

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
 Data File : BF127106.D
 Acq On : 28 Feb 2022 18:13
 Operator : CG\JU
 Sample : N1664-28
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-10

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: BF127106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.516	545	549	553	rBV	2204821	2098660	82.47%	11.128%
2	6.528	716	721	734	rVB	2417184	2277999	89.52%	12.079%
3	6.898	781	784	788	rBV	807664	646734	25.42%	3.429%
4	7.463	875	880	883	rBV	1701693	1481285	58.21%	7.855%
5	8.075	981	984	996	rBV	210367	219295	8.62%	1.163%
6	8.181	999	1002	1006	rBV	938333	834189	32.78%	4.423%
7	9.257	1181	1185	1188	rBV	3007506	2544661	100.00%	13.493%
8	9.369	1200	1204	1208	rBV	313968	277234	10.89%	1.470%
9	9.739	1264	1267	1275	rBV5	21619	39330	1.55%	0.209%
10	9.939	1298	1301	1305	rBV	1007854	864405	33.97%	4.584%
11	10.733	1432	1436	1439	rBV	1902657	1623601	63.80%	8.609%
12	11.375	1542	1545	1548	rVB	50535	35600	1.40%	0.189%
13	11.433	1551	1555	1557	rBV	973680	800739	31.47%	4.246%
14	11.457	1557	1559	1562	rVB	139067	109537	4.30%	0.581%
15	11.586	1578	1581	1587	rBV	39075	50474	1.98%	0.268%
16	11.663	1589	1594	1600	rVV3	32494	52348	2.06%	0.278%
17	11.816	1616	1620	1622	rBV	95460	80901	3.18%	0.429%
18	11.945	1635	1642	1647	rBV2	182152	217809	8.56%	1.155%
19	11.986	1647	1649	1651	rVB	53391	37324	1.47%	0.198%
20	12.045	1656	1659	1661	rBV2	32624	35091	1.38%	0.186%
21	12.198	1682	1685	1688	rBV	82291	65103	2.56%	0.345%
22	12.486	1730	1734	1736	rBV3	30070	42912	1.69%	0.228%
23	12.522	1737	1740	1743	rVB	210291	168368	6.62%	0.893%
24	12.604	1752	1754	1758	rVB	97064	88960	3.50%	0.472%
25	12.645	1758	1761	1764	rBV	227032	201619	7.92%	1.069%
26	12.880	1794	1801	1804	rBV	181226	209352	8.23%	1.110%
27	13.016	1820	1824	1828	rBV	1932194	1751842	68.84%	9.289%
28	13.239	1858	1862	1866	rBV2	35679	59423	2.34%	0.315%
29	13.457	1892	1899	1902	rBV3	90187	103977	4.09%	0.551%
30	13.710	1940	1942	1948	rVB	23683	29242	1.15%	0.155%
31	13.921	1974	1978	1988	rVB5	90976	174356	6.85%	0.925%
32	14.074	2000	2004	2007	rBV2	544552	579679	22.78%	3.074%
33	14.104	2007	2009	2011	rVB	86359	64609	2.54%	0.343%
34	14.927	2146	2149	2152	rBV	33227	32197	1.27%	0.171%
35	15.133	2180	2184	2187	rBV	103897	152419	5.99%	0.808%
36	15.445	2234	2237	2243	rVB	67023	77323	3.04%	0.410%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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37	15.510	2244	2248	2252	rBV	77134	98393	3.87%	0.522%
38	15.574	2254	2259	2264	rBV	425753	560484	22.03%	2.972%
39	17.086	2512	2516	2526	rVB2	34144	70990	2.79%	0.376%

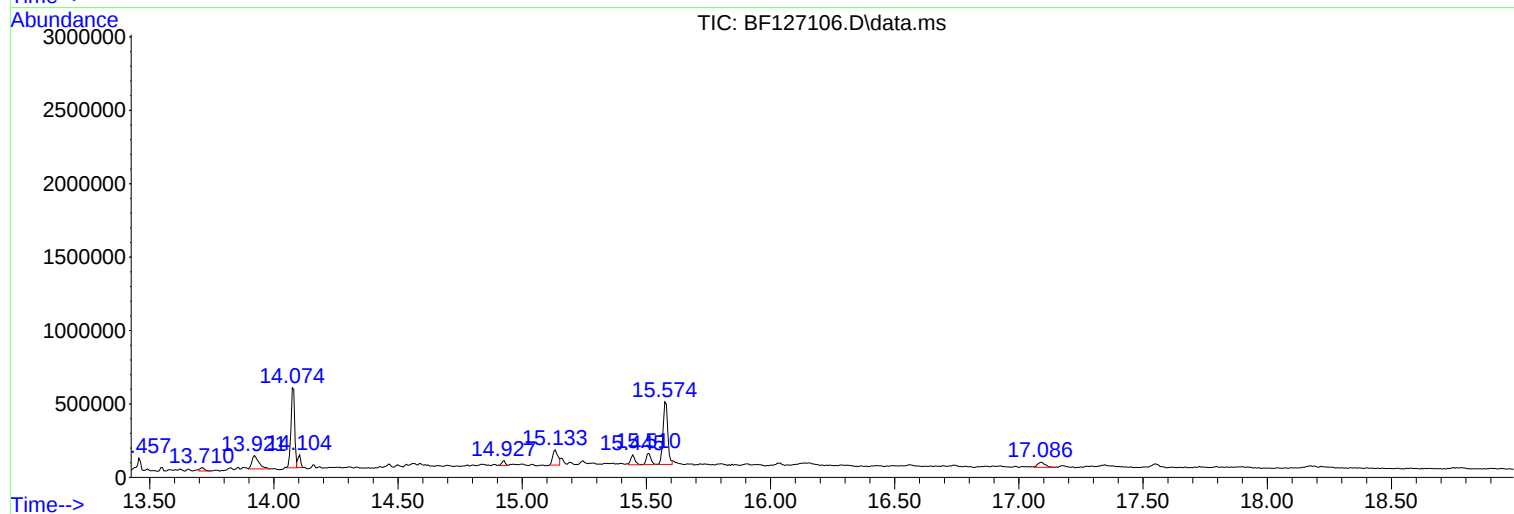
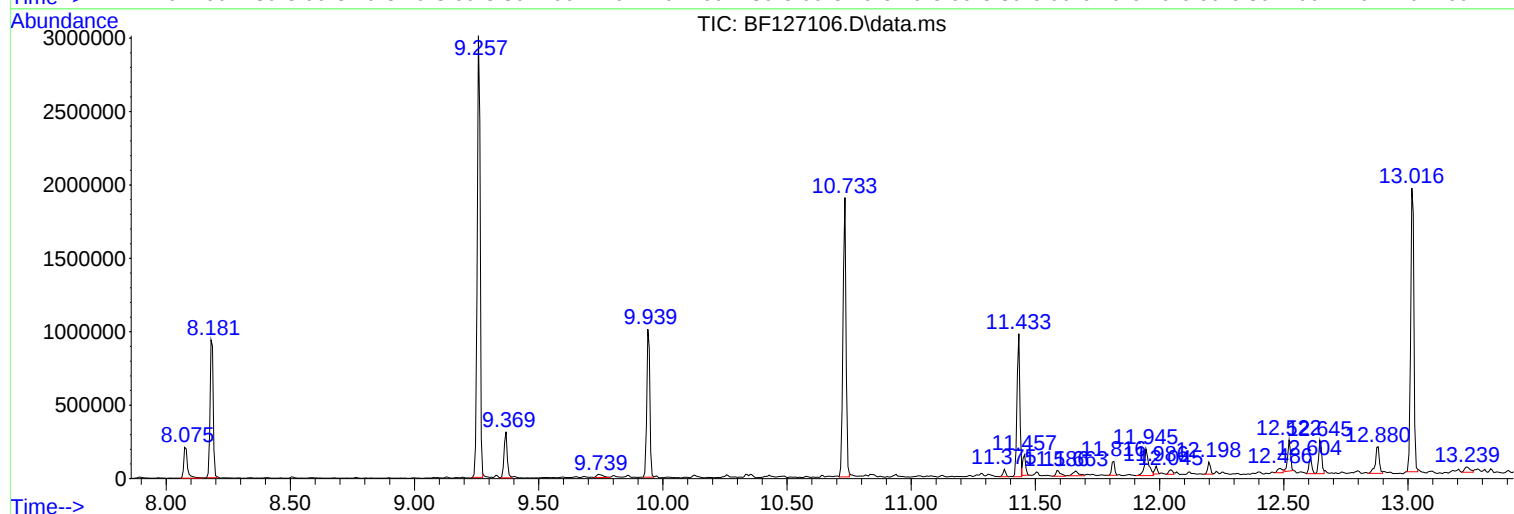
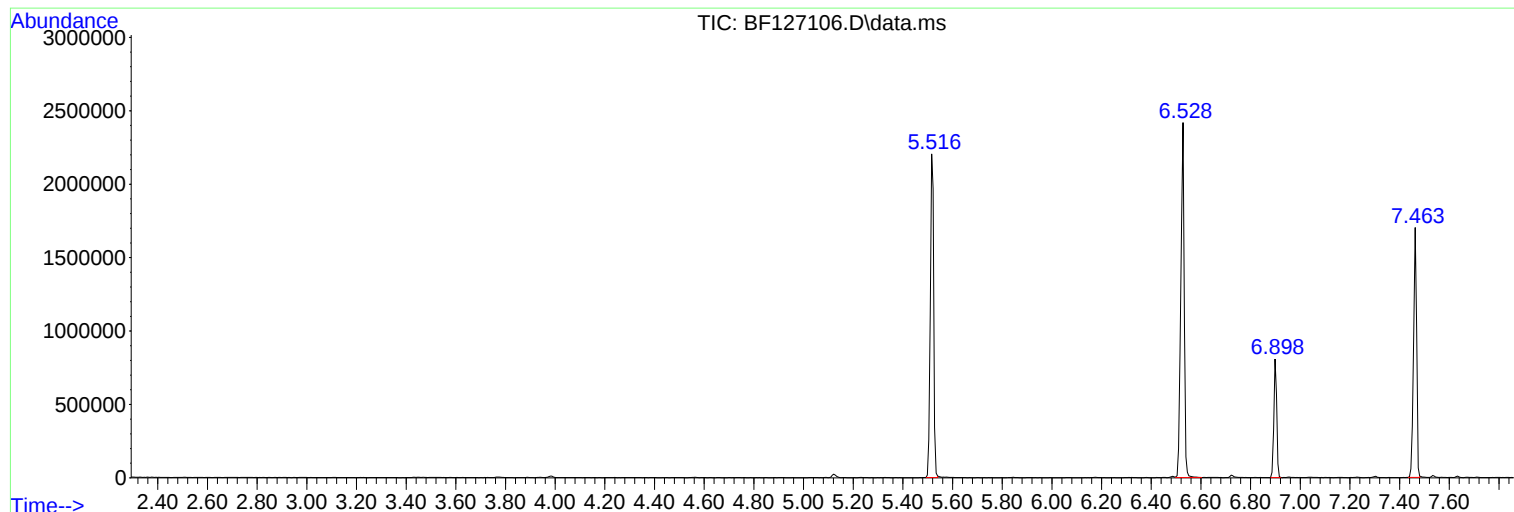
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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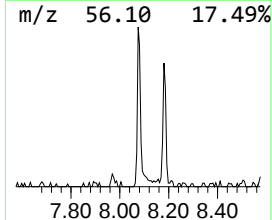
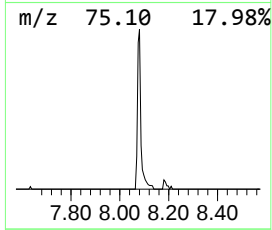
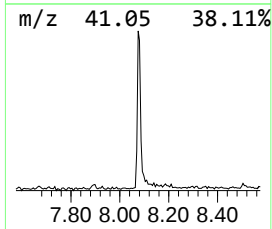
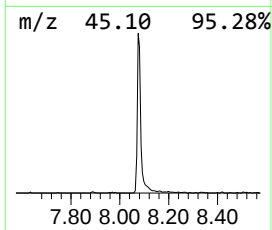
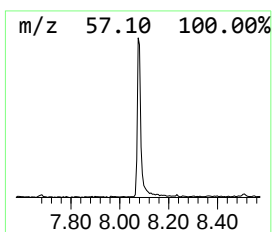
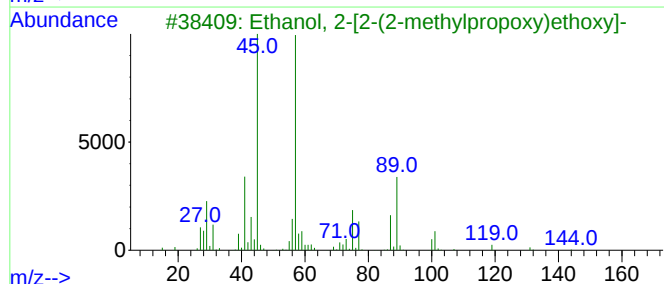
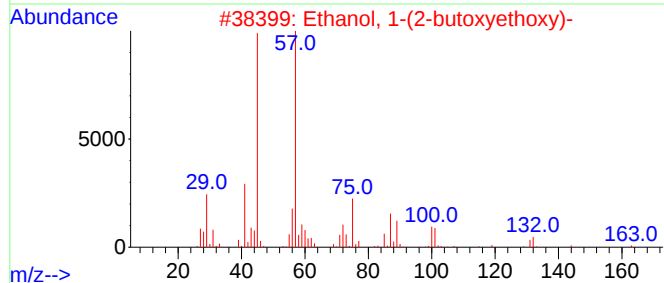
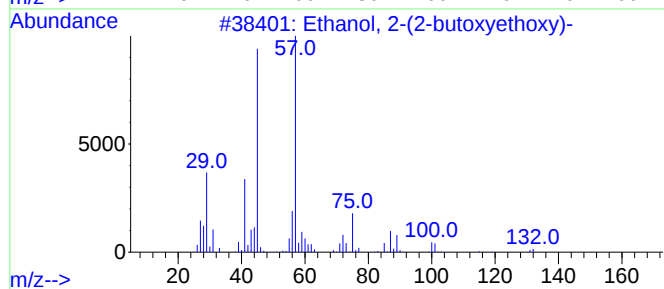
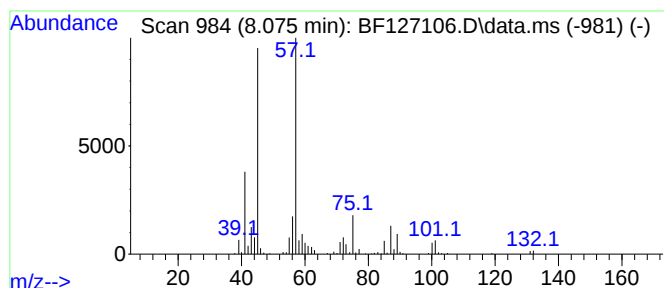
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.26 ng	219295	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	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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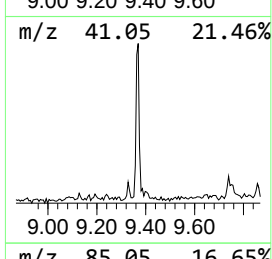
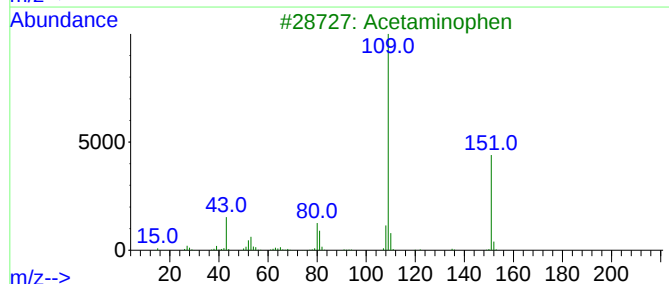
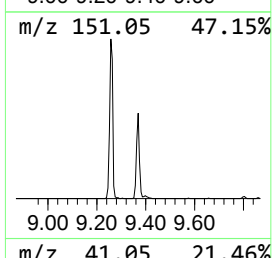
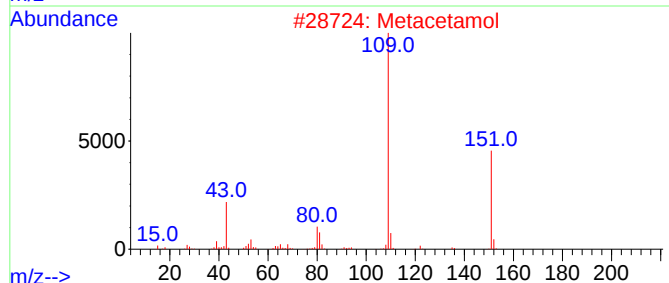
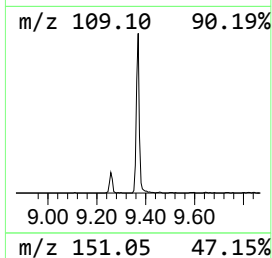
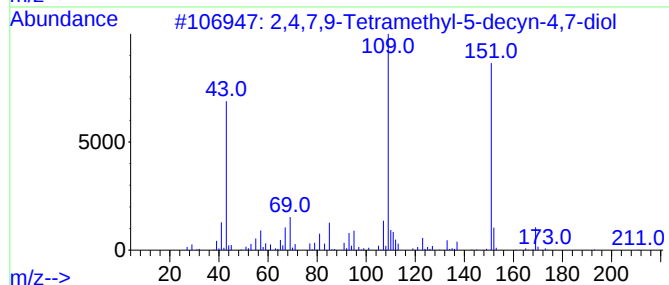
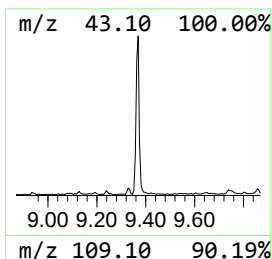
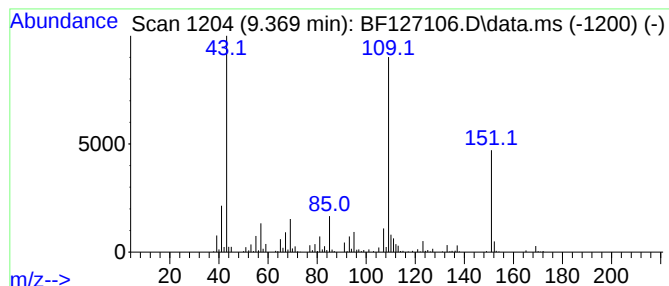
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	6.41 ng	277234	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	91
2	Metacetamol	151	C8H9NO2		000621-42-1	64
3	Acetaminophen	151	C8H9NO2		000103-90-2	59
4	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN		1000250-88-9	47
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O		000116-02-9	47



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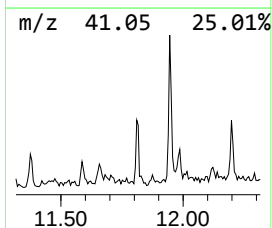
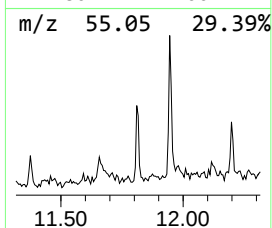
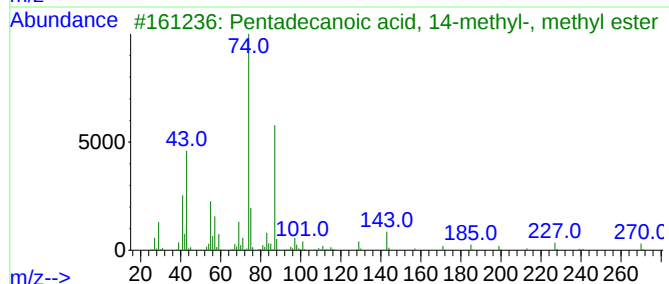
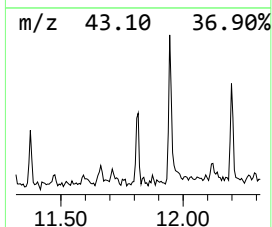
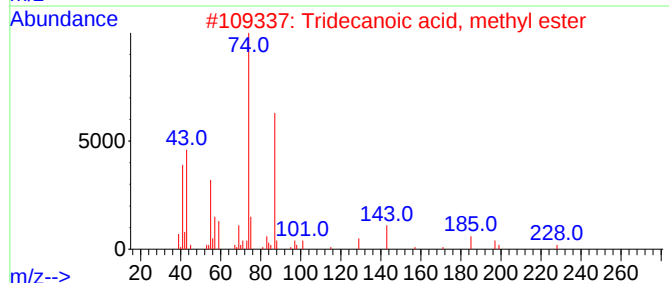
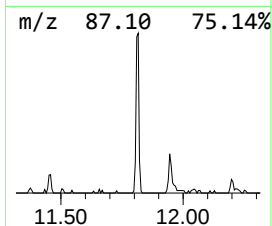
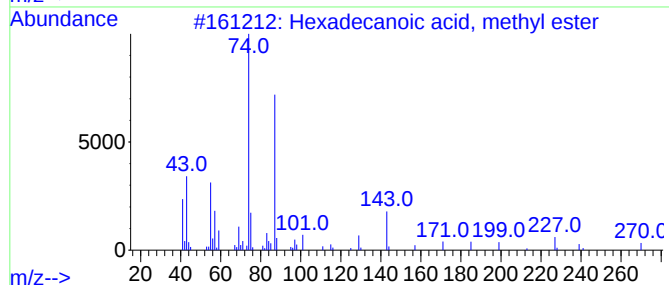
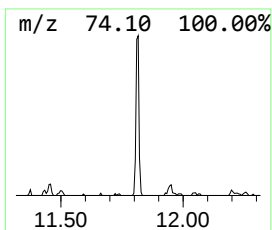
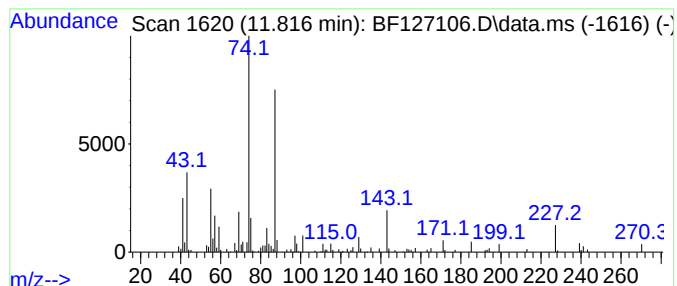
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	2.02 ng	80901	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	91
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
5			Methyl 13-methyltetradecanoate	256	C16H32O2	1000424-50-7	80



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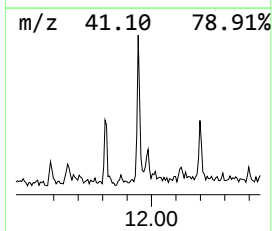
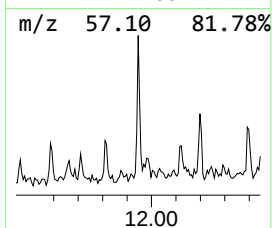
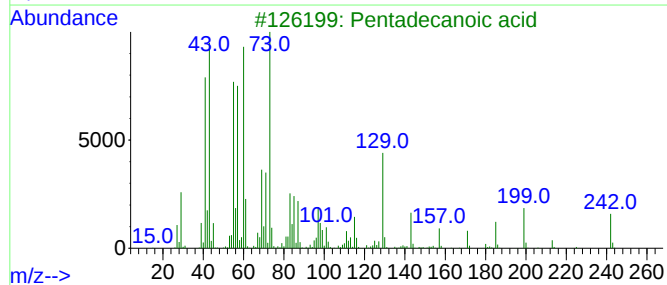
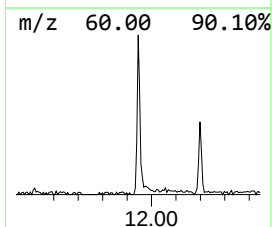
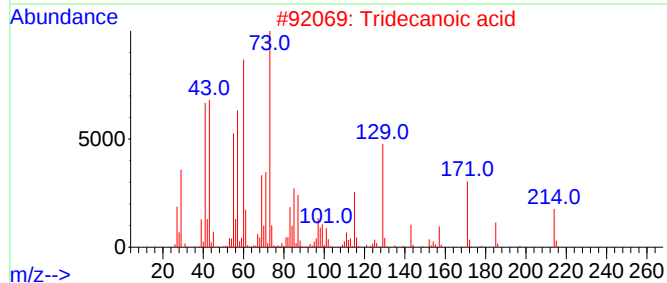
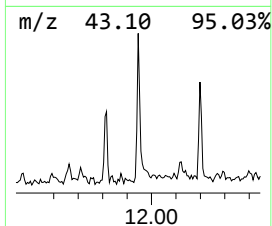
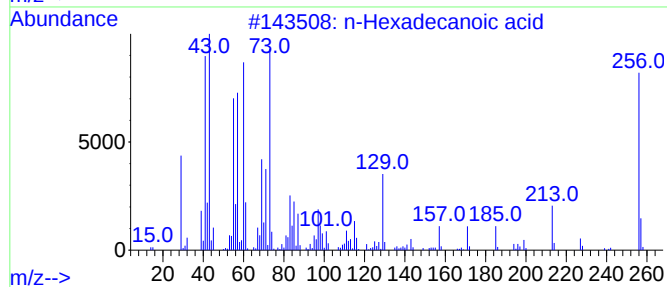
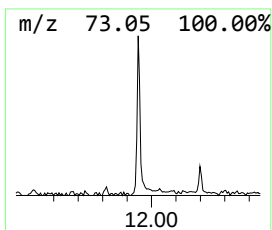
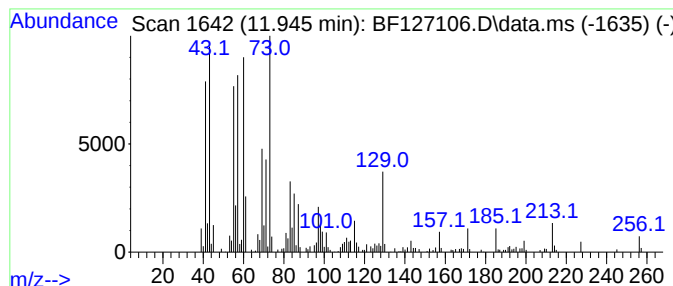
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.945	5.44 ng	217809	Phenanthrene-d10	11.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Octanoic acid	144	C8H16O2	000124-07-2	46



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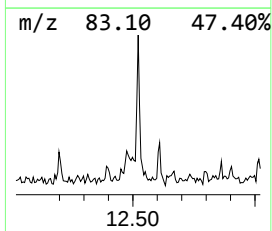
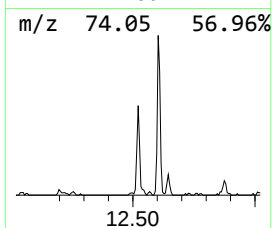
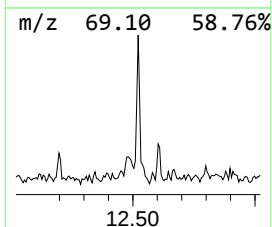
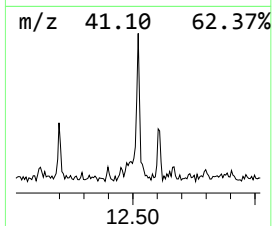
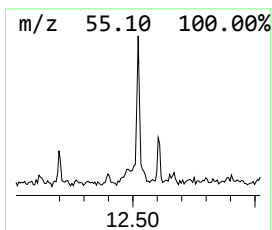
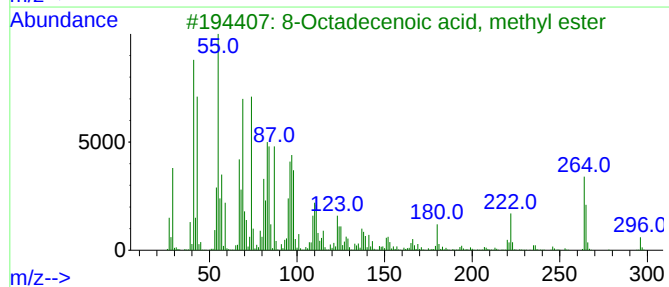
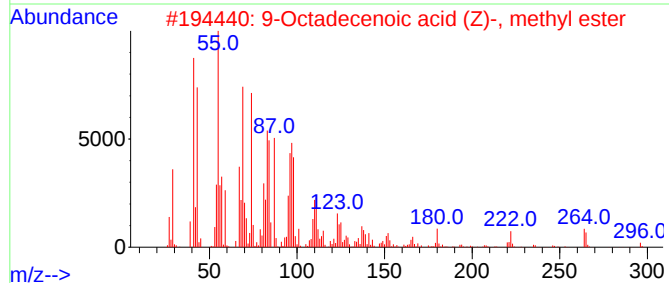
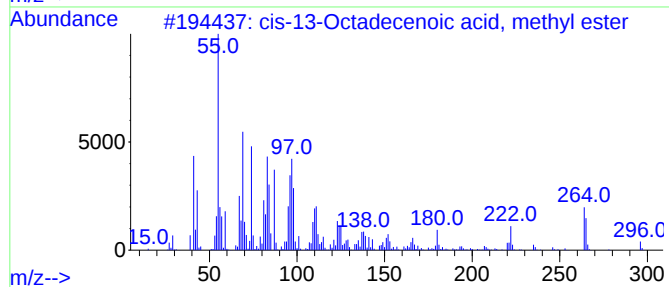
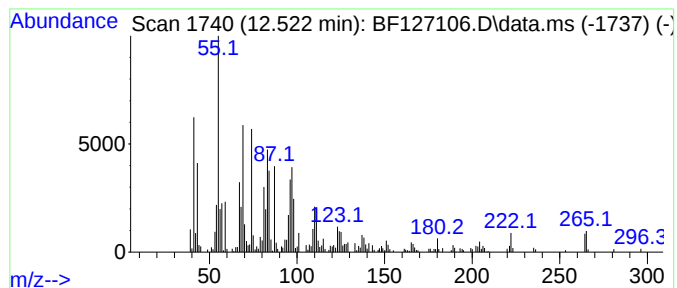
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 cis-13-Octadecenoic acid, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.522	4.21 ng	168368	Phenanthrene-d10	11.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
3	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127106.D
Acq On : 28 Feb 2022 18:13
Operator : CG\JU
Sample : N1664-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

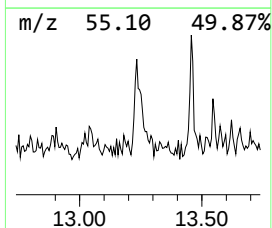
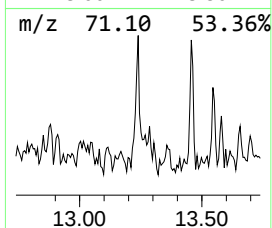
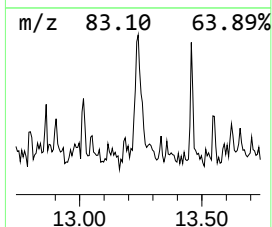
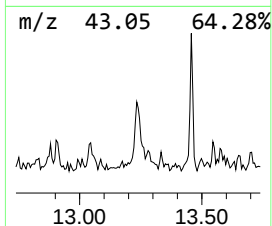
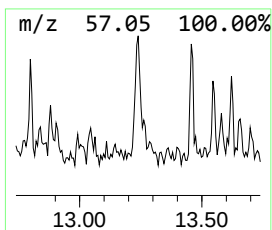
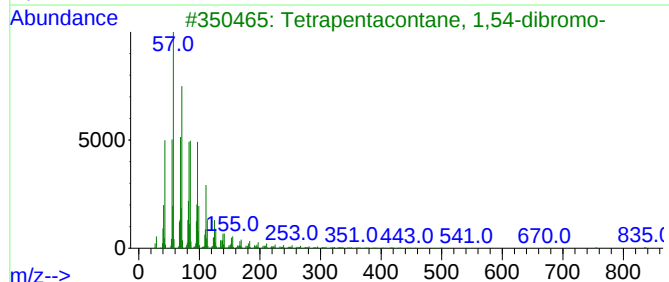
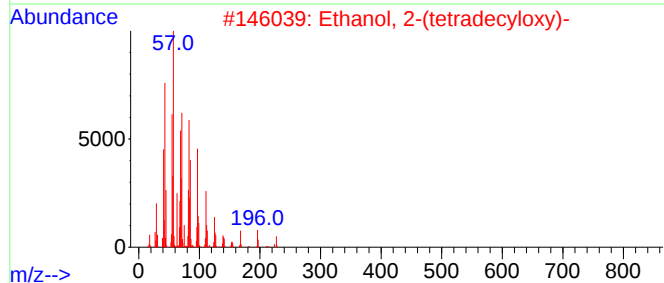
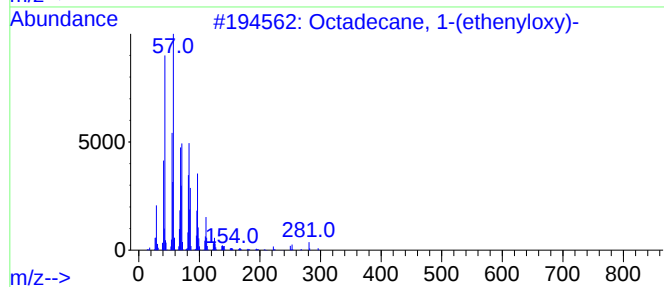
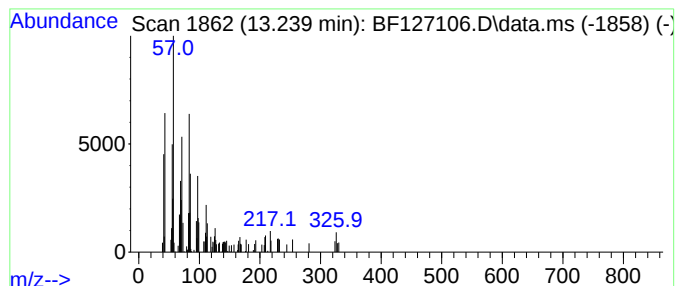
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane, 1-(ethenyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	2.05 ng	59423	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	80
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74
3			Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	70
4			Docosyl isobutyl ether	382	C26H54O	1000406-33-1	62
5			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127106.D
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Operator : CG\JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

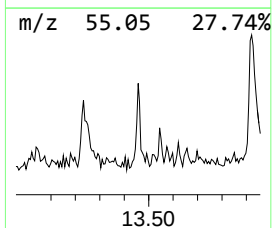
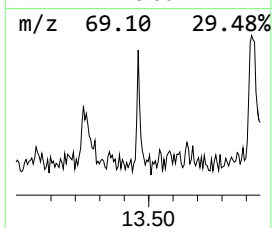
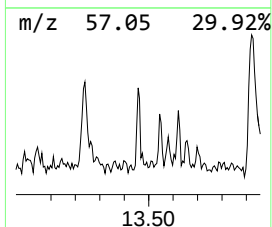
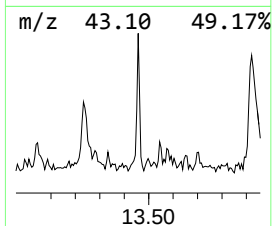
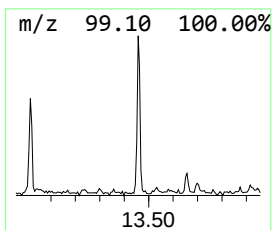
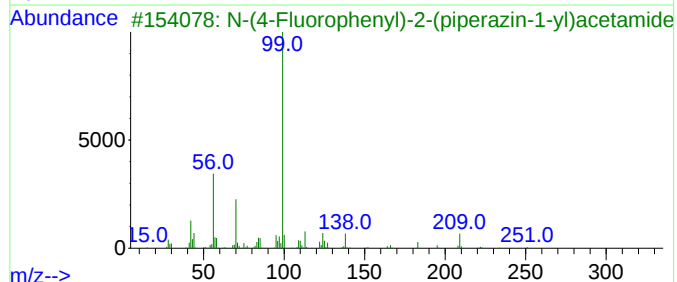
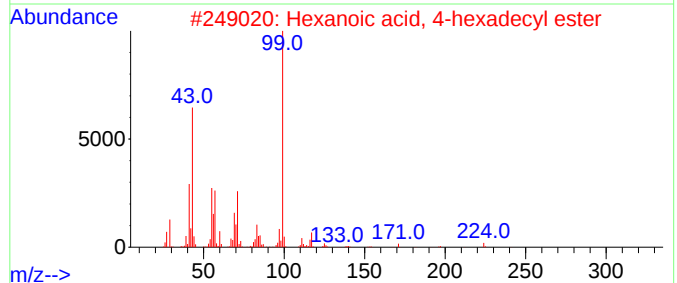
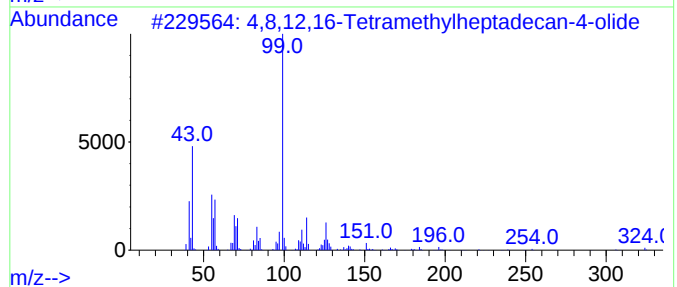
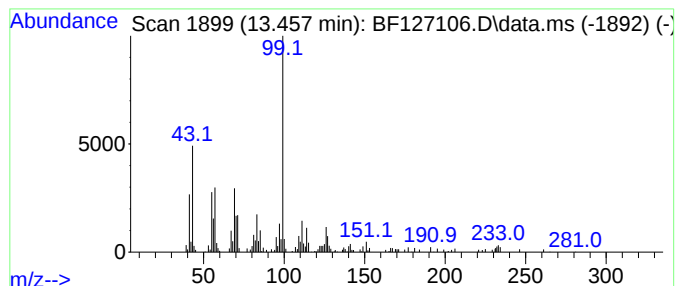
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4,8,12,16-Tetramethylheptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	3.59 ng	103977	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	87		
2	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	53		
3	N-(4-Fluorophenyl)-2-(piperazin-...	265	C14H20FN3O	1000502-16-3	52		
4	1-Isobutyl-3-methylbutyl methylp...	224	C10H22FO2P	193090-16-3	50		
5	Hexanoic acid, tridec-2-ynyl ester	294	C19H34O2	1000299-36-0	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

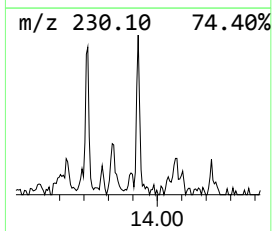
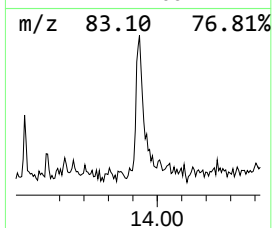
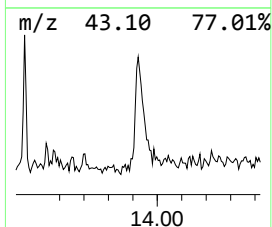
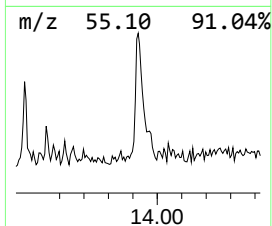
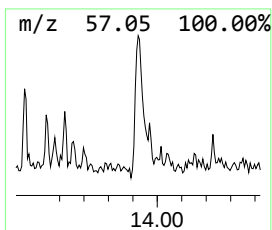
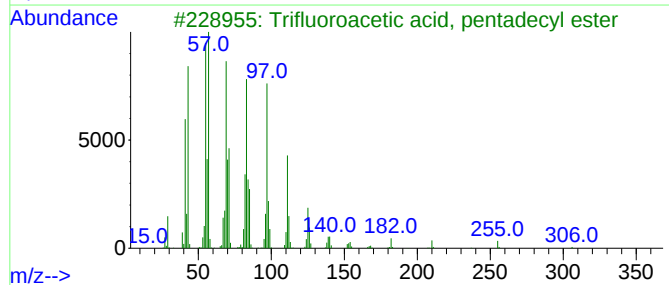
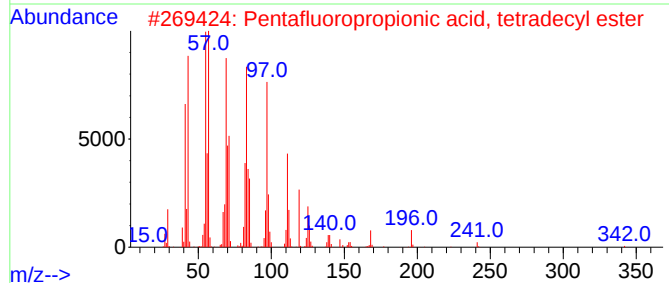
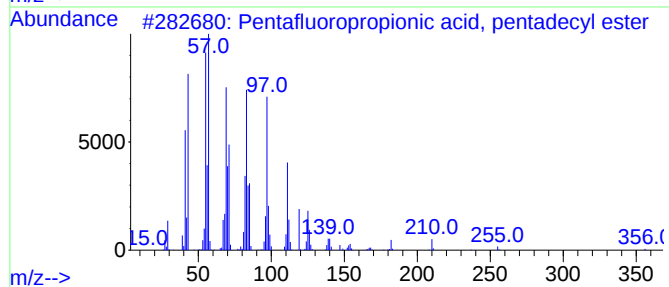
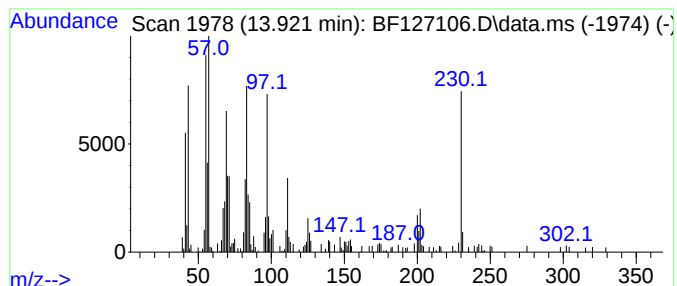
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	6.02 ng	174356	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83
2			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	83
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	83
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	83
5			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127106.D
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Sample : N1664-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-10

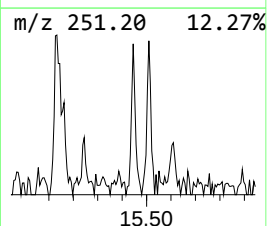
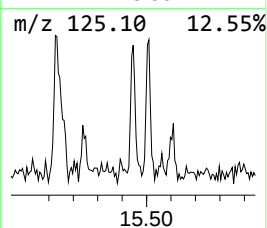
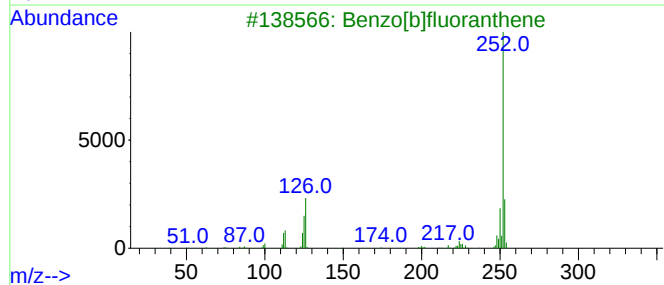
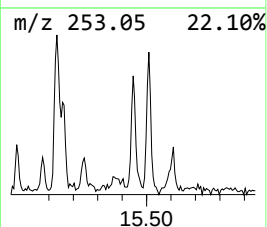
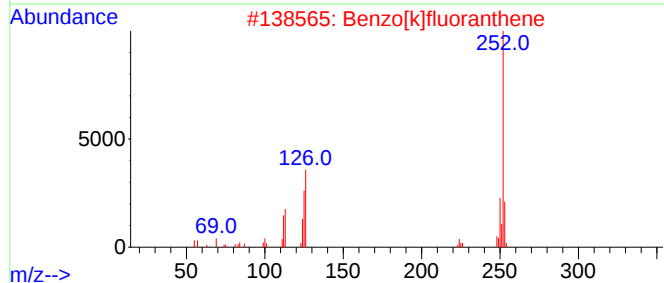
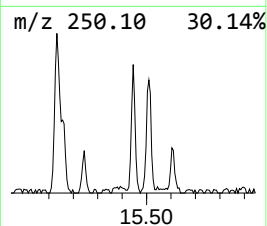
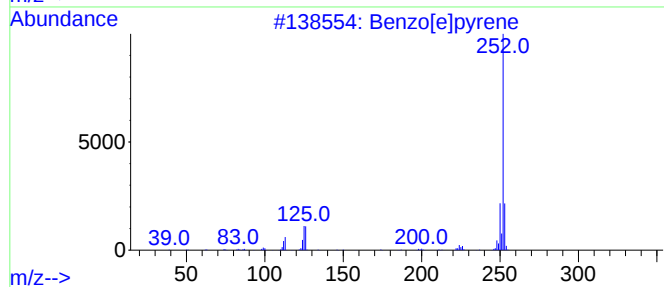
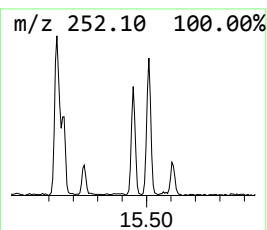
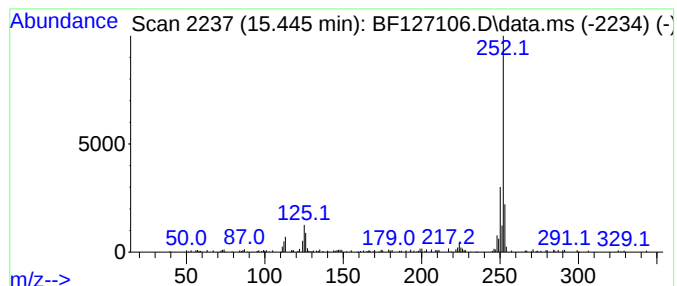
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	2.76 ng	77323	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[k]fluoranthene	252	C20H12	000207-08-9	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127106.D
Acq On : 28 Feb 2022 18:13
Operator : CG\JU
Sample : N1664-28
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-10

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	5.3	ng	219295	2	8.181	834189	20.0
2,4,7,9-Tetrame...	9.369	6.4	ng	277234	3	9.939	864405	20.0
Hexadecanoic ac...	11.816	2.0	ng	80901	4	11.433	800739	20.0
n-Hexadecanoic ...	11.945	5.4	ng	217809	4	11.433	800739	20.0
cis-13-Octadece...	12.522	4.2	ng	168368	4	11.433	800739	20.0
Octadecane, 1-(...	13.239	2.0	ng	59423	5	14.080	579679	20.0
4,8,12,16-Tetra...	13.457	3.6	ng	103977	5	14.080	579679	20.0
Pentafluoroprop...	13.922	6.0	ng	174356	5	14.080	579679	20.0
Benzo[e]pyrene	15.445	2.8	ng	77323	6	15.574	560484	20.0