

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
 Data File : BF125334.D
 Acq On : 2 Sep 2021 22:20
 Operator : JU/CG
 Sample : M3614-01 5X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-8-083121

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125334.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	18	rVB	222413	273978	17.91%	1.480%
2	3.975	317	321	326	rVB	13721	17744	1.16%	0.096%
3	5.516	579	583	593	rBV	920839	838477	54.81%	4.529%
4	6.528	752	755	774	rBV	941819	856001	55.96%	4.624%
5	6.904	816	819	823	rBV	1185612	1012062	66.16%	5.467%
6	7.469	911	915	927	rBV	547689	537870	35.16%	2.905%
7	8.104	1019	1023	1032	rBV6	13121	46499	3.04%	0.251%
8	8.192	1034	1038	1052	rVB	1610662	1406432	91.94%	7.597%
9	8.904	1156	1159	1166	rBV	58870	55537	3.63%	0.300%
10	9.004	1171	1176	1183	rBV	69128	65204	4.26%	0.352%
11	9.263	1217	1220	1231	rBV	1254008	1039208	67.93%	5.613%
12	9.369	1235	1238	1243	rVB2	23501	27159	1.78%	0.147%
13	9.533	1261	1266	1269	rBV	47537	58610	3.83%	0.317%
14	9.604	1274	1278	1280	rBV	71626	71139	4.65%	0.384%
15	9.633	1280	1283	1285	rVB	39108	33975	2.22%	0.184%
16	9.722	1295	1298	1304	rBV	36956	42468	2.78%	0.229%
17	9.804	1309	1312	1316	rBV	43071	39929	2.61%	0.216%
18	9.945	1333	1336	1340	rBV	1718901	1529782	100.00%	8.263%
19	9.981	1340	1342	1345	rVB	90955	72689	4.75%	0.393%
20	10.051	1350	1354	1358	rVB3	12556	17353	1.13%	0.094%
21	10.151	1367	1371	1374	rBV2	55355	55211	3.61%	0.298%
22	10.186	1374	1377	1382	rVB2	29807	28616	1.87%	0.155%
23	10.257	1387	1389	1393	rBV3	25911	29558	1.93%	0.160%
24	10.292	1393	1395	1401	rVB2	20106	21471	1.40%	0.116%
25	10.351	1401	1405	1407	rBV2	21142	32032	2.09%	0.173%
26	10.492	1426	1429	1436	rVB	109712	117832	7.70%	0.636%
27	10.651	1451	1456	1460	rVB3	27971	34820	2.28%	0.188%
28	10.733	1467	1470	1483	rVB	702762	643809	42.09%	3.478%
29	10.857	1486	1491	1498	rVB5	39312	55110	3.60%	0.298%
30	11.045	1518	1523	1525	rBV2	37875	46806	3.06%	0.253%
31	11.069	1525	1527	1531	rVB2	30238	25674	1.68%	0.139%
32	11.127	1534	1537	1539	rVB	27592	23675	1.55%	0.128%
33	11.169	1539	1544	1545	rBV4	12059	16705	1.09%	0.090%
34	11.286	1560	1564	1567	rBV4	20736	25083	1.64%	0.135%
35	11.333	1567	1572	1578	rVB3	41128	62476	4.08%	0.337%
36	11.433	1586	1589	1592	rBV	1576039	1528532	99.92%	8.256%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
 Data File : BF125334.D
 Acq On : 2 Sep 2021 22:20
 Operator : JU/CG
 Sample : M3614-01 5X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-8-083121

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-BF081821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.457	1592	1593	1597	rVV	490990	353432	23.10%	1.909%
38	11.510	1599	1602	1605	rVB	120443	103696	6.78%	0.560%
39	11.669	1626	1629	1632	rBV3	22575	27041	1.77%	0.146%
40	11.727	1635	1639	1644	rVV3	20833	33350	2.18%	0.180%
41	11.769	1644	1646	1651	rVB2	32557	30395	1.99%	0.164%
42	11.822	1651	1655	1658	rBV	210217	193992	12.68%	1.048%
43	11.939	1672	1675	1676	rBV	87890	83807	5.48%	0.453%
44	11.963	1677	1679	1685	rVV	114154	124591	8.14%	0.673%
45	12.016	1685	1688	1691	rVV	38764	40983	2.68%	0.221%
46	12.051	1691	1694	1696	rVV2	152981	162607	10.63%	0.878%
47	12.069	1696	1697	1702	rVB	61073	49048	3.21%	0.265%
48	12.233	1721	1725	1727	rBV	60548	54455	3.56%	0.294%
49	12.410	1753	1755	1757	rBV2	21928	18275	1.19%	0.099%
50	12.486	1765	1768	1769	rBV	61222	59622	3.90%	0.322%
51	12.504	1769	1771	1773	rVV	400293	392352	25.65%	2.119%
52	12.527	1773	1775	1778	rVV	776430	612559	40.04%	3.309%
53	12.574	1781	1783	1787	rVV4	22750	30809	2.01%	0.166%
54	12.610	1787	1789	1792	rVB	122252	102904	6.73%	0.556%
55	12.651	1792	1796	1800	rBV	481611	415349	27.15%	2.244%
56	12.745	1809	1812	1815	rBV3	20019	19473	1.27%	0.105%
57	12.804	1819	1822	1824	rBV	22829	17205	1.12%	0.093%
58	12.880	1829	1835	1841	rVV	458356	481499	31.48%	2.601%
59	12.933	1841	1844	1848	rVB3	25494	27316	1.79%	0.148%
60	13.016	1855	1858	1862	rBV	944128	816930	53.40%	4.413%
61	13.092	1867	1871	1876	rBV4	38957	66424	4.34%	0.359%
62	13.180	1883	1886	1887	rBV	33266	28494	1.86%	0.154%
63	13.204	1888	1890	1893	rVB	81500	78738	5.15%	0.425%
64	13.274	1899	1902	1905	rVB	69453	60070	3.93%	0.324%
65	13.310	1905	1908	1911	rBV2	55674	57346	3.75%	0.310%
66	13.404	1921	1924	1927	rVB	38362	33878	2.21%	0.183%
67	13.439	1927	1930	1932	rBV	35896	37895	2.48%	0.205%
68	13.586	1952	1955	1957	rBV3	19340	21291	1.39%	0.115%
69	13.827	1994	1996	1999	rBV	27469	24555	1.61%	0.133%
70	13.857	1999	2001	2003	rVB	29999	20189	1.32%	0.109%
71	13.880	2003	2005	2009	rBV3	22524	22917	1.50%	0.124%
72	14.080	2034	2039	2042	rBV	1237794	1273278	83.23%	6.878%
73	14.104	2042	2043	2050	rVB	178093	129675	8.48%	0.700%
74	14.186	2055	2057	2059	rBV	29434	22008	1.44%	0.119%
75	14.463	2102	2104	2108	rVB	43660	41237	2.70%	0.223%
76	14.504	2108	2111	2113	rBV	29131	30500	1.99%	0.165%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.139	2215	2219	2222	rBV2	125724	205108	13.41%	1.108%
78	15.451	2269	2272	2278	rVB	80233	107383	7.02%	0.580%
79	15.510	2279	2282	2289	rVB	101967	147630	9.65%	0.797%
80	15.580	2289	2294	2304	rBV	809062	1063588	69.53%	5.745%

Sum of corrected areas: 18513420

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

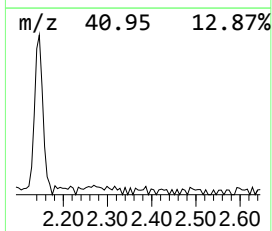
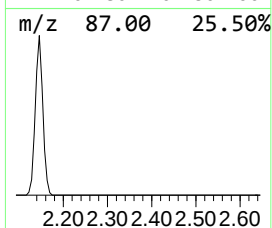
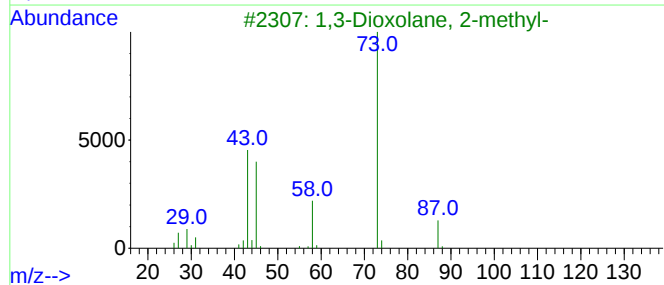
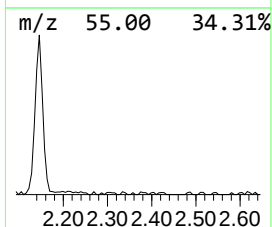
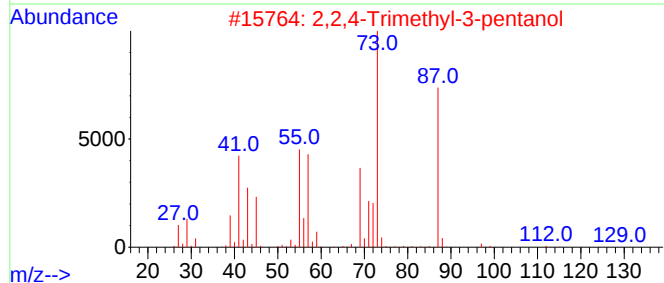
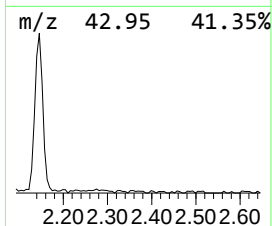
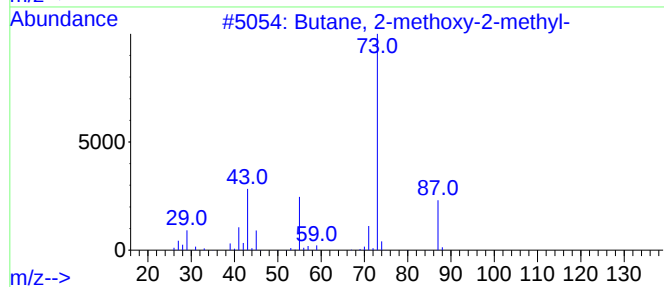
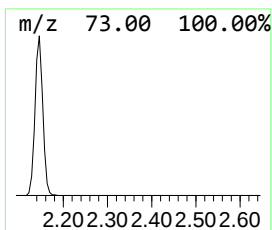
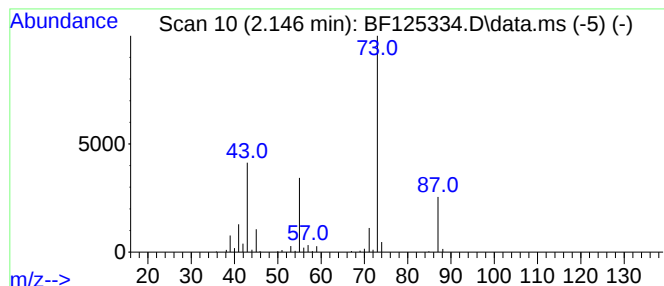
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	5.41 ng	273978	1,4-Dichlorobenzene-d4	6.904

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	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5		Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

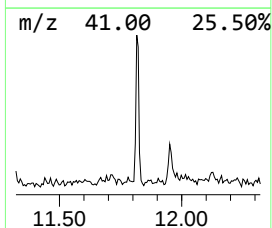
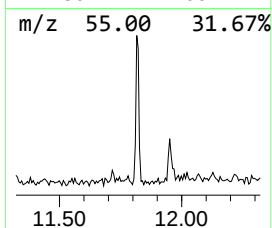
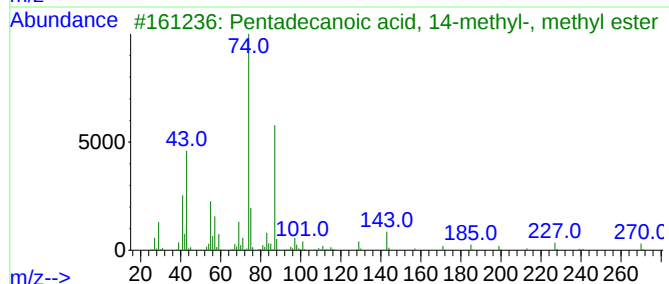
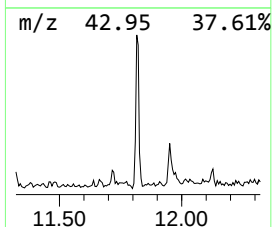
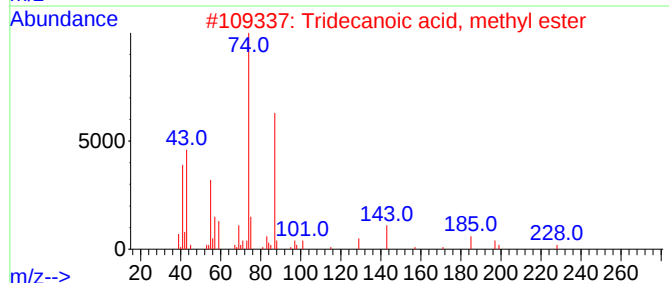
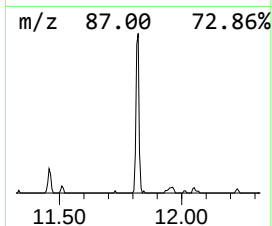
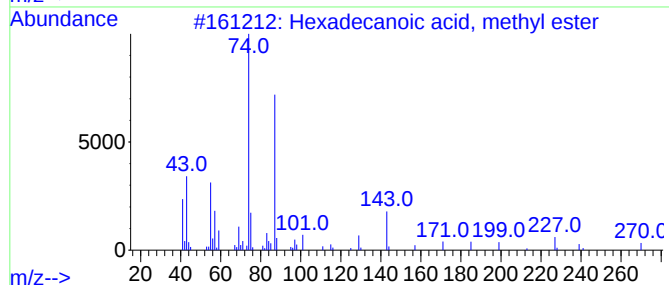
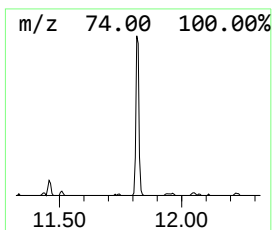
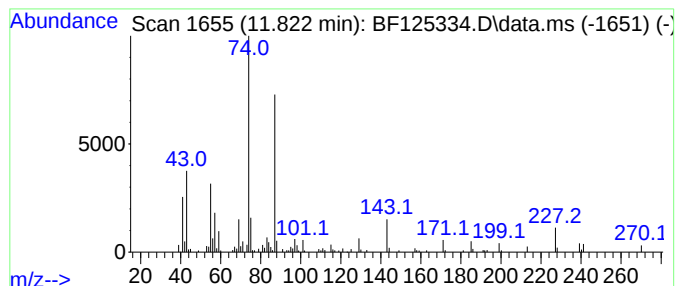
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	2.54 ng	193992	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	83
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

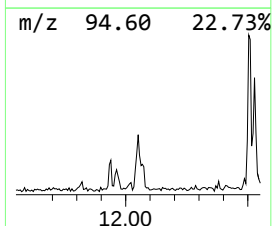
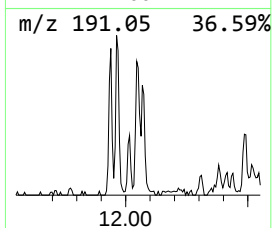
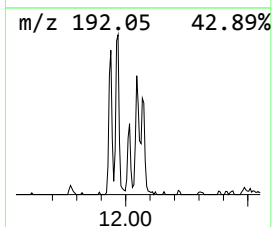
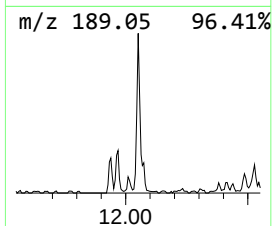
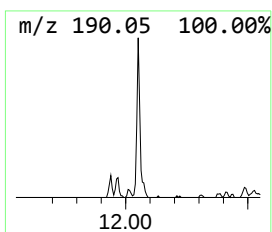
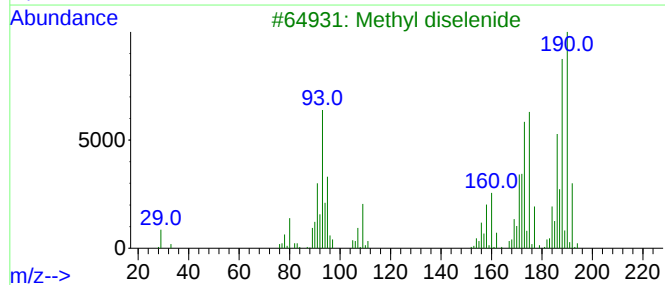
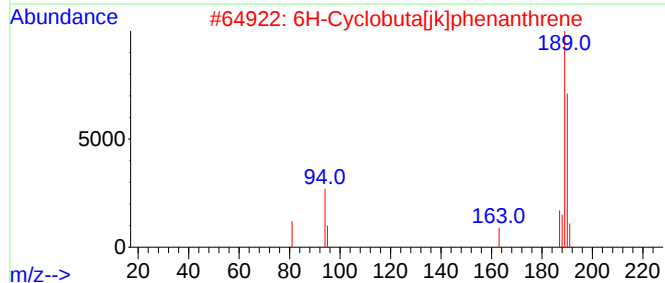
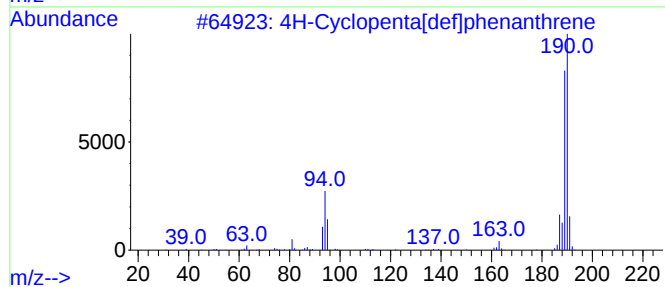
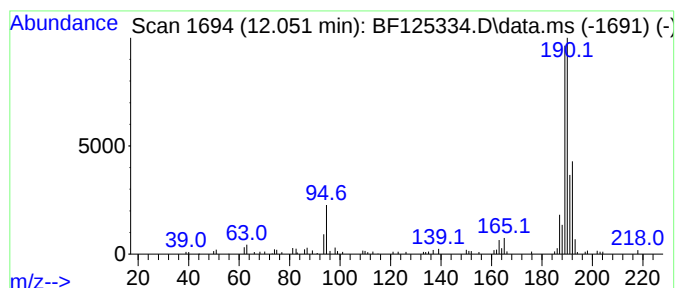
Instrument :
BNA_F
ClientSampleId :
NB-8-083121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.051	2.13 ng	162607	Phenanthrene-d10		11.433	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	74
2	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	45
3	Methyl diselenide		190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)		190	C10H14N4	069286-06-2	42
5	Carbonic acid, ethyl 2-formyl-4,...		262	C10H8Cl2O4	1000331-34-4	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

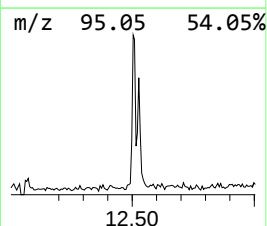
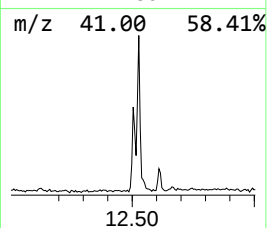
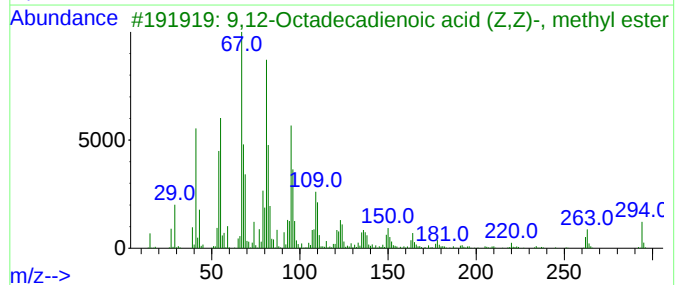
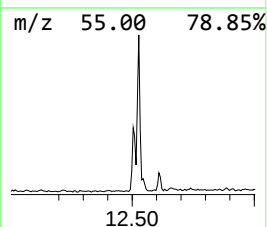
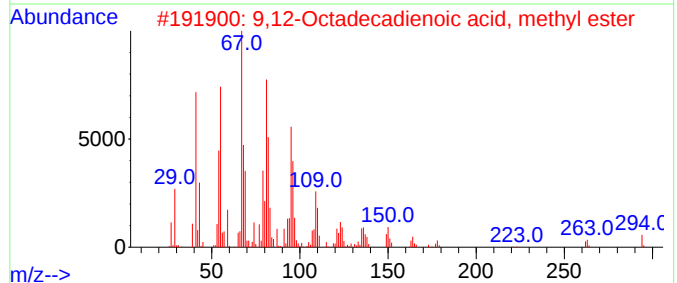
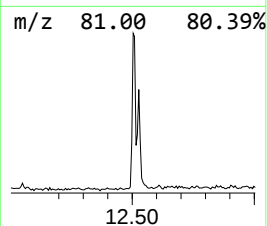
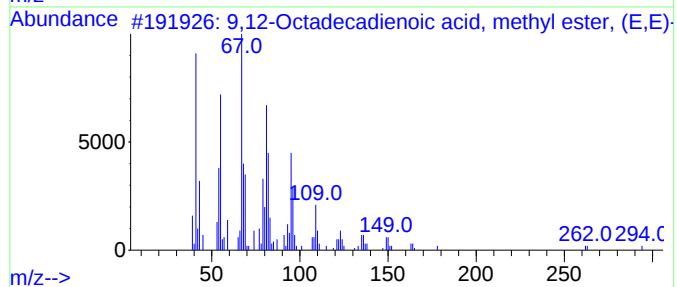
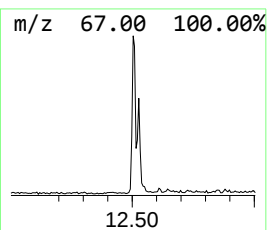
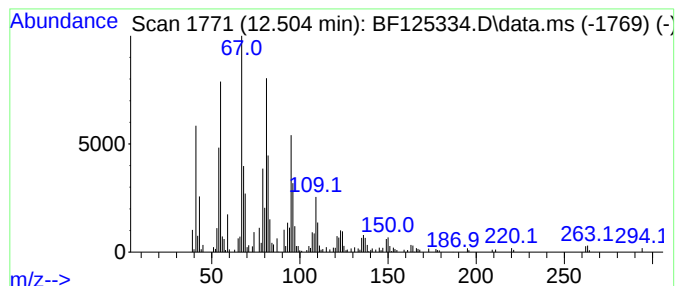
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	5.13 ng	392352	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98		
4	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	97		
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	96		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

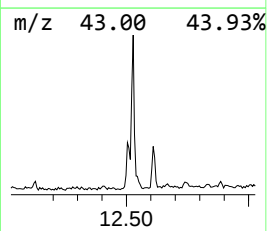
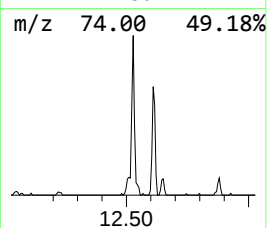
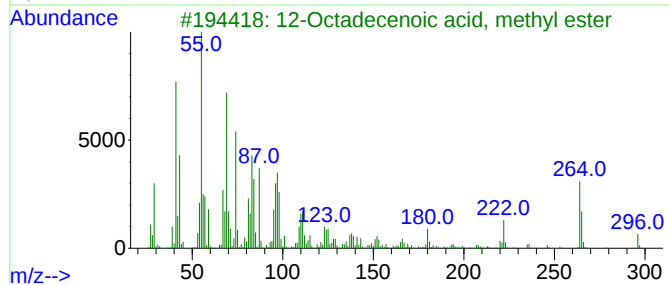
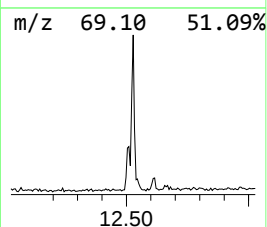
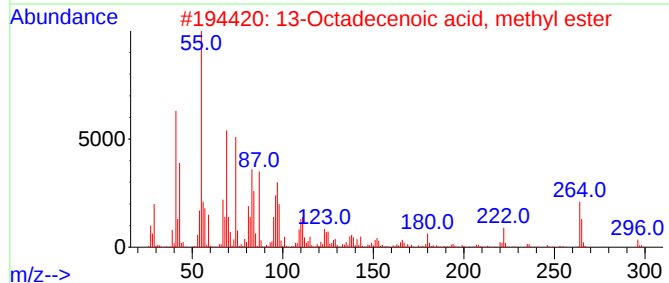
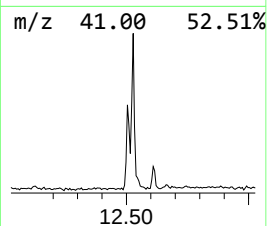
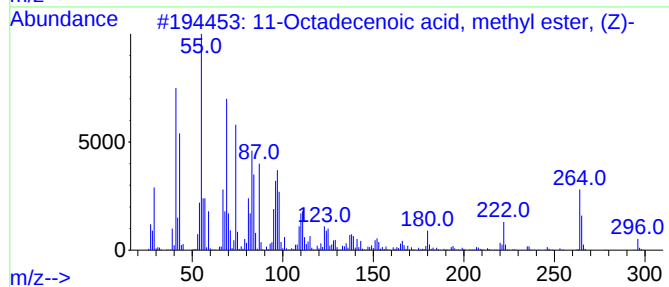
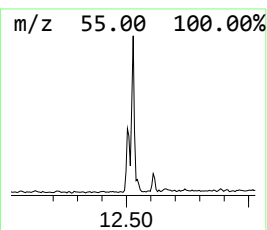
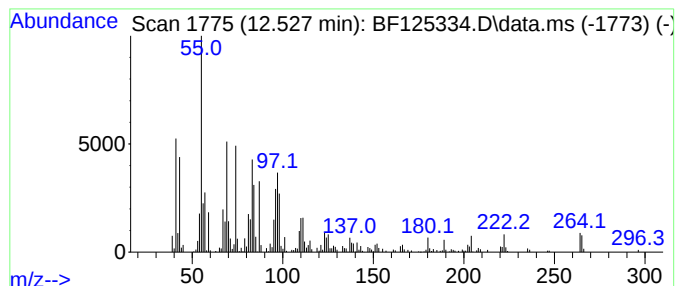
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 11-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	8.02 ng	612559	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

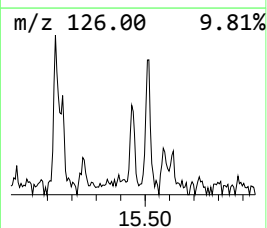
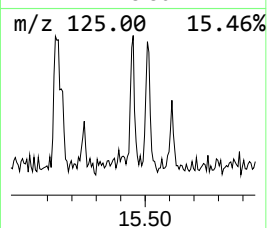
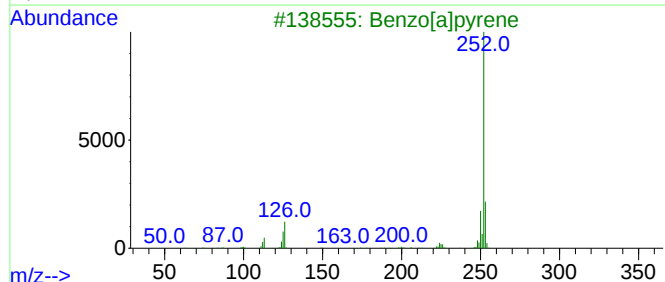
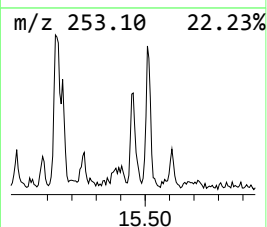
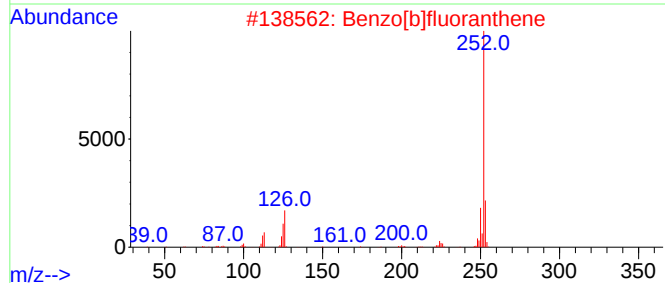
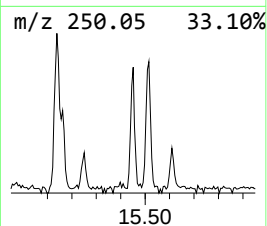
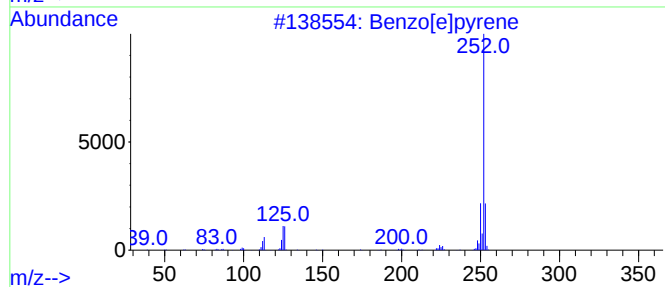
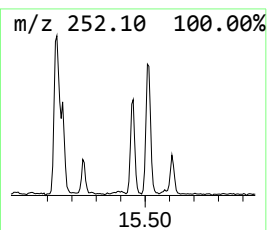
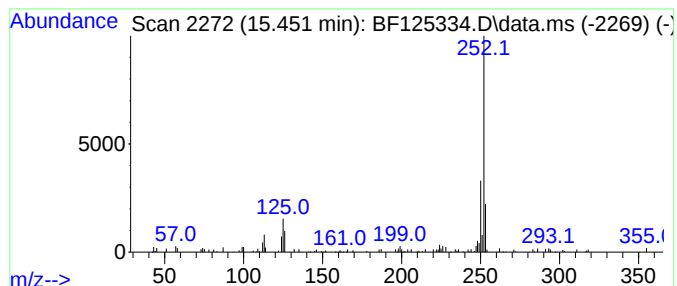
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	2.02 ng	107383	Perylene-d12	15.580

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125334.D
Acq On : 2 Sep 2021 22:20
Operator : JU/CG
Sample : M3614-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-8-083121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.146	5.4	ng	273978	1	6.904	1012060	20.0
Hexadecanoic ac...	11.822	2.5	ng	193992	4	11.433	1528530	20.0
4H-Cyclopenta[d...	12.051	2.1	ng	162607	4	11.433	1528530	20.0
9,12-Octadecadi...	12.504	5.1	ng	392352	4	11.433	1528530	20.0
11-Octadecenoic...	12.527	8.0	ng	612559	4	11.433	1528530	20.0
Benzo[e]pyrene	15.451	2.0	ng	107383	6	15.580	1063590	20.0