

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
 Data File : BF134919.D
 Acq On : 24 Aug 2023 12:28
 Operator : CG\JU
 Sample : 04090-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-K

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-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	563	567	570	rBV	2212022	1910767	91.52%	8.972%
2	6.428	733	738	741	rBV	2154390	1943919	93.11%	9.128%
3	6.622	768	771	777	rBV	126318	99985	4.79%	0.470%
4	6.792	796	800	803	rBV	938927	725899	34.77%	3.409%
5	7.351	891	895	898	rBV	1489294	1255397	60.13%	5.895%
6	8.069	1013	1017	1021	rBV	1090151	950896	45.55%	4.465%
7	9.151	1196	1201	1204	rBV	2344730	2087761	100.00%	9.804%
8	9.275	1217	1222	1225	rBV	1215605	1199079	57.43%	5.631%
9	9.828	1312	1316	1320	rBV	1294996	1076789	51.58%	5.056%
10	9.863	1320	1322	1325	rVB	40600	33150	1.59%	0.156%
11	10.375	1407	1409	1414	rVB	28602	27305	1.31%	0.128%
12	10.622	1447	1451	1454	rBV	1760118	1491665	71.45%	7.004%
13	10.904	1496	1499	1502	rBV	40271	44582	2.14%	0.209%
14	10.963	1506	1509	1512	rBV2	27038	34841	1.67%	0.164%
15	11.180	1540	1546	1550	rBV5	24565	33534	1.61%	0.157%
16	11.216	1550	1552	1560	rVB	27671	27313	1.31%	0.128%
17	11.322	1566	1570	1572	rBV	1317079	1071798	51.34%	5.033%
18	11.345	1572	1574	1577	rVV	424308	318750	15.27%	1.497%
19	11.398	1577	1583	1586	rVB	56131	58680	2.81%	0.276%
20	11.557	1604	1610	1612	rBV2	23586	26227	1.26%	0.123%
21	11.727	1633	1639	1645	rVB4	34266	49452	2.37%	0.232%
22	11.827	1652	1656	1658	rBV	74604	71960	3.45%	0.338%
23	11.857	1658	1661	1666	rBV	436718	420535	20.14%	1.975%
24	11.933	1671	1674	1677	rVV2	90802	111826	5.36%	0.525%
25	11.963	1677	1679	1684	rVB	53598	47961	2.30%	0.225%
26	12.127	1700	1707	1709	rBV	44632	57083	2.73%	0.268%
27	12.145	1709	1710	1717	rVB2	38923	40021	1.92%	0.188%
28	12.380	1746	1750	1753	rBV	43707	50097	2.40%	0.235%
29	12.416	1753	1756	1757	rVV2	54132	50767	2.43%	0.238%
30	12.433	1757	1759	1762	rVV	141709	124695	5.97%	0.586%
31	12.463	1762	1764	1768	rVB2	31202	29498	1.41%	0.139%
32	12.539	1771	1777	1781	rBV	399154	352897	16.90%	1.657%
33	12.580	1781	1784	1787	rVB4	26004	25902	1.24%	0.122%
34	12.651	1792	1796	1802	rBV2	146040	177309	8.49%	0.833%
35	12.769	1810	1816	1819	rBV	364013	365053	17.49%	1.714%
36	12.821	1823	1825	1830	rVB2	38867	36669	1.76%	0.172%

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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

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37	12.921	1838	1842	1845	rVV	1774441	1671370	80.06%	7.848%
38	12.992	1849	1854	1858	rBV3	31150	45433	2.18%	0.213%
39	13.080	1866	1869	1870	rBV2	21939	25989	1.24%	0.122%
40	13.098	1870	1872	1876	rVB	49483	49093	2.35%	0.231%
41	13.163	1876	1883	1887	rBV2	45117	73470	3.52%	0.345%
42	13.204	1887	1890	1893	rBV2	41879	41505	1.99%	0.195%
43	13.298	1903	1906	1909	rVB	25316	22567	1.08%	0.106%
44	13.327	1909	1911	1914	rBV	28588	27825	1.33%	0.131%
45	13.504	1934	1941	1944	rBV2	62961	80642	3.86%	0.379%
46	13.610	1956	1959	1964	rVB	31302	38102	1.83%	0.179%
47	13.721	1974	1978	1981	rBV3	38422	48668	2.33%	0.229%
48	13.827	1992	1996	2004	rVB2	128113	178397	8.54%	0.838%
49	13.974	2016	2021	2024	rBV2	766772	873751	41.85%	4.103%
50	14.004	2024	2026	2029	rVB	134706	104769	5.02%	0.492%
51	14.074	2034	2038	2043	rVB2	112459	118866	5.69%	0.558%
52	14.157	2048	2052	2056	rVB2	53684	59718	2.86%	0.280%
53	14.368	2085	2088	2091	rVB	30080	25056	1.20%	0.118%
54	14.463	2101	2104	2107	rBV2	58780	53076	2.54%	0.249%
55	14.751	2150	2153	2154	rBV2	26597	25262	1.21%	0.119%
56	14.768	2154	2156	2162	rVB	41143	51789	2.48%	0.243%
57	15.021	2195	2199	2202	rBV	103580	155188	7.43%	0.729%
58	15.115	2211	2215	2220	rVB4	36691	55251	2.65%	0.259%
59	15.321	2247	2250	2257	rVB	62633	78399	3.76%	0.368%
60	15.386	2257	2261	2265	rBV	85941	101722	4.87%	0.478%
61	15.451	2267	2272	2277	rBV	583932	748275	35.84%	3.514%
62	15.951	2354	2357	2362	rVB3	19374	26494	1.27%	0.124%
63	16.939	2520	2525	2534	rVB2	39707	85169	4.08%	0.400%

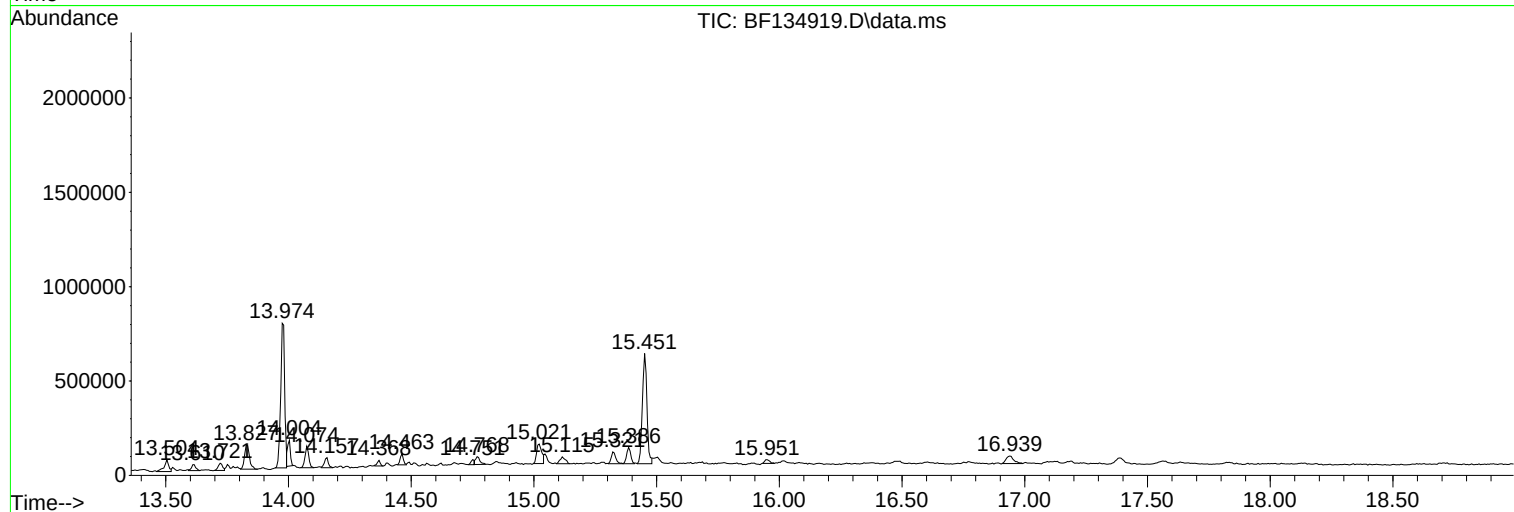
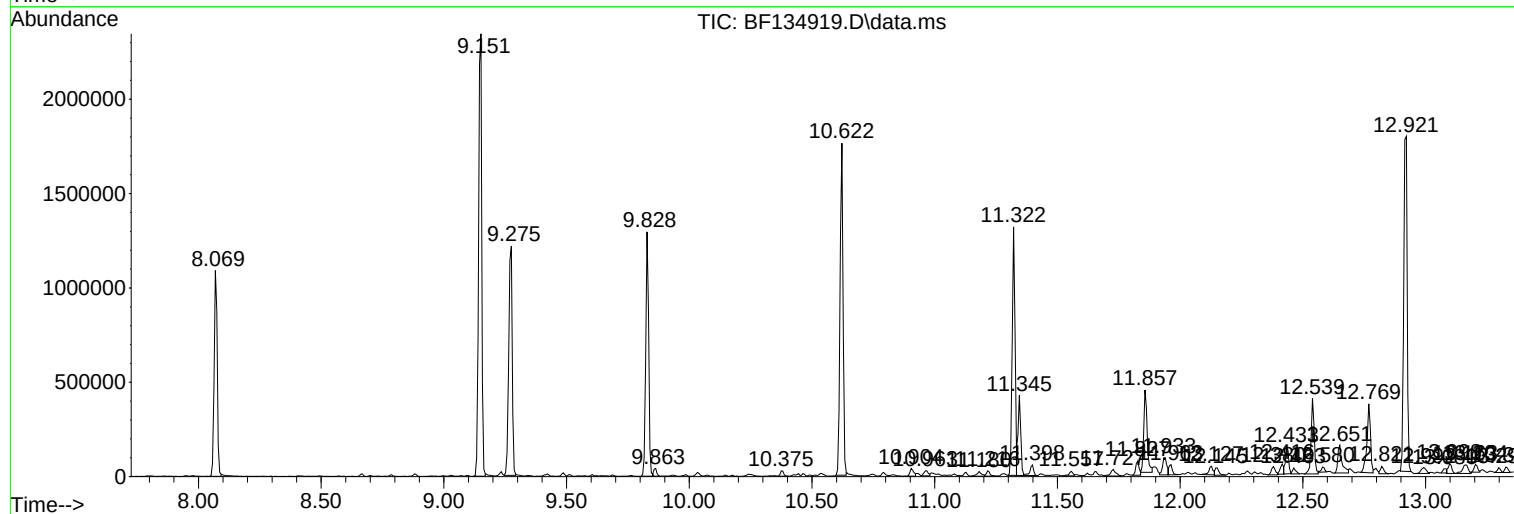
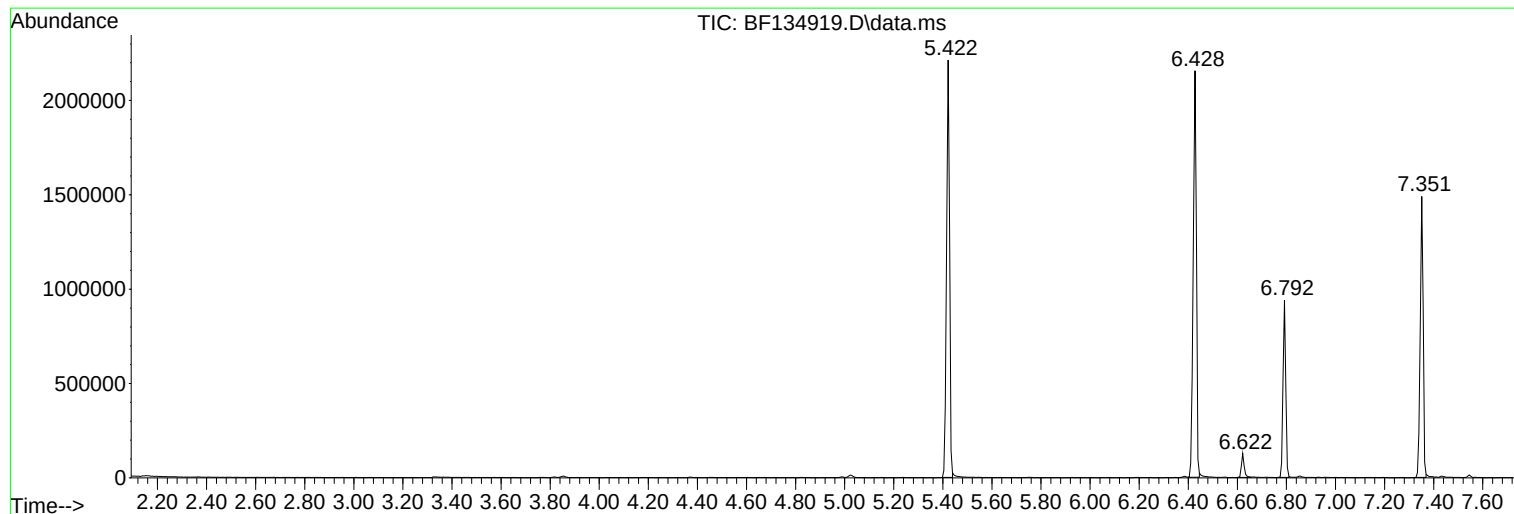
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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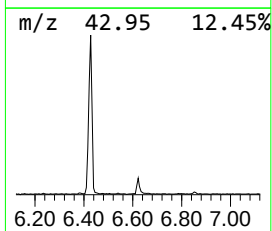
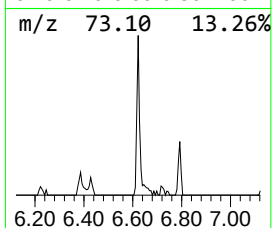
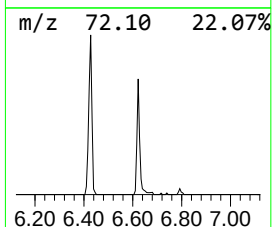
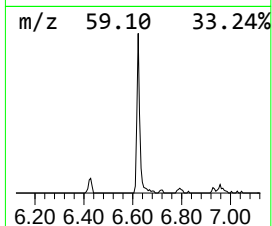
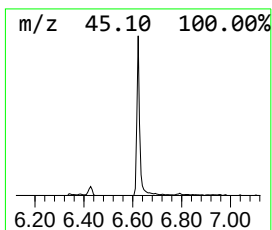
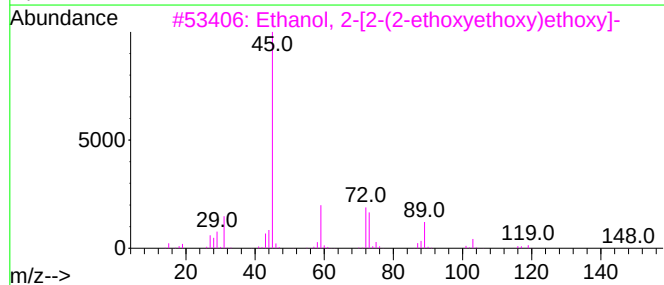
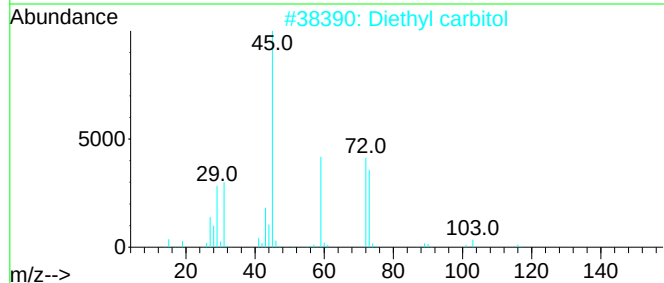
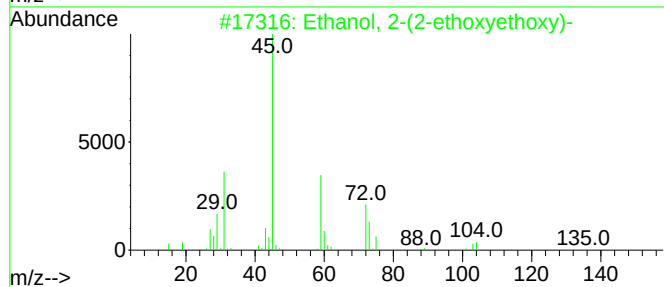
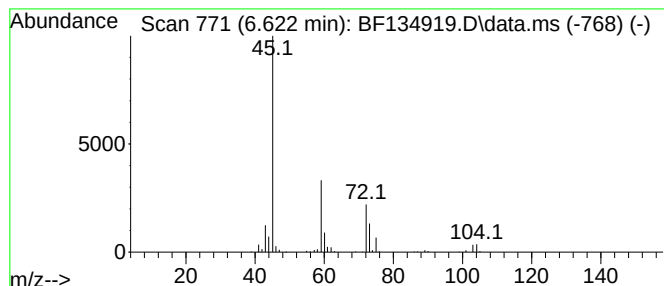
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.622	2.75 ng	99985	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42



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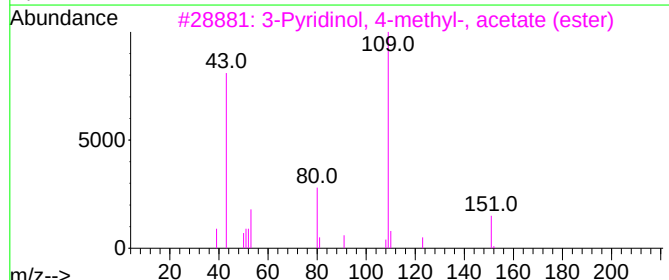
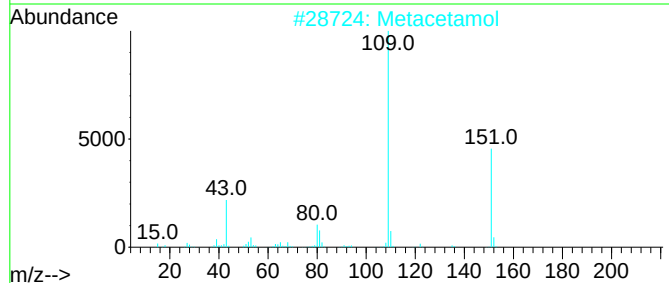
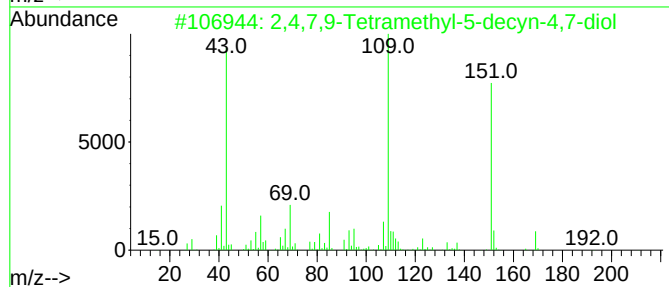
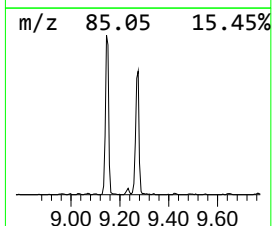
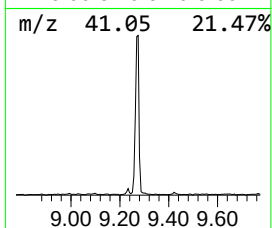
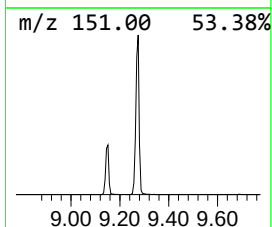
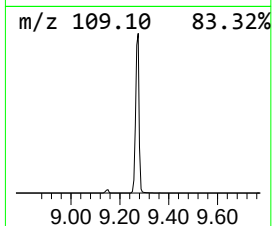
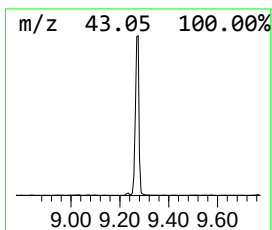
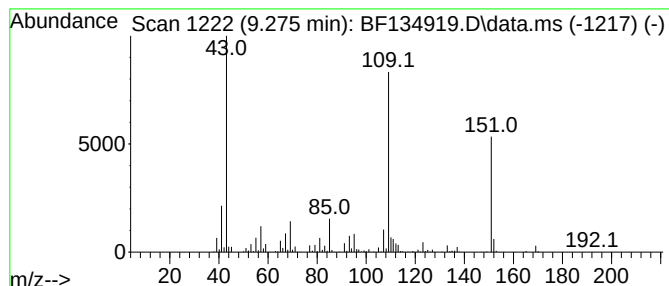
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.275	22.27 ng	1199080	Acenaphthene-d10	9.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	64	
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59	
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59	



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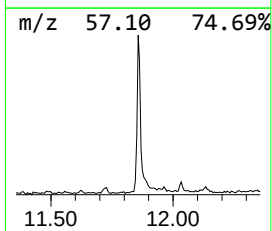
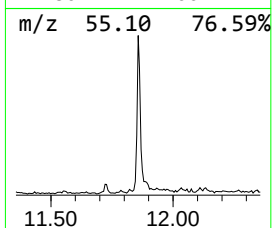
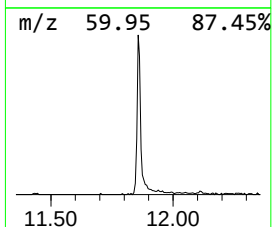
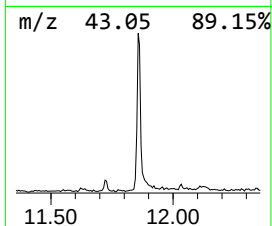
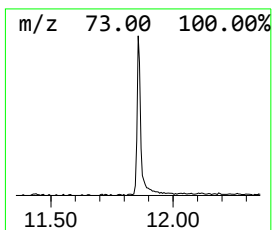
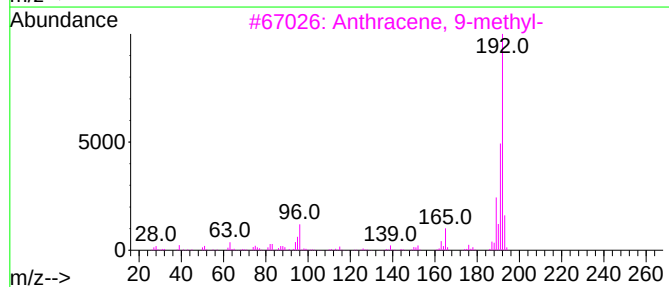
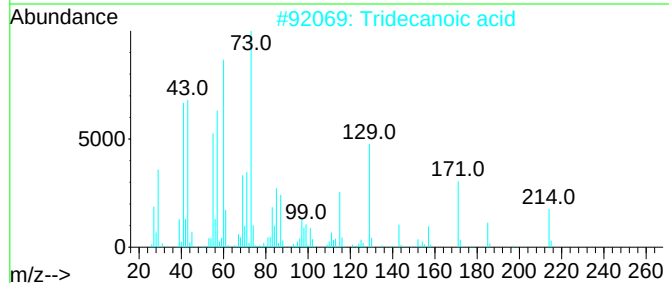
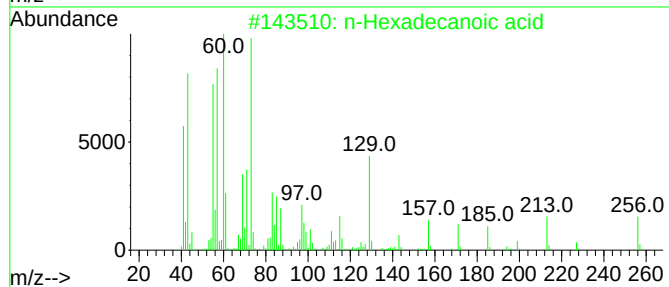
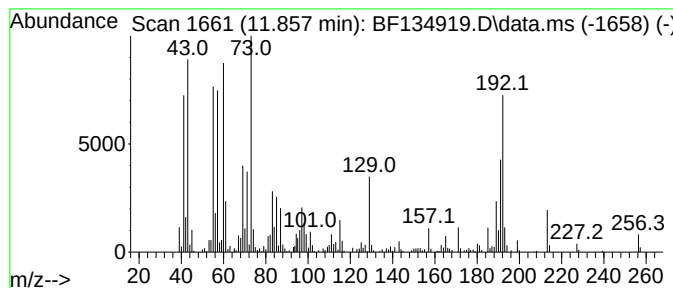
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.857	7.85 ng	420535	Phenanthrene-d10	11.322	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	59



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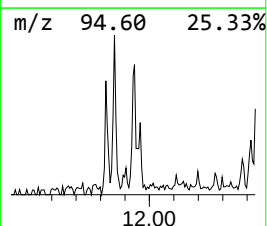
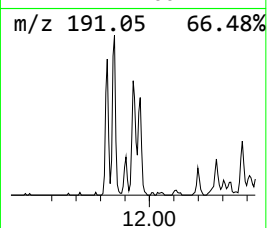
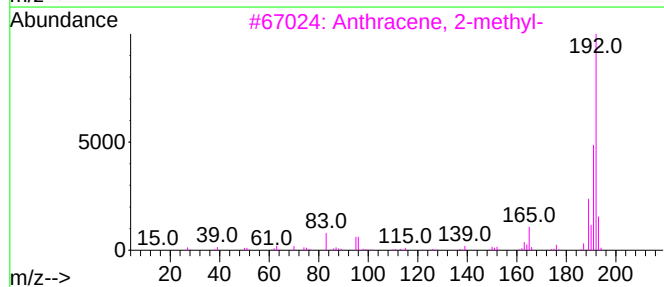
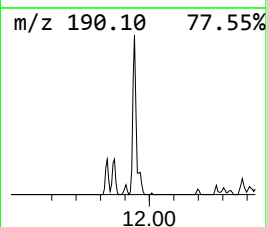
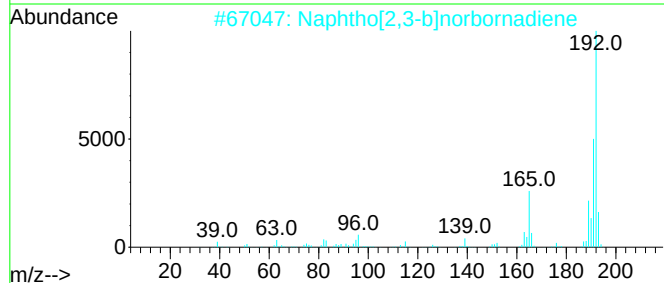
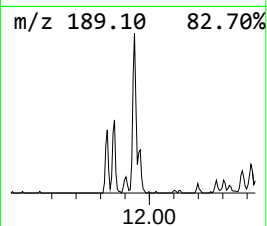
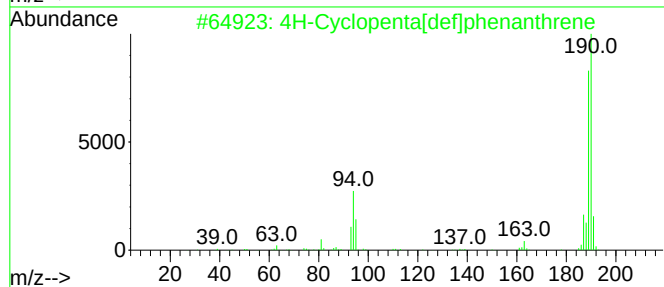
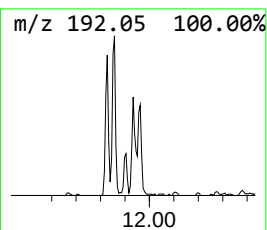
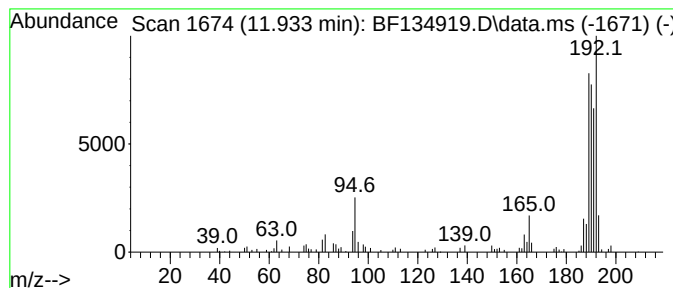
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.933 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.09 ng	111826	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	46
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	46
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	45
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42



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Misc :
ALS Vial : 6 Sample Multiplier: 1

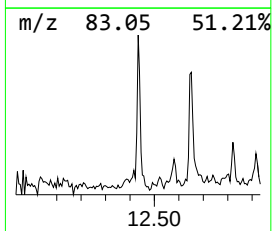
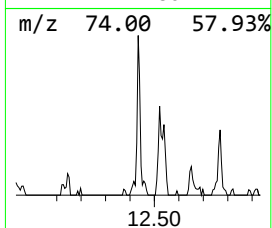
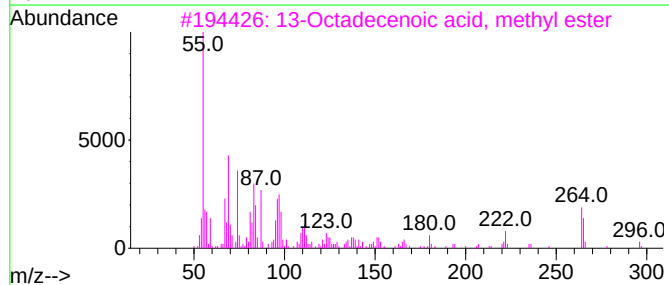
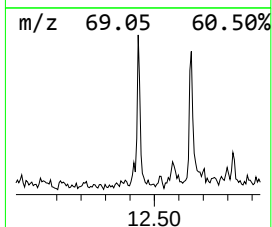
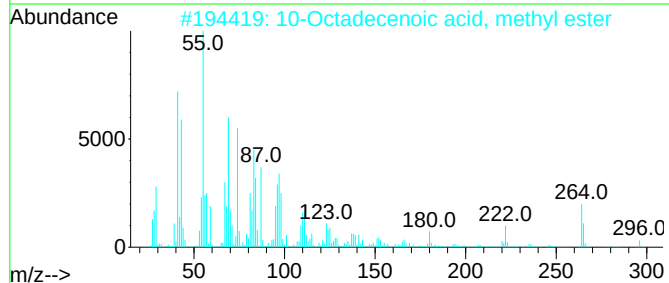
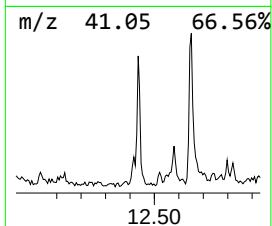
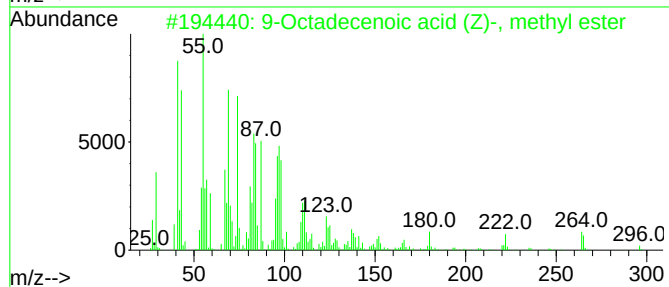
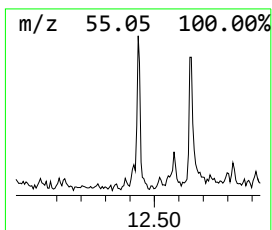
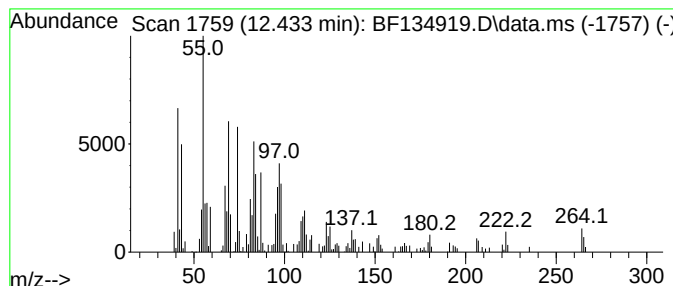
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BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.433	2.33 ng	124695	Phenanthrene-d10	11.322	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134919.D
Acq On : 24 Aug 2023 12:28
Operator : CG\JU
Sample : 04090-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

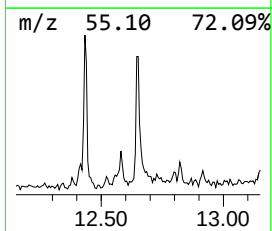
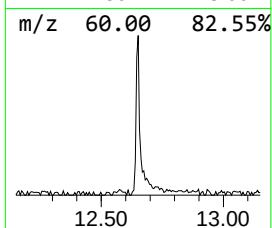
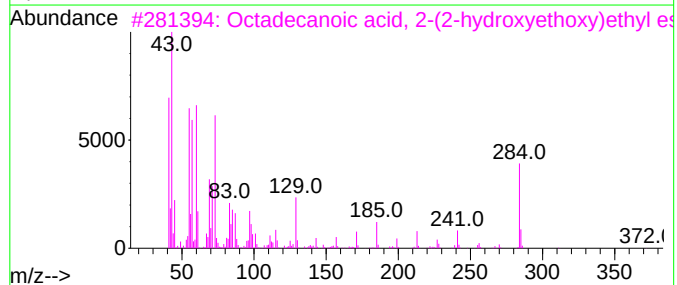
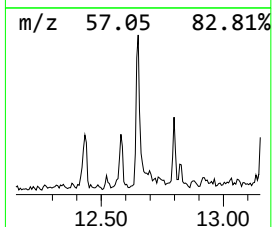
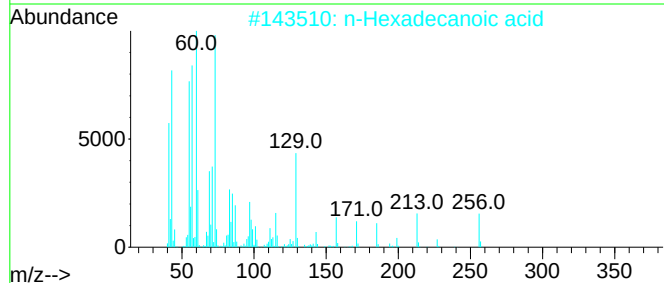
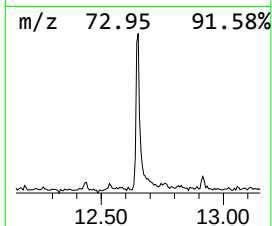
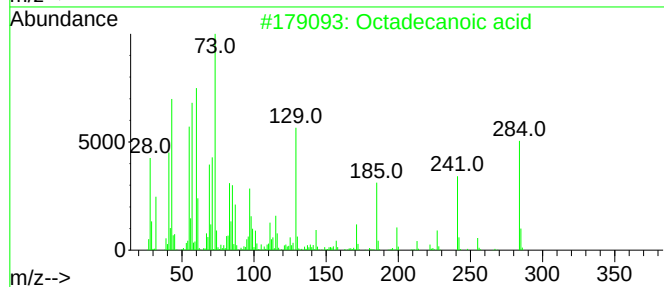
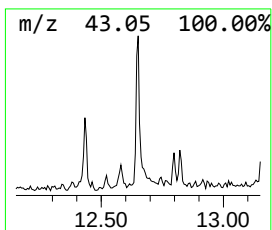
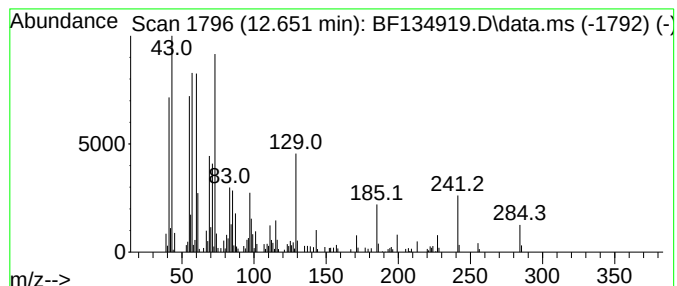
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	4.06 ng	177309	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134919.D
Acq On : 24 Aug 2023 12:28
Operator : CG\JU
Sample : 04090-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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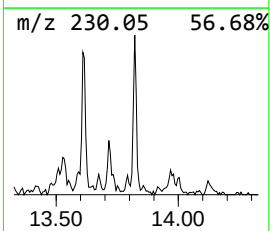
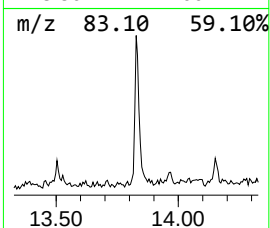
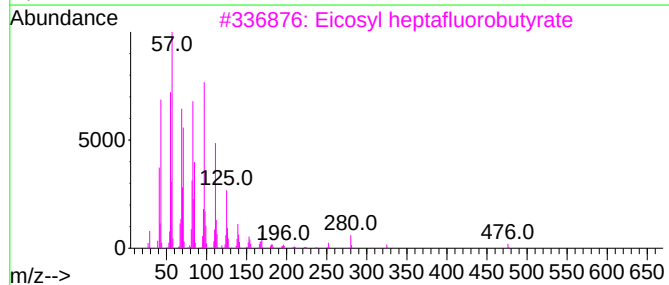
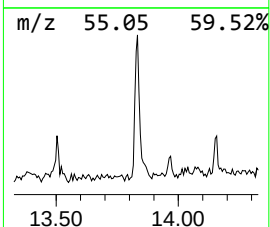
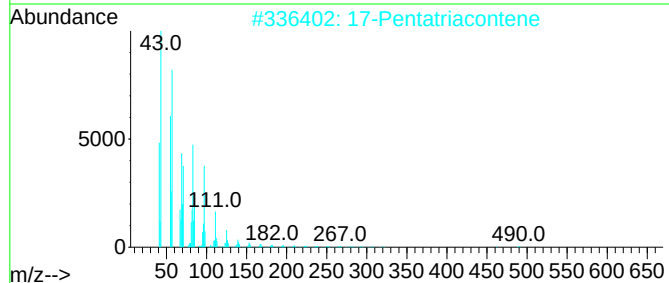
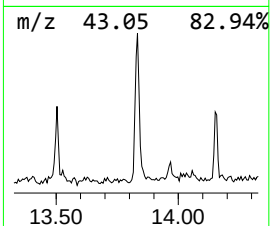
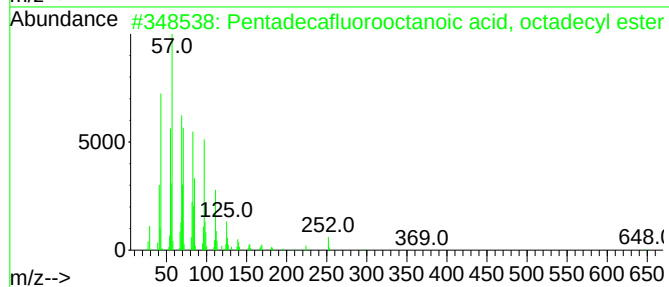
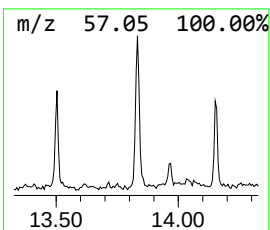
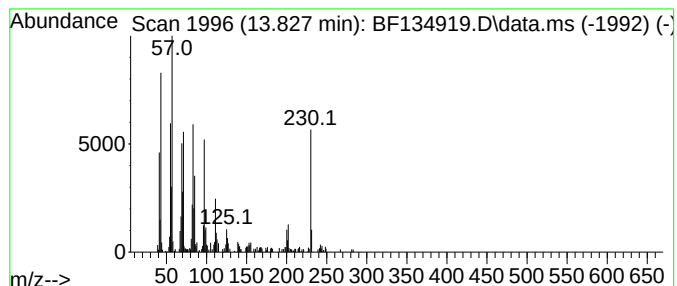
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.08 ng	178397	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			17-Pentatriacontene	491	C35H70	006971-40-0	70
3			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	70
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	62
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134919.D
Acq On : 24 Aug 2023 12:28
Operator : CG\JU
Sample : 04090-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

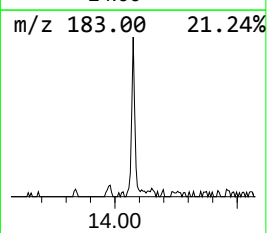
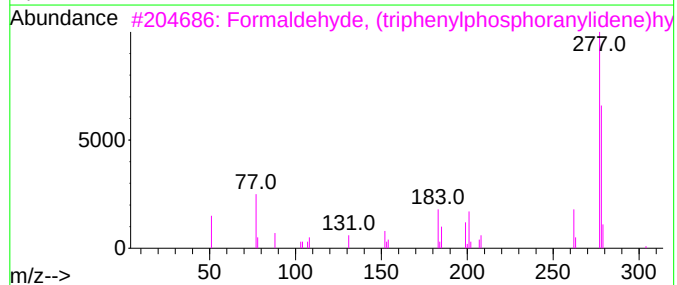
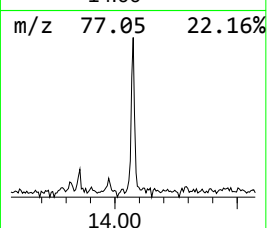
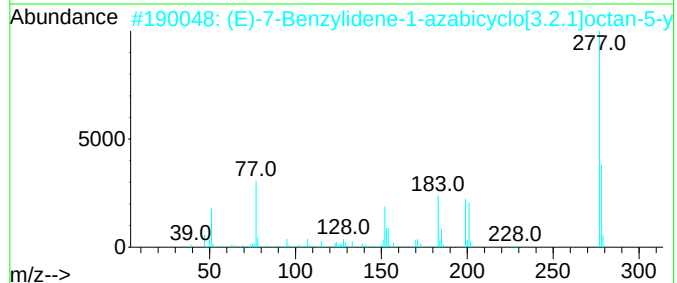
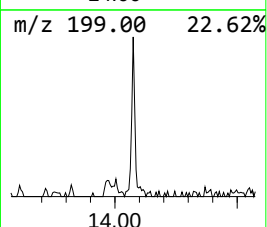
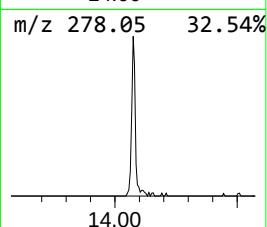
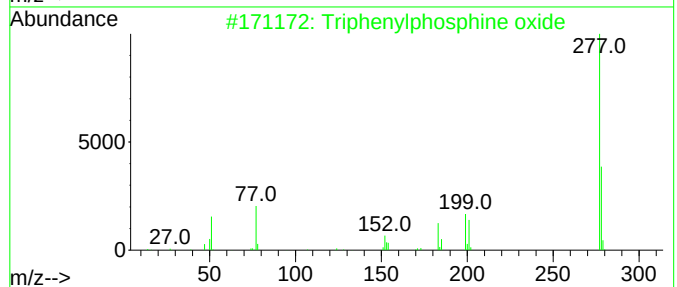
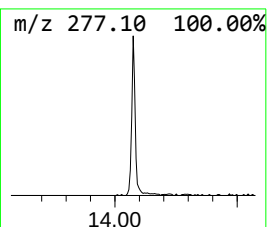
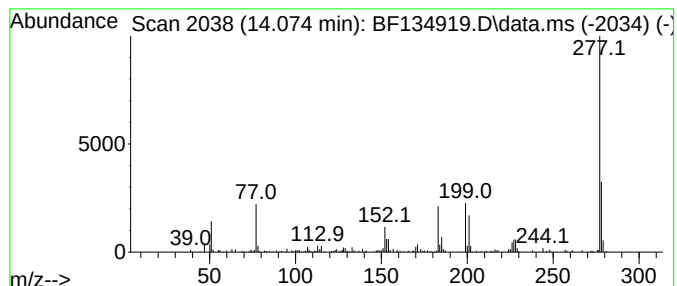
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	2.72 ng	118866	Chrysene-d12	13.980

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	64
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	43
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134919.D
Acq On : 24 Aug 2023 12:28
Operator : CG\JU
Sample : 04090-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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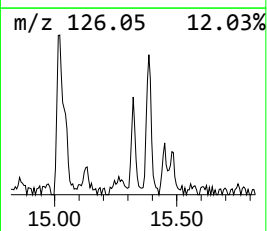
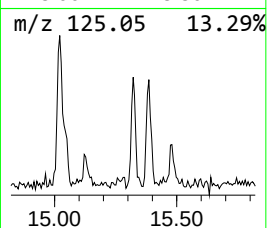
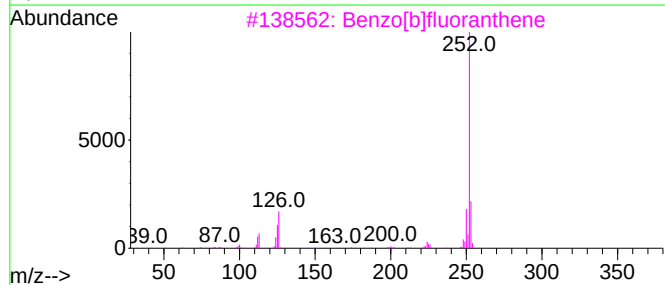
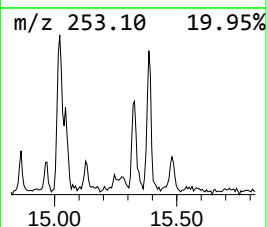
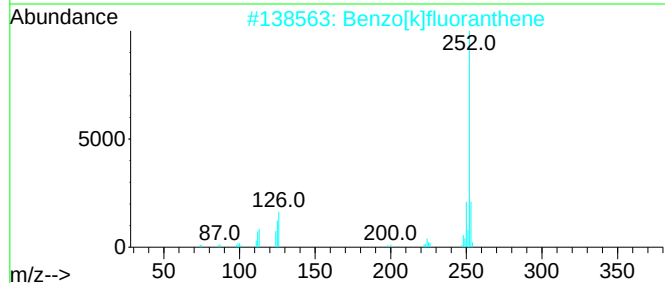
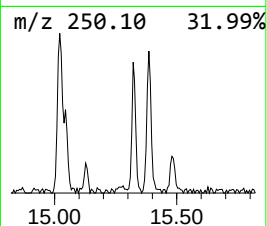
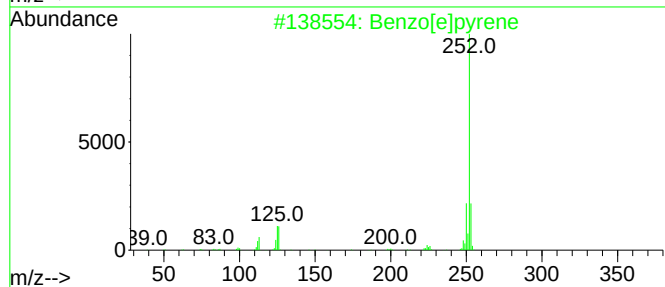
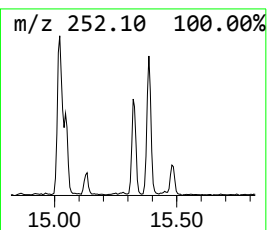
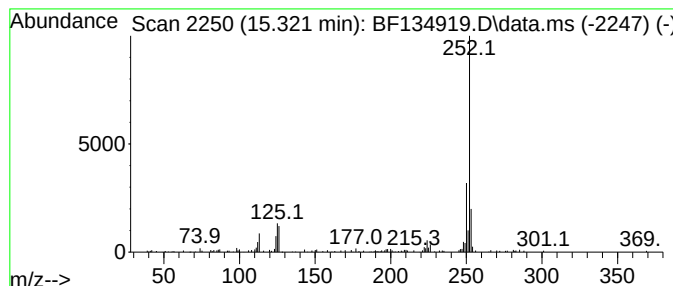
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	2.10 ng	78399	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082423\
Data File : BF134919.D
Acq On : 24 Aug 2023 12:28
Operator : CG\JU
Sample : 04090-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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
Ethanol, 2-(2-e...	6.622	2.8	ng	99985	1	6.792	725899	20.0
2,4,7,9-Tetrame...	9.275	22.3	ng	1199080	3	9.828	1076790	20.0
n-Hexadecanoic ...	11.857	7.8	ng	420535	4	11.322	1071800	20.0
unknown11.933	11.933	2.1	ng	111826	4	11.322	1071800	20.0
9-Octadecenoic ...	12.433	2.3	ng	124695	4	11.322	1071800	20.0
Octadecanoic acid	12.651	4.1	ng	177309	5	13.980	873751	20.0
Pentadecafluoro...	13.827	4.1	ng	178397	5	13.980	873751	20.0
Triphenylphosph...	14.074	2.7	ng	118866	5	13.980	873751	20.0
Benzo[e]pyrene	15.321	2.1	ng	78399	6	15.451	748275	20.0