

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
 Data File : BF127105.D
 Acq On : 28 Feb 2022 17:44
 Operator : CG\JU
 Sample : N1664-25
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-9

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.122	479	482	488	rVB	32447	34501	1.42%	0.188%
2	5.516	545	549	553	rBV	2064889	1981508	81.35%	10.776%
3	6.528	716	721	724	rBV	2344975	2178265	89.43%	11.846%
4	6.898	781	784	788	rBV	738003	600678	24.66%	3.267%
5	7.463	875	880	883	rBV	1671762	1438484	59.06%	7.823%
6	8.075	981	984	994	rBV	164852	167306	6.87%	0.910%
7	8.181	999	1002	1006	rBV	905239	812731	33.37%	4.420%
8	9.257	1181	1185	1188	rBV	2947853	2435692	100.00%	13.245%
9	9.363	1200	1203	1207	rBV	127156	116959	4.80%	0.636%
10	9.745	1264	1268	1275	rBV6	18546	29272	1.20%	0.159%
11	9.939	1298	1301	1305	rBV	1029976	831436	34.14%	4.521%
12	10.733	1432	1436	1439	rBV	2033421	1699479	69.77%	9.242%
13	10.951	1466	1473	1476	rBV6	22203	36520	1.50%	0.199%
14	11.310	1531	1534	1541	rVB3	21451	34825	1.43%	0.189%
15	11.433	1551	1555	1557	rBV	978689	797110	32.73%	4.335%
16	11.457	1557	1559	1562	rVB	138475	105814	4.34%	0.575%
17	11.663	1589	1594	1600	rBV	33513	40229	1.65%	0.219%
18	11.816	1616	1620	1623	rBV	129184	116228	4.77%	0.632%
19	11.945	1637	1642	1643	rBV2	65056	68341	2.81%	0.372%
20	11.963	1643	1645	1647	rVB	39997	32173	1.32%	0.175%
21	12.045	1655	1659	1661	rBV2	41126	42199	1.73%	0.229%
22	12.480	1730	1733	1736	rBV2	27561	37047	1.52%	0.201%
23	12.521	1736	1740	1742	rVV	215307	167892	6.89%	0.913%
24	12.610	1752	1755	1758	rVB	45995	41228	1.69%	0.224%
25	12.645	1758	1761	1765	rBV	291592	238499	9.79%	1.297%
26	12.874	1795	1800	1804	rBV	219964	242637	9.96%	1.319%
27	13.016	1820	1824	1828	rBV	1803503	1616018	66.35%	8.788%
28	13.086	1833	1836	1842	rBV5	22879	40213	1.65%	0.219%
29	13.180	1849	1852	1854	rBV4	22739	28328	1.16%	0.154%
30	13.715	1940	1943	1946	rVB	32196	33519	1.38%	0.182%
31	13.827	1958	1962	1964	rBV2	29718	39165	1.61%	0.213%
32	13.921	1974	1978	1987	rVB6	103499	184691	7.58%	1.004%
33	14.074	1996	2004	2007	rBV2	541621	660176	27.10%	3.590%
34	14.104	2007	2009	2014	rVB	129384	115562	4.74%	0.628%
35	14.592	2090	2092	2099	rVB5	38570	61741	2.53%	0.336%
36	15.133	2180	2184	2191	rBV	170728	323288	13.27%	1.758%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.192	2191	2194	2199	rVB6	23275	31857	1.31%	0.173%
38	15.245	2200	2203	2206	rBV	36528	44144	1.81%	0.240%
39	15.445	2233	2237	2242	rVB	93965	117443	4.82%	0.639%
40	15.509	2244	2248	2253	rVB	103144	128619	5.28%	0.699%
41	15.574	2254	2259	2263	rBV	410074	544699	22.36%	2.962%
42	17.092	2512	2517	2525	rVB3	43383	92342	3.79%	0.502%

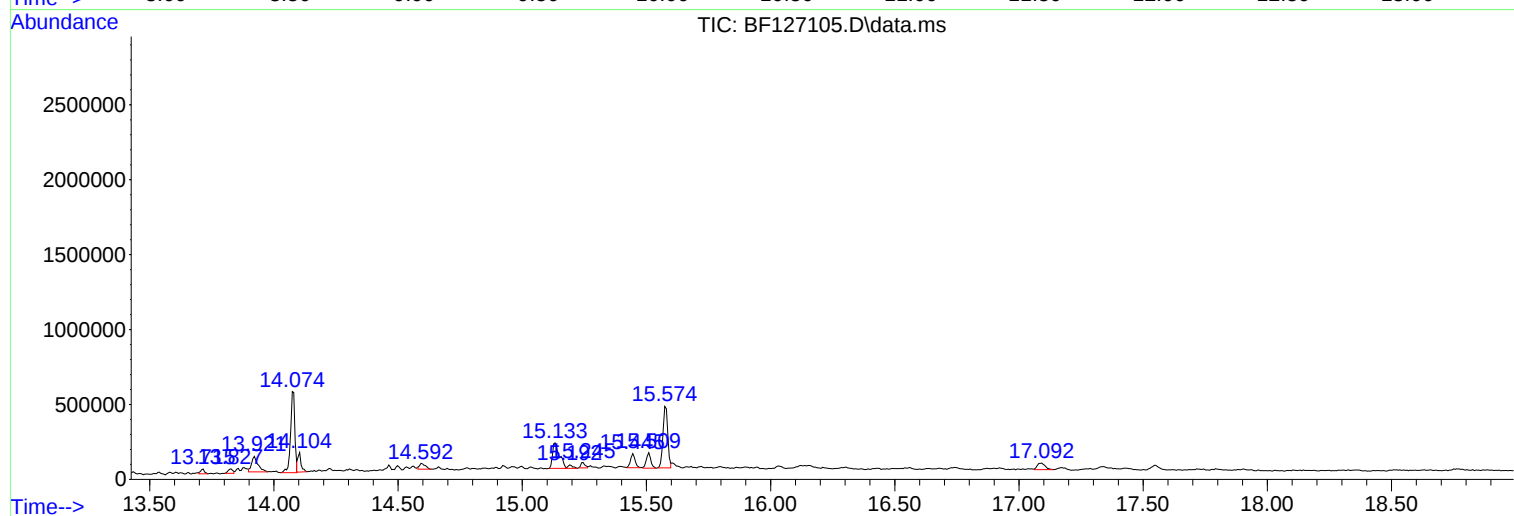
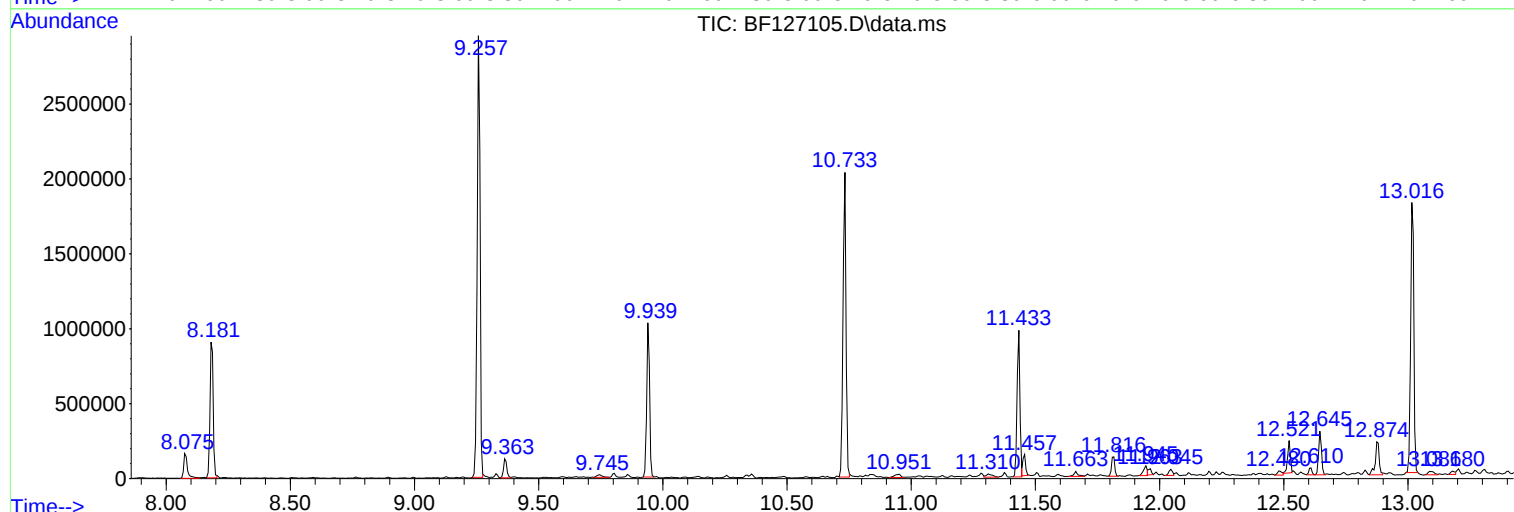
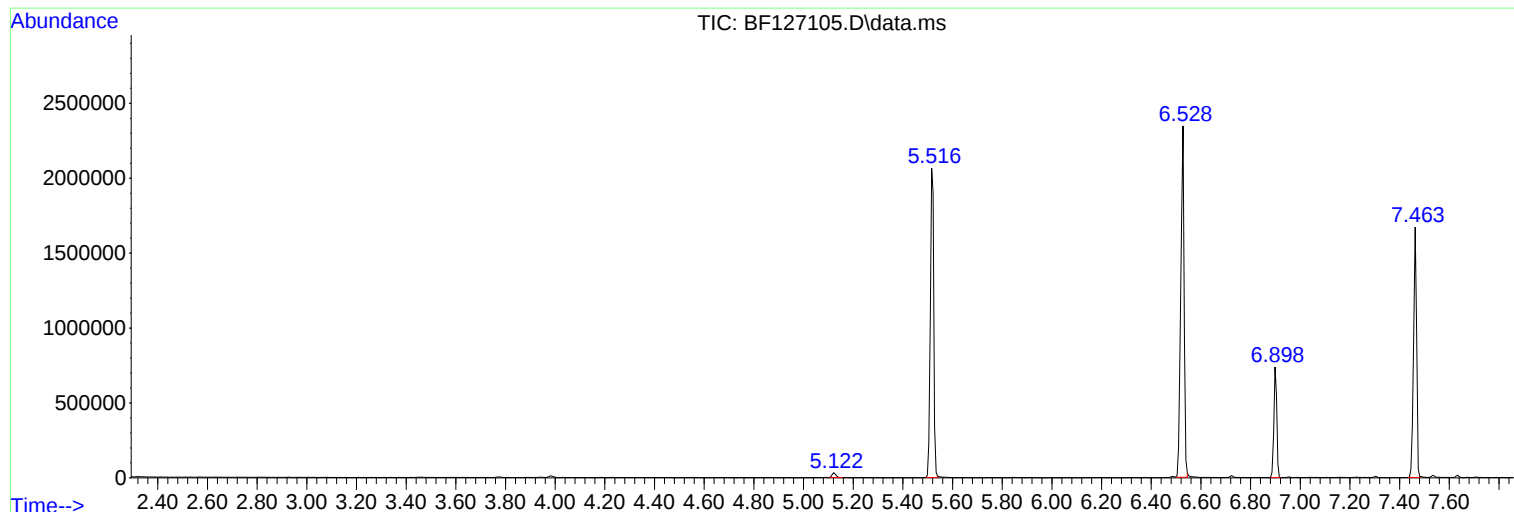
Sum of corrected areas: 18388858

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

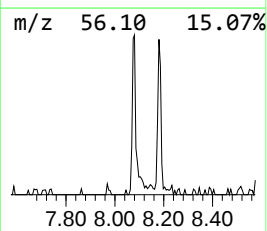
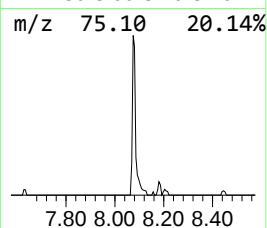
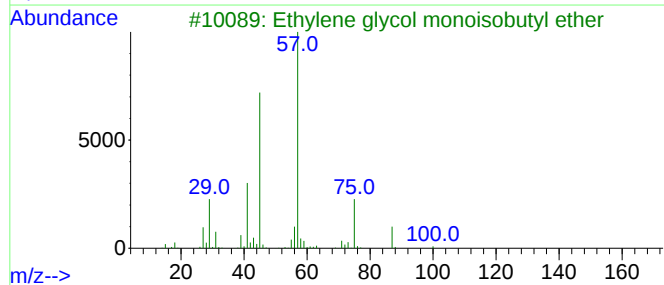
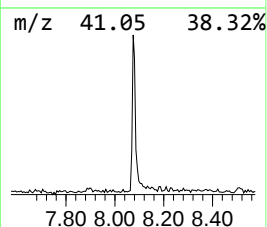
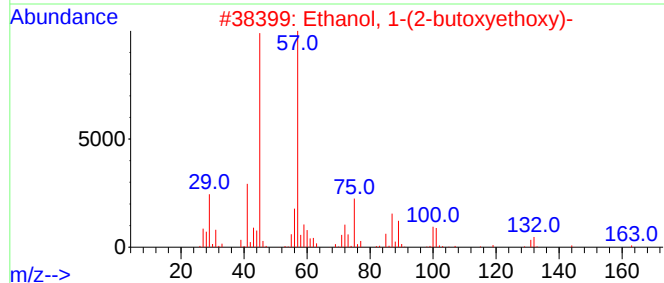
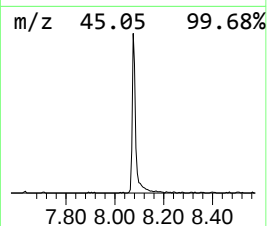
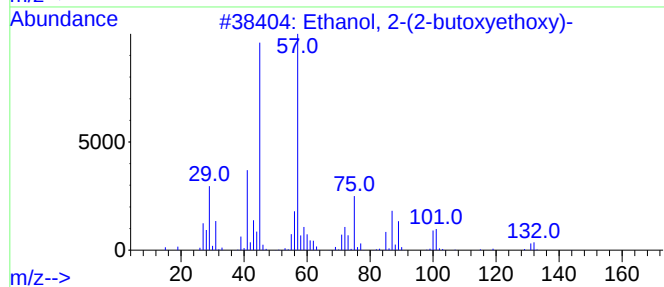
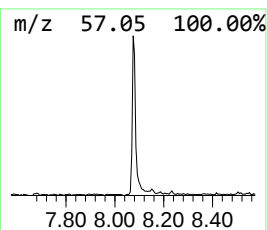
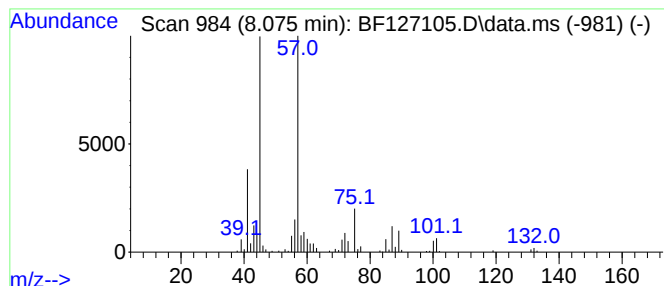
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	4.12 ng	167306	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

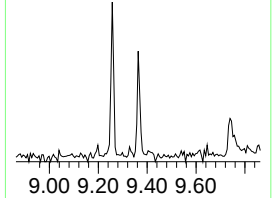
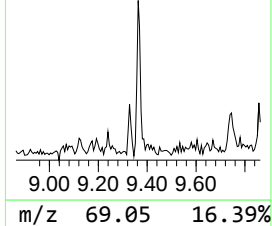
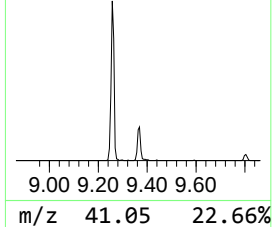
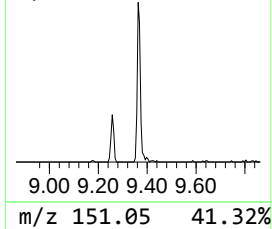
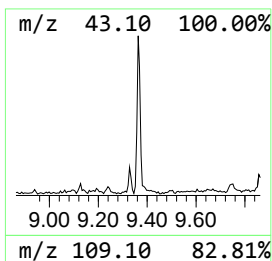
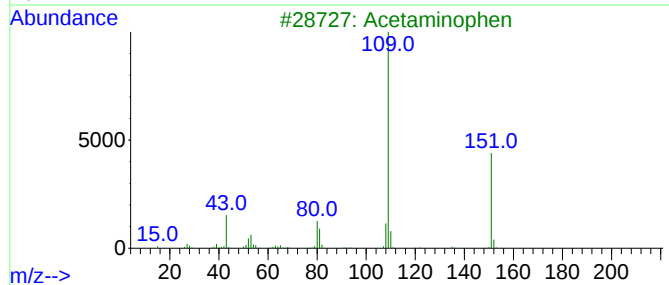
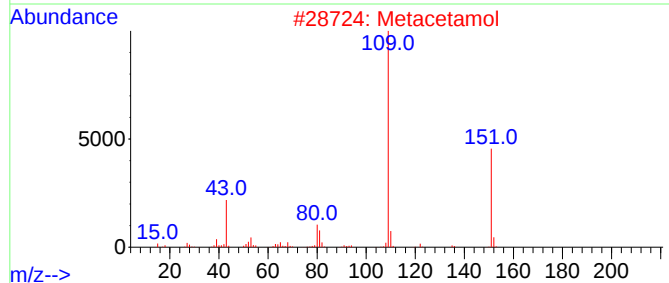
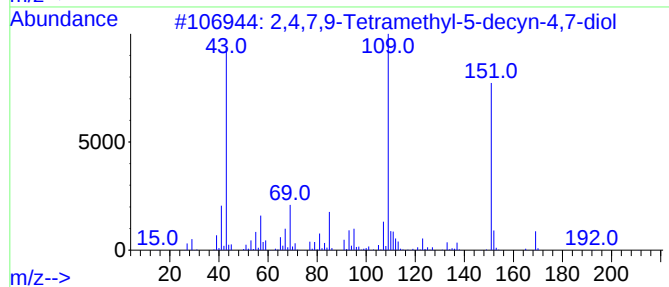
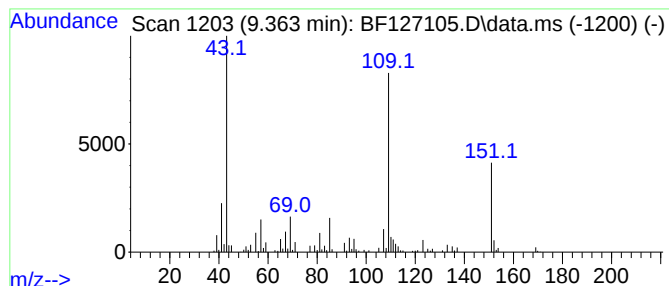
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.363	2.81 ng	116959	Acenaphthene-d10		9.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	68
2	Metacetamol	151	C8H9NO2		000621-42-1	64
3	Acetaminophen	151	C8H9NO2		000103-90-2	59
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
5	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

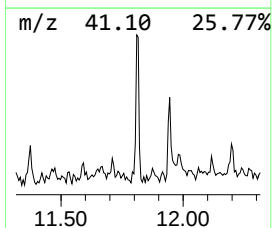
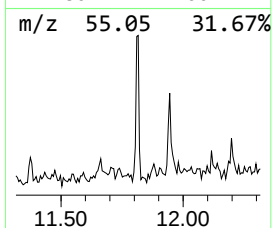
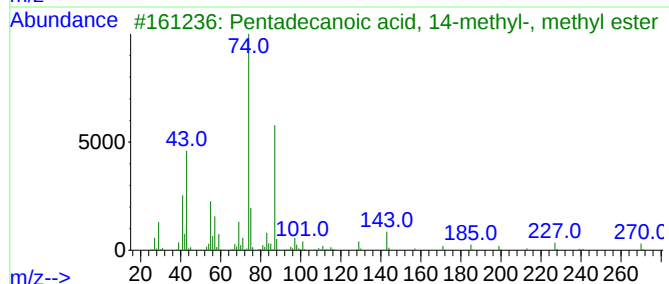
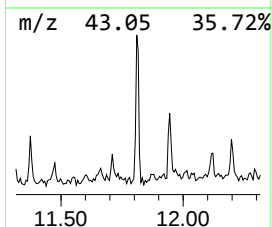
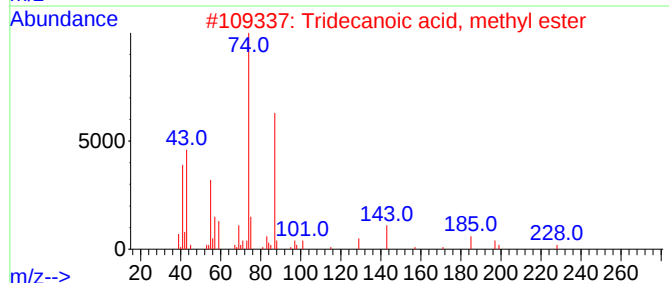
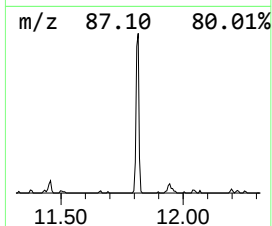
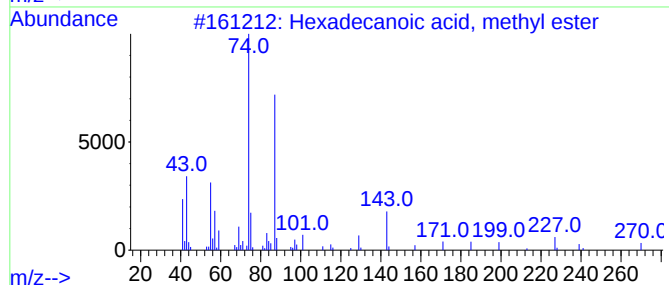
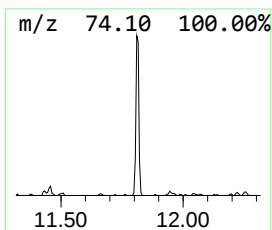
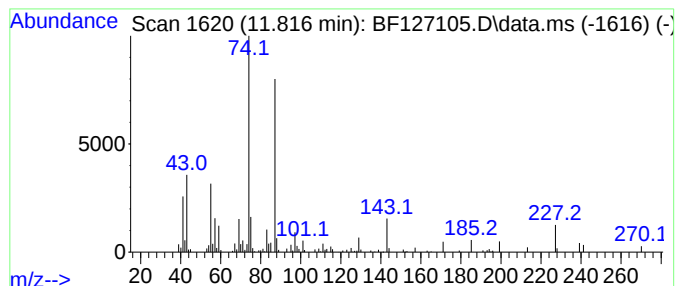
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	2.92 ng	116228	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	94
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

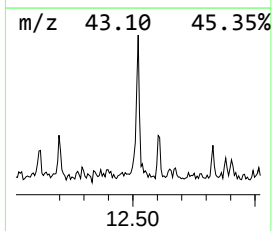
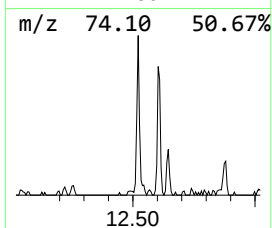
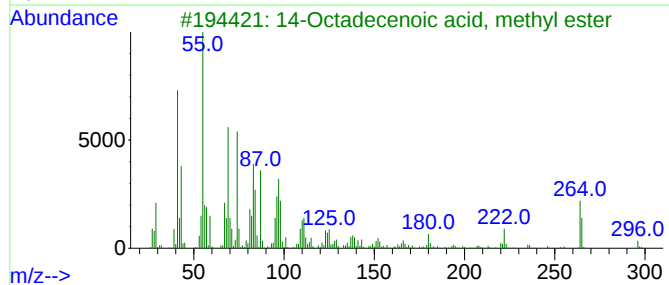
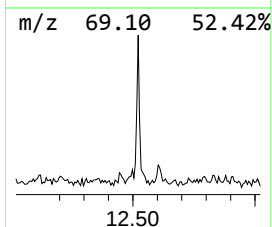
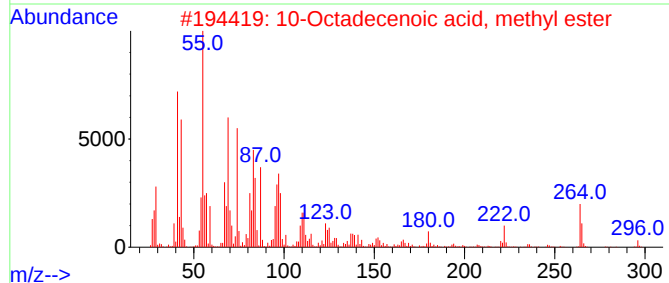
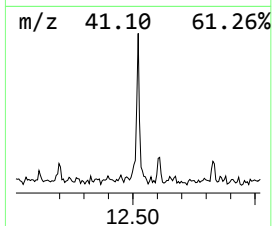
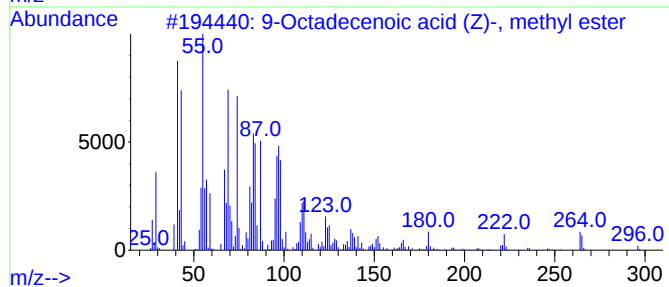
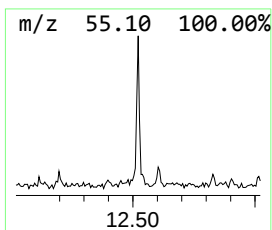
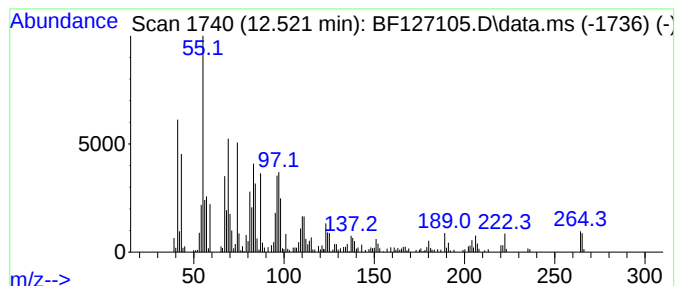
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.521	4.21 ng	167892	Phenanthrene-d10	11.433

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			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

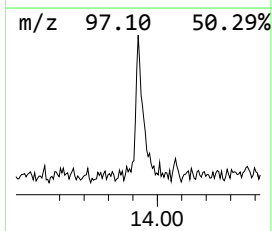
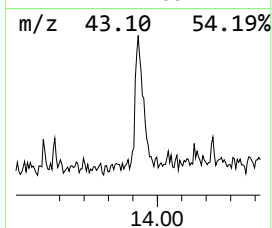
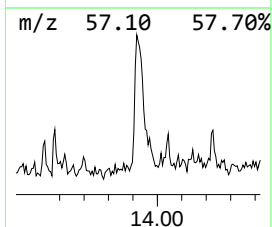
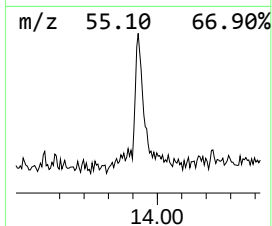
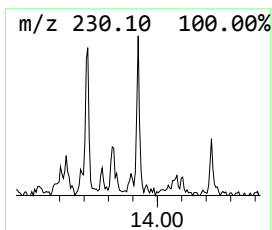
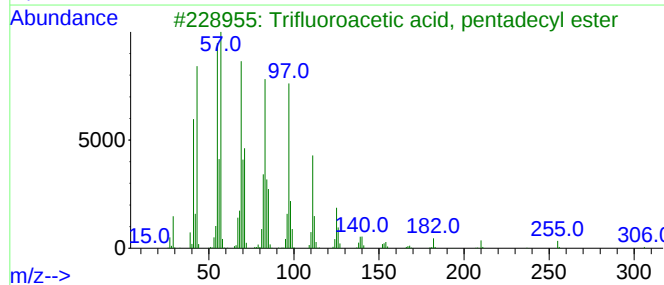
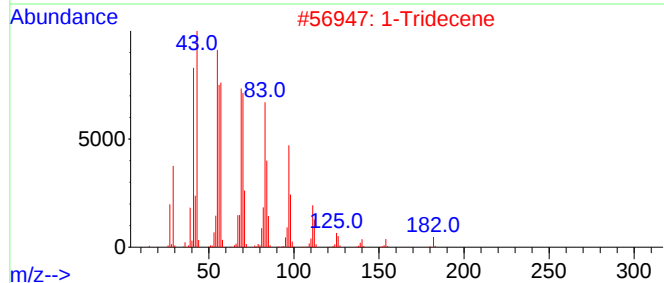
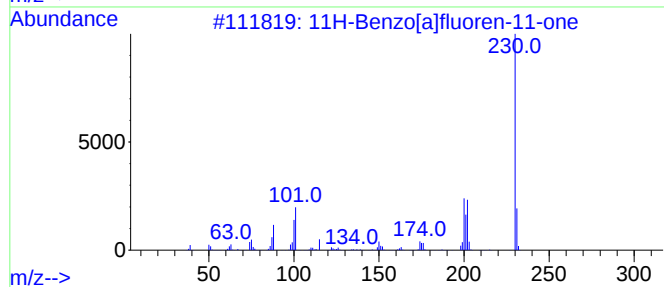
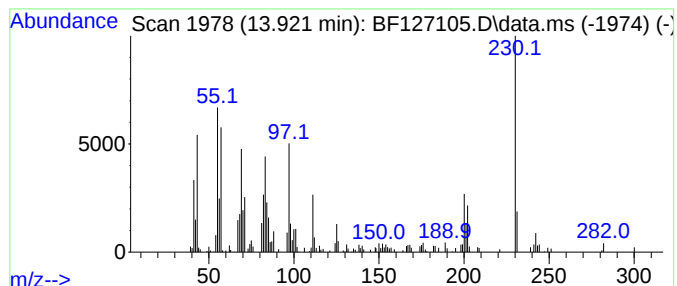
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.60 ng	184691	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	84
2			1-Tridecene	182	C13H26	002437-56-1	50
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	46
4			1-Tetracosene	336	C24H48	010192-32-2	42
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

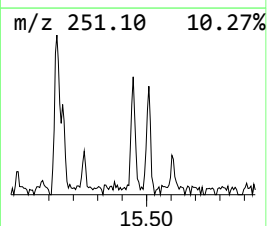
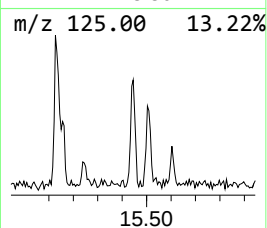
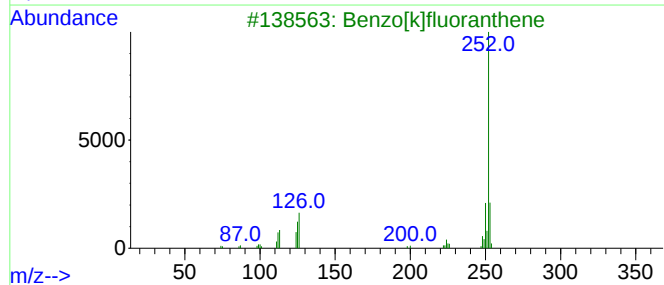
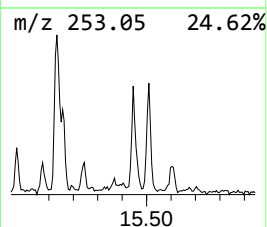
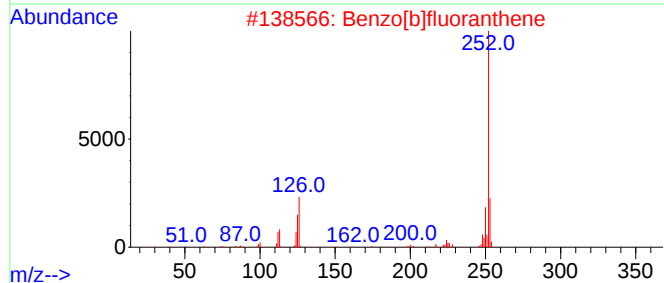
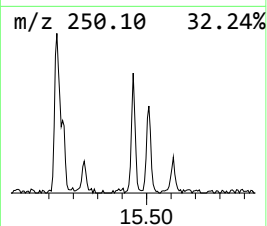
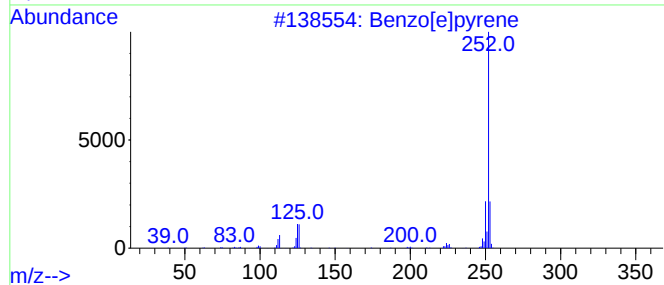
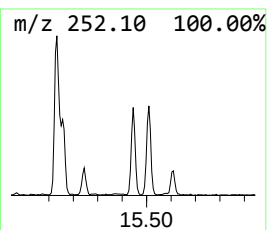
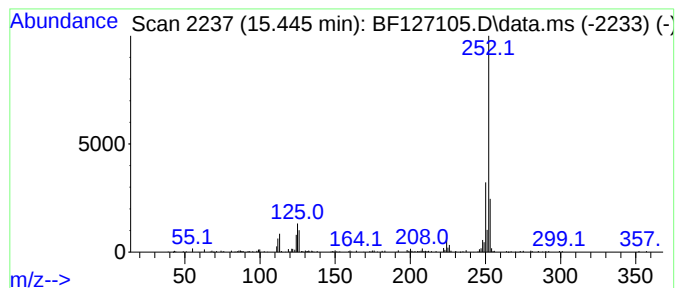
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	4.31 ng	117443	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127105.D
Acq On : 28 Feb 2022 17:44
Operator : CG\JU
Sample : N1664-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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-b...	8.075	4.1	ng	167306	2	8.181	812731	20.0
2,4,7,9-Tetrame...	9.363	2.8	ng	116959	3	9.939	831436	20.0
Hexadecanoic ac...	11.816	2.9	ng	116228	4	11.433	797110	20.0
9-Octadecenoic ...	12.521	4.2	ng	167892	4	11.433	797110	20.0
11H-Benzo[a]flu...	13.921	5.6	ng	184691	5	14.080	660176	20.0
Benzo[e]pyrene	15.445	4.3	ng	117443	6	15.574	544699	20.0