV	4950825	4685065	100.00%	12.154%
8	9.525	1133	1137	1140	rVB	60399	56636	1.21%	0.147%
9	9.760	1174	1177	1180	rBV2	45956	47785	1.02%	0.124%
10	10.107	1232	1236	1240	rVB	2340744	1904351	40.65%	4.940%
11	10.519	1299	1306	1310	rVB4	52464	83410	1.78%	0.216%
12	10.819	1351	1357	1361	rBV	527125	449057	9.58%	1.165%
13	10.901	1366	1371	1374	rBV	3482483	3083806	65.82%	8.000%
14	11.013	1385	1390	1397	rVB4	100119	160593	3.43%	0.417%
15	11.130	1406	1410	1414	rBV	58942	49318	1.05%	0.128%
16	11.448	1461	1464	1467	rBV	54901	49271	1.05%	0.128%
17	11.607	1487	1491	1493	rBV	2273042	1938276	41.37%	5.028%
18	11.630	1493	1495	1498	rVV	168292	139622	2.98%	0.362%
19	11.666	1498	1501	1505	rVV2	56316	73921	1.58%	0.192%
20	11.830	1524	1529	1534	rBV2	55809	92160	1.97%	0.239%
21	12.113	1573	1577	1580	rBV	689897	648999	13.85%	1.684%
22	12.219	1592	1595	1598	rBV2	55438	66261	1.41%	0.172%
23	12.289	1603	1607	1609	rBV	58660	53579	1.14%	0.139%
24	12.366	1617	1620	1624	rBV	122444	105923	2.26%	0.275%
25	12.660	1664	1670	1672	rBV2	107844	163696	3.49%	0.425%
26	12.748	1682	1685	1689	rVB	44875	48131	1.03%	0.125%
27	12.824	1692	1698	1703	rBV	550414	525746	11.22%	1.364%
28	12.901	1707	1711	1717	rBV2	166785	189236	4.04%	0.491%
29	12.995	1722	1727	1731	rVV3	70376	84345	1.80%	0.219%
30	13.060	1731	1738	1743	rVV	488958	566355	12.09%	1.469%
31	13.201	1757	1762	1765	rBV	4478751	4070411	86.88%	10.560%
32	13.277	1770	1775	1781	rBV4	45326	91998	1.96%	0.239%
33	13.360	1786	1789	1792	rBV4	40202	54563	1.16%	0.142%
34	13.413	1795	1798	1801	rBV	128697	94686	2.02%	0.246%
35	13.489	1807	1811	1814	rVB2	51464	68459	1.46%	0.178%
36	13.760	1851	1857	1859	rBV2	137877	143328	3.06%	0.372%

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37	13.895	1878	1880	1885	rVB	62162	57614	1.23%	0.149%
38	14.013	1895	1900	1903	rBV2	40577	59587	1.27%	0.155%
39	14.089	1910	1913	1927	rVB2	361972	657059	14.02%	1.705%
40	14.265	1938	1943	1946	rBV2	1327370	1371958	29.28%	3.559%
41	14.289	1946	1947	1952	rVB	251666	176809	3.77%	0.459%
42	14.354	1953	1958	1963	rBV	350781	342671	7.31%	0.889%
43	14.407	1964	1967	1970	rVB	117543	95321	2.03%	0.247%
44	14.718	2017	2020	2023	rBV	102585	82351	1.76%	0.214%
45	15.054	2074	2077	2085	rBV	83228	91710	1.96%	0.238%
46	15.142	2089	2092	2095	rBV	120312	123518	2.64%	0.320%
47	15.365	2126	2130	2134	rBV	194131	308280	6.58%	0.800%
48	15.430	2138	2141	2147	rVB2	78536	100331	2.14%	0.260%
49	15.701	2184	2187	2194	rVB	99078	129675	2.77%	0.336%
50	15.771	2195	2199	2205	rVB	106811	143617	3.07%	0.373%
51	15.848	2206	2212	2224	rVB	725723	1083469	23.13%	2.811%
52	16.342	2292	2296	2305	rVB2	48426	79061	1.69%	0.205%
53	16.912	2389	2393	2401	rVB2	34936	65062	1.39%	0.169%
54	17.283	2451	2456	2466	rVB6	18018	58597	1.25%	0.152%
55	17.471	2483	2488	2498	rVB2	63149	142484	3.04%	0.370%
56	17.589	2502	2508	2514	rVB3	24722	62962	1.34%	0.163%
57	17.971	2567	2573	2579	rBV	42619	89139	1.90%	0.231%

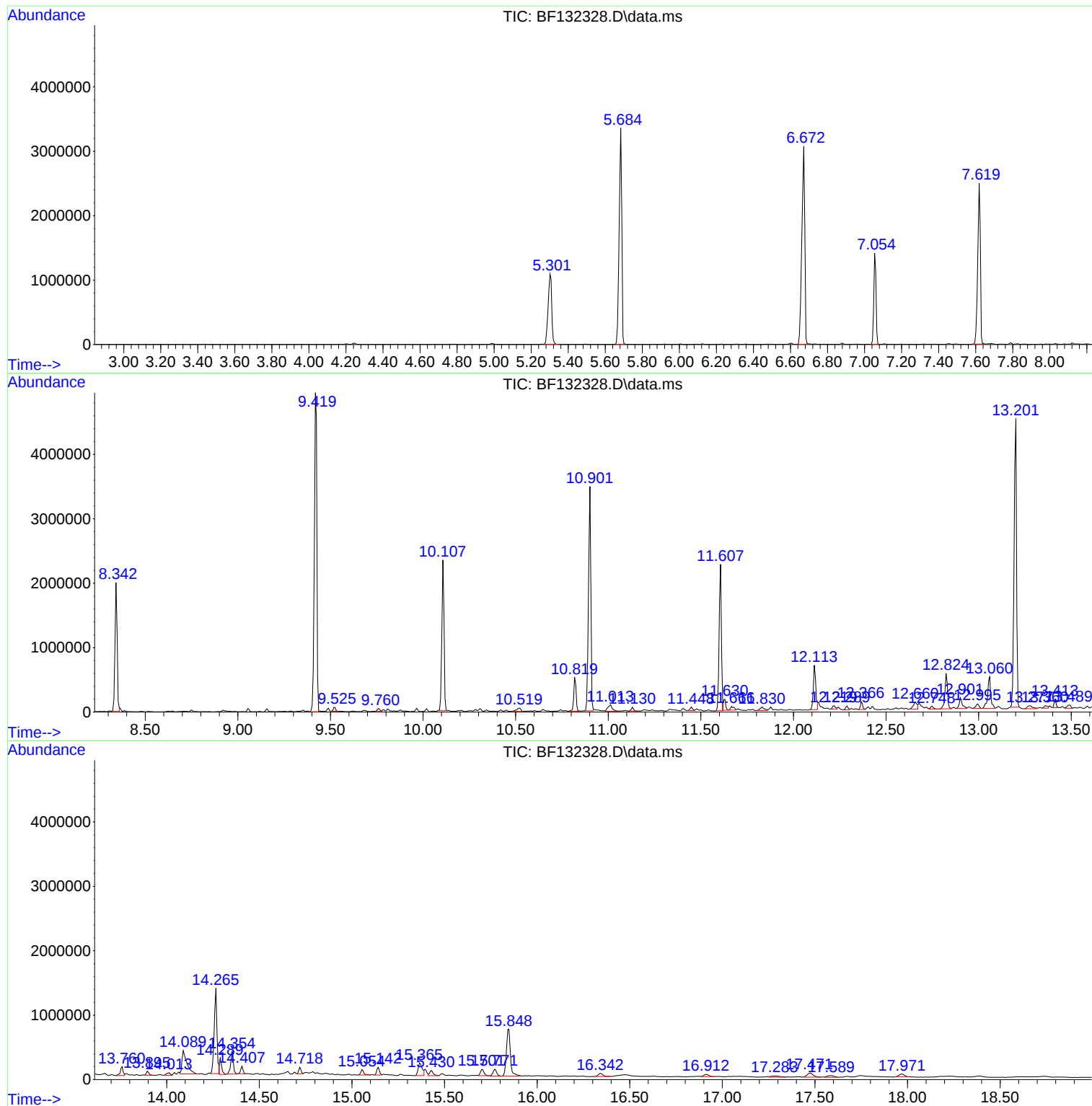
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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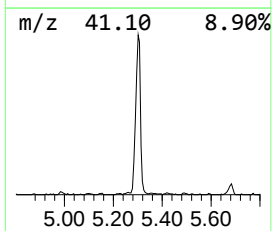
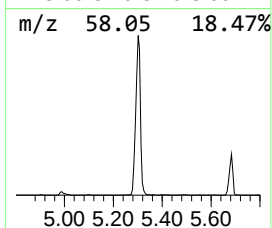
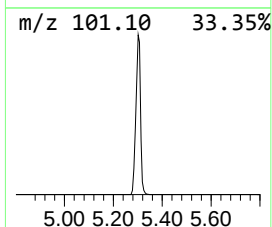
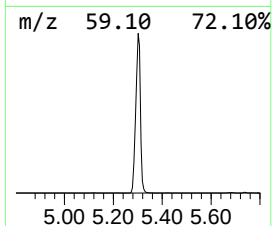
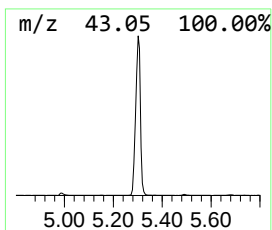
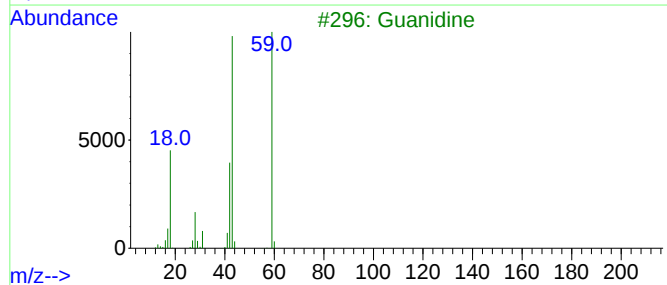
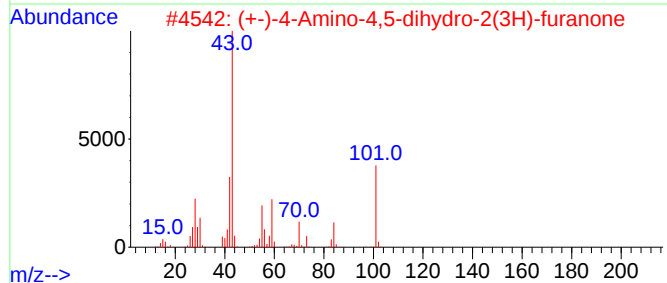
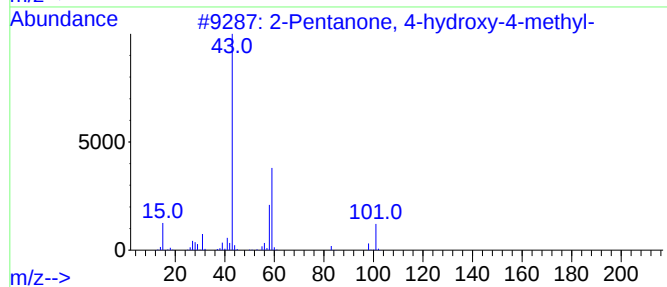
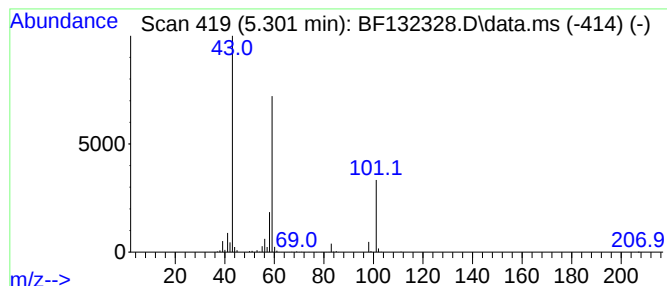
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.301	24.81 ng	1454080	1,4-Dichlorobenzene-d4	7.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47		
3	Guanidine	59	CH5N3	000113-00-8	43		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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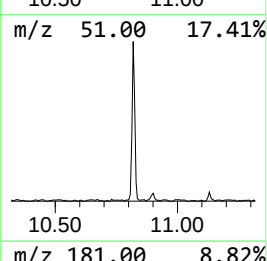
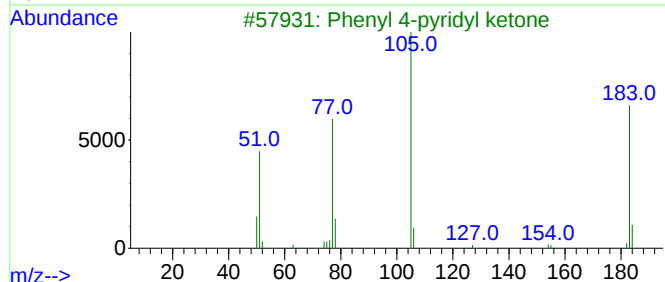
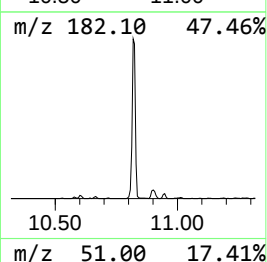
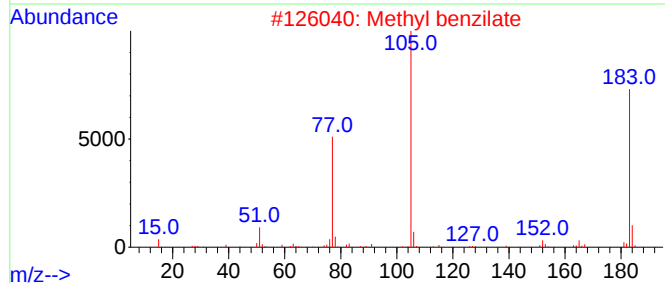
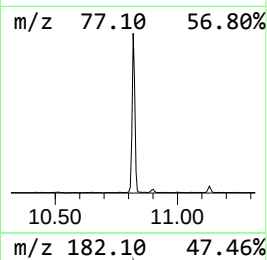
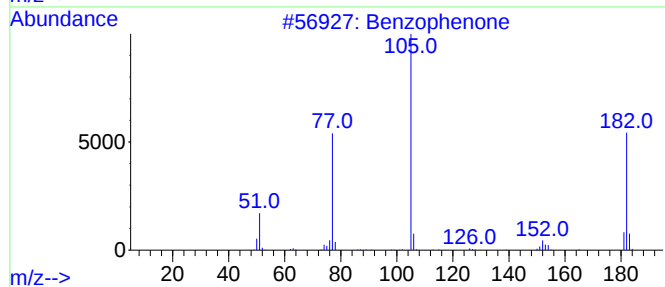
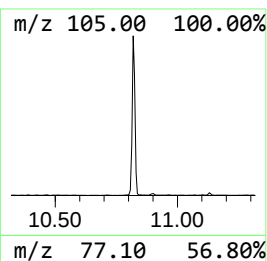
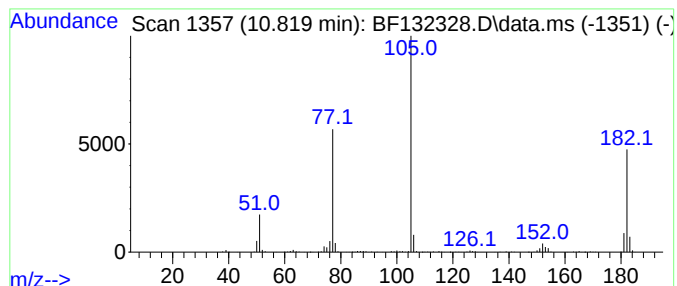
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.819	4.72 ng	449057	Acenaphthene-d10	10.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Methyl benzoate	242	C15H14O3	000076-89-1	50
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47



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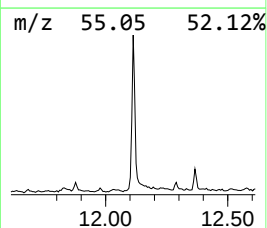
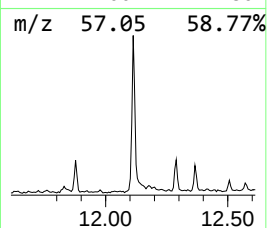
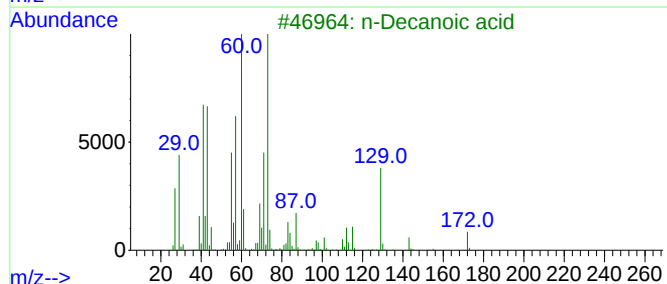
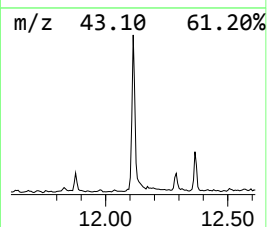
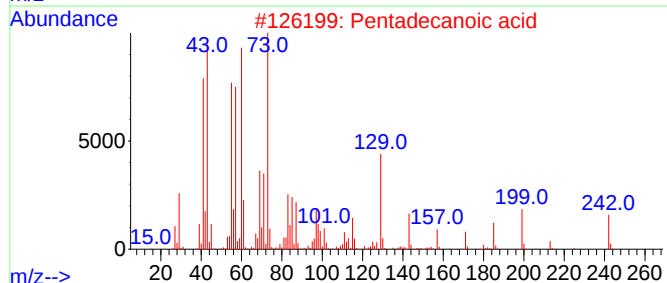
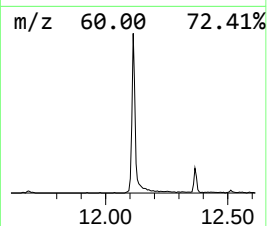
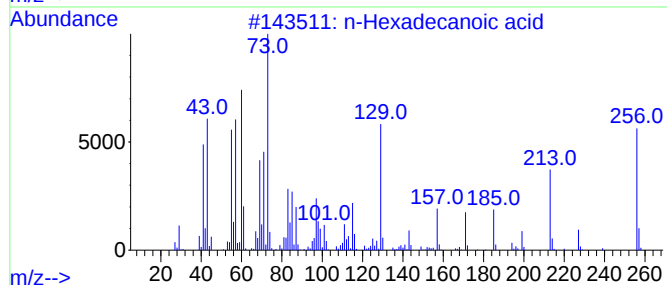
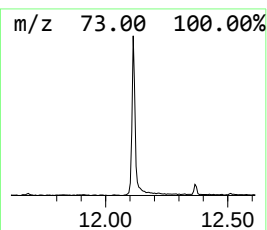
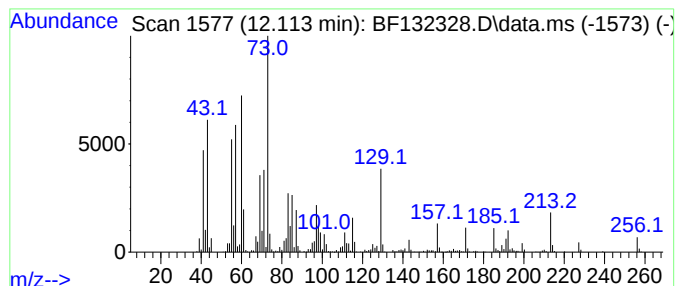
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.113	6.70 ng	648999	Phenanthrene-d10	11.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	27



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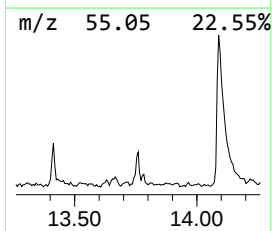
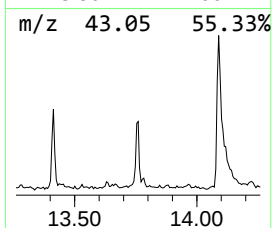
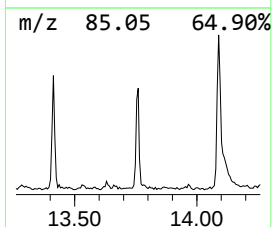
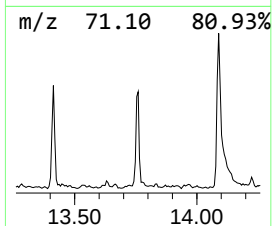
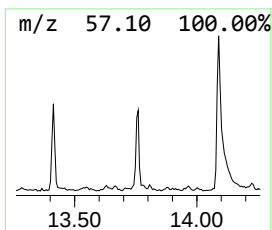
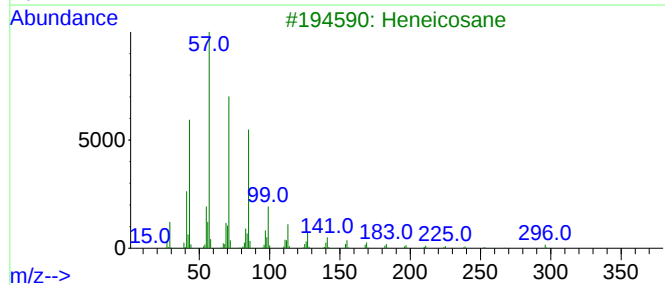
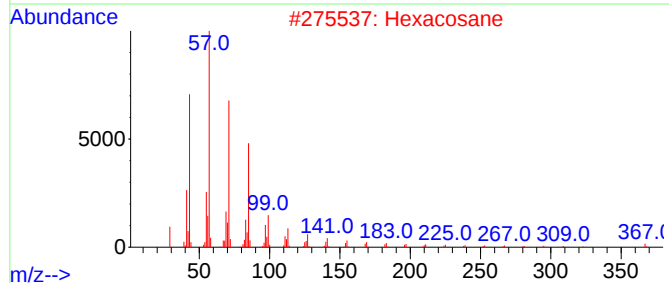
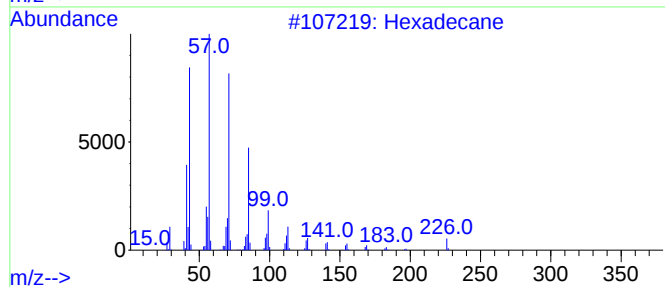
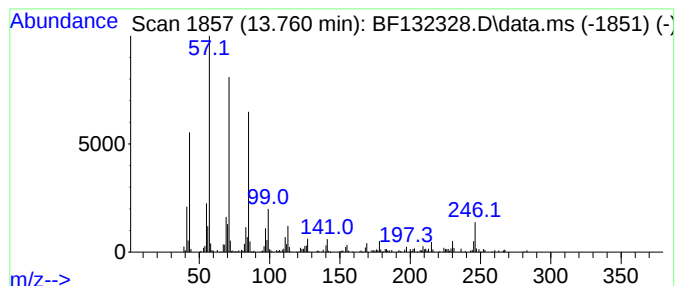
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Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.760	2.09 ng	143328	Chrysene-d12	14.265

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Hexacosane	366	C26H54	000630-01-3	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
5			Pentacosane	352	C25H52	000629-99-2	83



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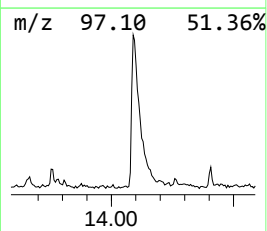
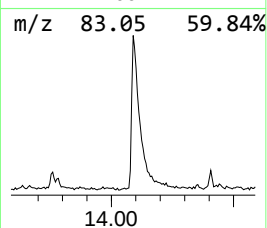
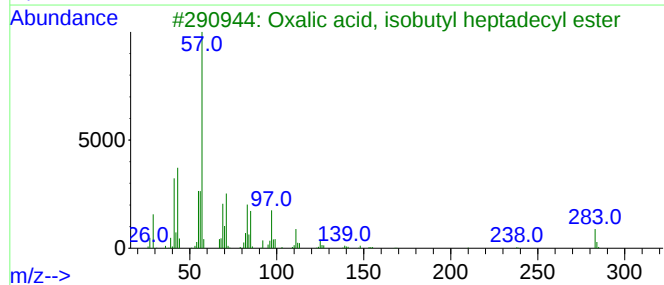
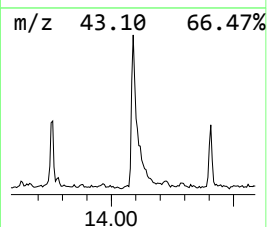
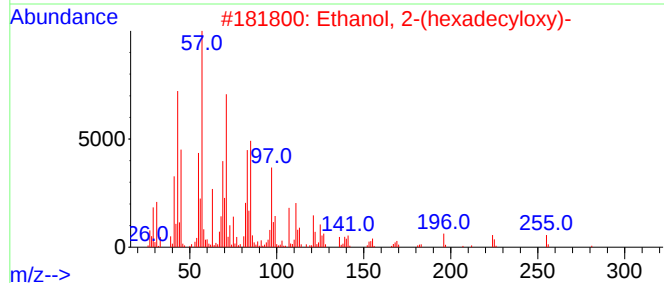
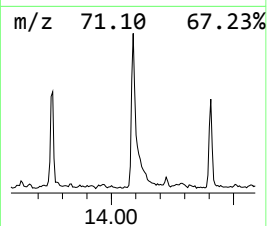
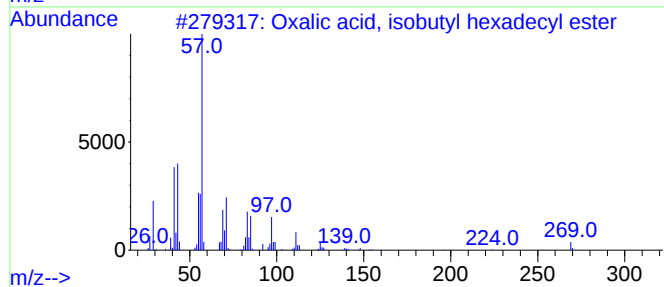
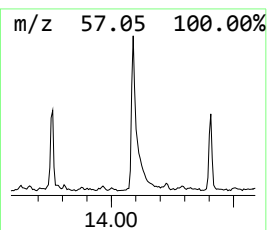
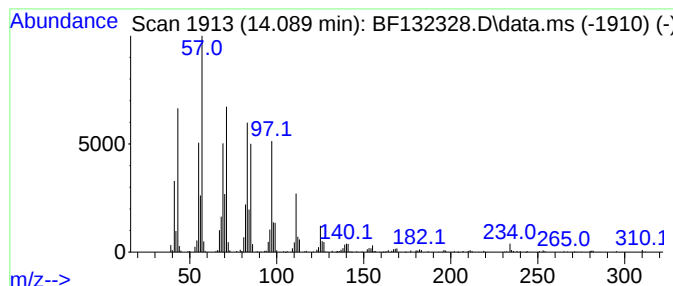
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Oxalic acid, isobutyl hexadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	9.58 ng	657059	Chrysene-d12	14.265

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
3			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
4			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132328.D
Acq On : 03 Feb 2023 18:35
Operator : CG\JU
Sample : 01416-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-01-SB01

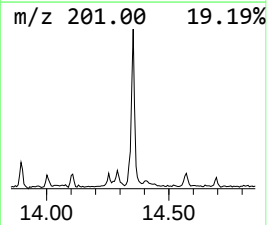
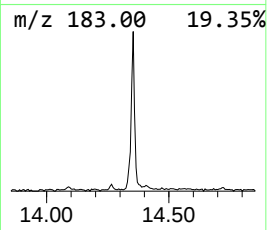
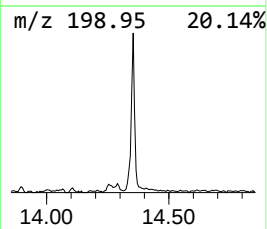
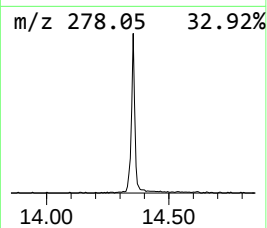
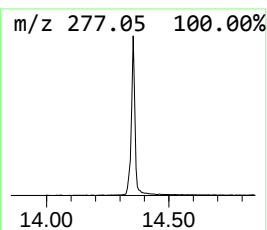
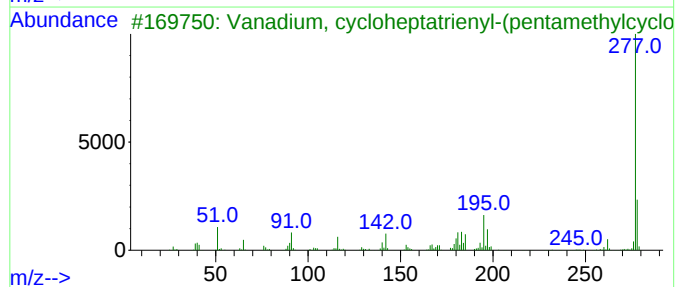
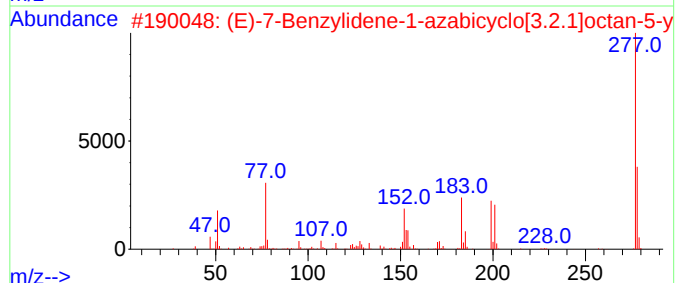
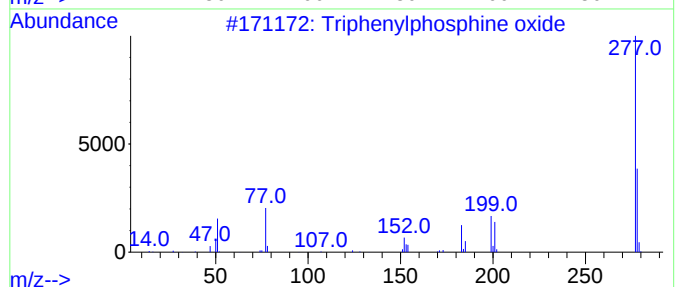
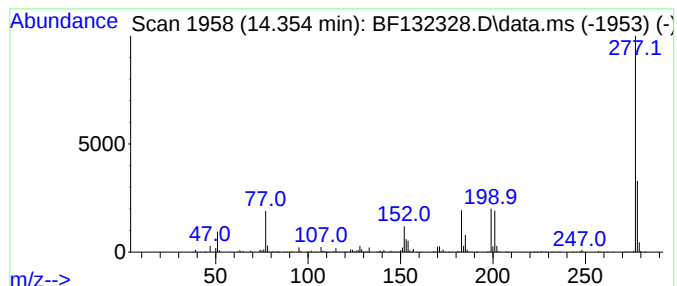
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.354	5.00 ng	342671	Chrysene-d12	14.265

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	C15H19NO3S	1000483-83-4	91
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132328.D
Acq On : 03 Feb 2023 18:35
Operator : CG\JU
Sample : 01416-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-01-SB01

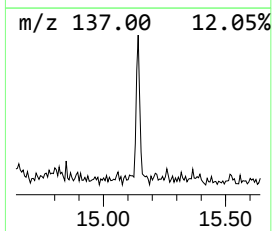
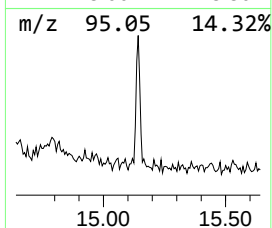
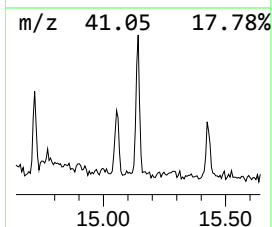
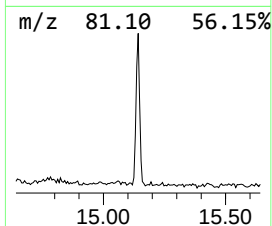
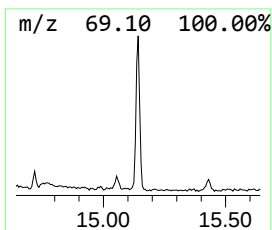
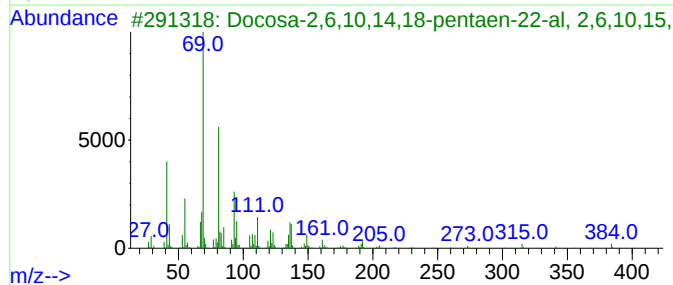
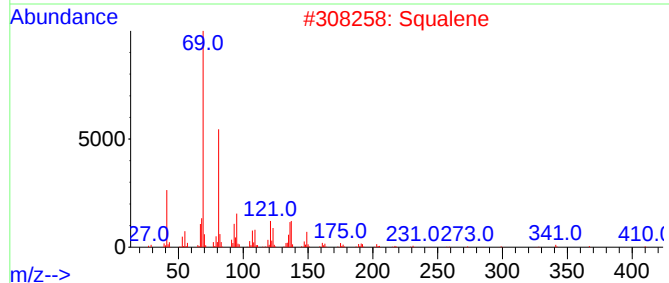
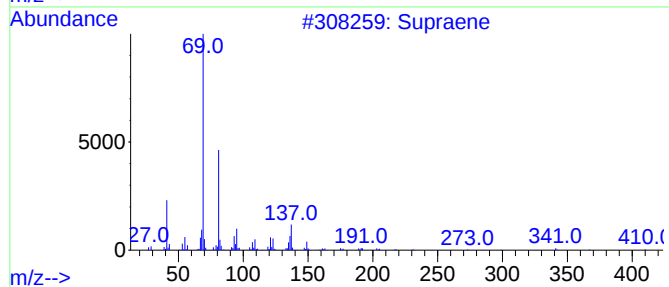
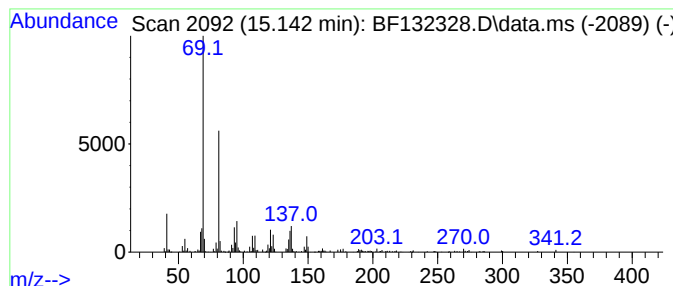
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.142	2.28 ng	123518	Perylene-d12	15.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59
5			Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132328.D
Acq On : 03 Feb 2023 18:35
Operator : CG\JU
Sample : 01416-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-01-SB01

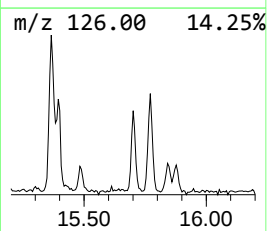
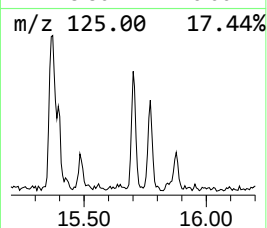
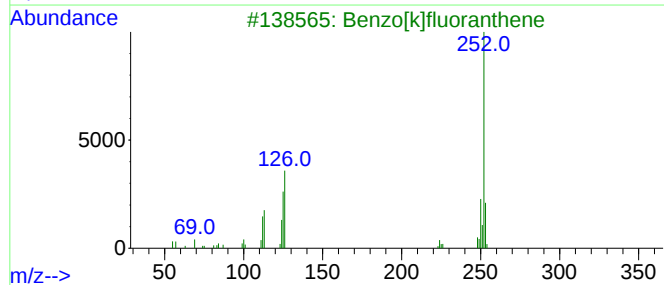
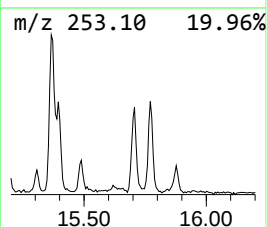
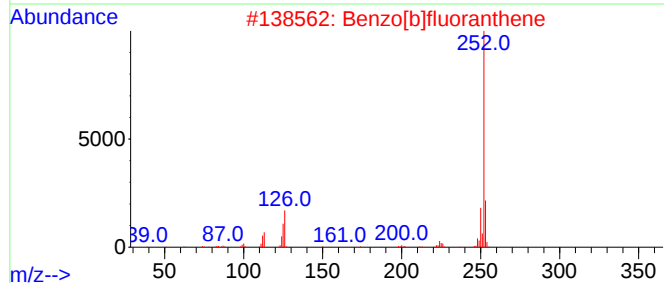
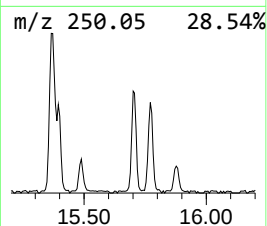
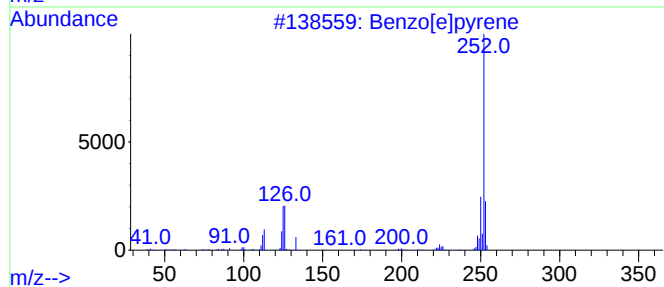
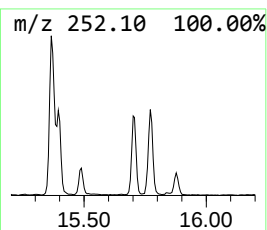
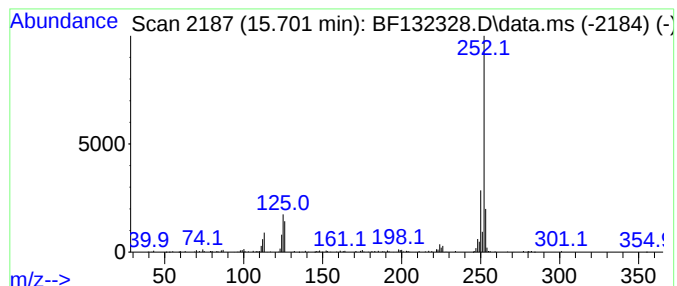
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.701	2.39 ng	129675	Perylene-d12	15.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132328.D
Acq On : 03 Feb 2023 18:35
Operator : CG\JU
Sample : 01416-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-01-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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-...	5.301	24.8	ng	1454080	1	7.054	1172290	20.0
Benzophenone	10.819	4.7	ng	449057	3	10.107	1904350	20.0
n-Hexadecanoic ...	12.113	6.7	ng	648999	4	11.607	1938280	20.0
Hexadecane	13.760	2.1	ng	143328	5	14.265	1371960	20.0
Oxalic acid, is...	14.089	9.6	ng	657059	5	14.265	1371960	20.0
Triphenylphosph...	14.354	5.0	ng	342671	5	14.265	1371960	20.0
Supraene	15.142	2.3	ng	123518	6	15.842	1083470	20.0
Benzo[e]pyrene	15.701	2.4	ng	129675	6	15.842	1083470	20.0