

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
 Data File : BF142457.D
 Acq On : 19 May 2025 17:58
 Operator : RC/JU
 Sample : Q2062-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 L1-WC-3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF050525.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	487	496	505	rBV	134022	199837	8.72%	1.116%
2	5.510	558	564	584	rVB	1142872	1519628	66.28%	8.487%
3	6.522	730	736	741	rBV	1358303	1793871	78.24%	10.019%
4	6.904	795	801	806	rBV	491883	616124	26.87%	3.441%
5	7.463	890	896	901	rBV	787646	1024997	44.71%	5.725%
6	8.187	1013	1019	1034	rVB	631967	805391	35.13%	4.498%
7	9.257	1195	1201	1206	rBV	1853762	2266654	98.86%	12.660%
8	9.939	1311	1317	1326	rBV	716138	900146	39.26%	5.027%
9	10.651	1433	1438	1445	rBV	275383	342091	14.92%	1.911%
10	10.728	1445	1451	1464	rVV	1103037	1457803	63.58%	8.142%
11	10.957	1482	1490	1498	rBV	58308	75649	3.30%	0.423%
12	11.427	1564	1570	1578	rBV2	650753	975137	42.53%	5.446%
13	11.498	1578	1582	1586	rVB	19517	25351	1.11%	0.142%
14	11.945	1650	1658	1670	rBV3	165653	297370	12.97%	1.661%
15	12.039	1670	1674	1682	rVB	24677	52466	2.29%	0.293%
16	12.451	1738	1744	1746	rBV	16271	24609	1.07%	0.137%
17	12.639	1770	1776	1781	rBV	249979	326629	14.25%	1.824%
18	12.733	1788	1792	1797	rBV	17678	28480	1.24%	0.159%
19	12.863	1807	1814	1820	rBV	223988	330023	14.39%	1.843%
20	13.010	1830	1839	1844	rBV	1798308	2292722	100.00%	12.805%
21	13.086	1847	1852	1859	rVB5	14822	28427	1.24%	0.159%
22	13.298	1884	1888	1895	rVB2	17199	23128	1.01%	0.129%
23	13.580	1931	1936	1944	rBV7	11228	25660	1.12%	0.143%
24	13.698	1952	1956	1962	rVB	19903	27147	1.18%	0.152%
25	13.810	1970	1975	1978	rBV2	13364	25541	1.11%	0.143%
26	13.904	1987	1991	2002	rVB	88003	137047	5.98%	0.765%
27	14.063	2011	2018	2029	rVB2	577250	950992	41.48%	5.311%
28	14.227	2042	2046	2052	rBV3	16159	27757	1.21%	0.155%
29	14.533	2094	2098	2102	rBV4	27106	43697	1.91%	0.244%
30	14.827	2144	2148	2162	rVB2	53872	107818	4.70%	0.602%
31	15.115	2191	2197	2206	rBV	98361	240149	10.47%	1.341%
32	15.427	2245	2250	2256	rVB	53089	83100	3.62%	0.464%
33	15.486	2256	2260	2266	rVV	67054	105887	4.62%	0.591%
34	15.557	2266	2272	2286	rVB	349407	596146	26.00%	3.330%
35	17.057	2521	2527	2535	rVB2	31472	72861	3.18%	0.407%
36	17.504	2598	2603	2611	rVB	24471	54206	2.36%	0.303%

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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-BF050525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

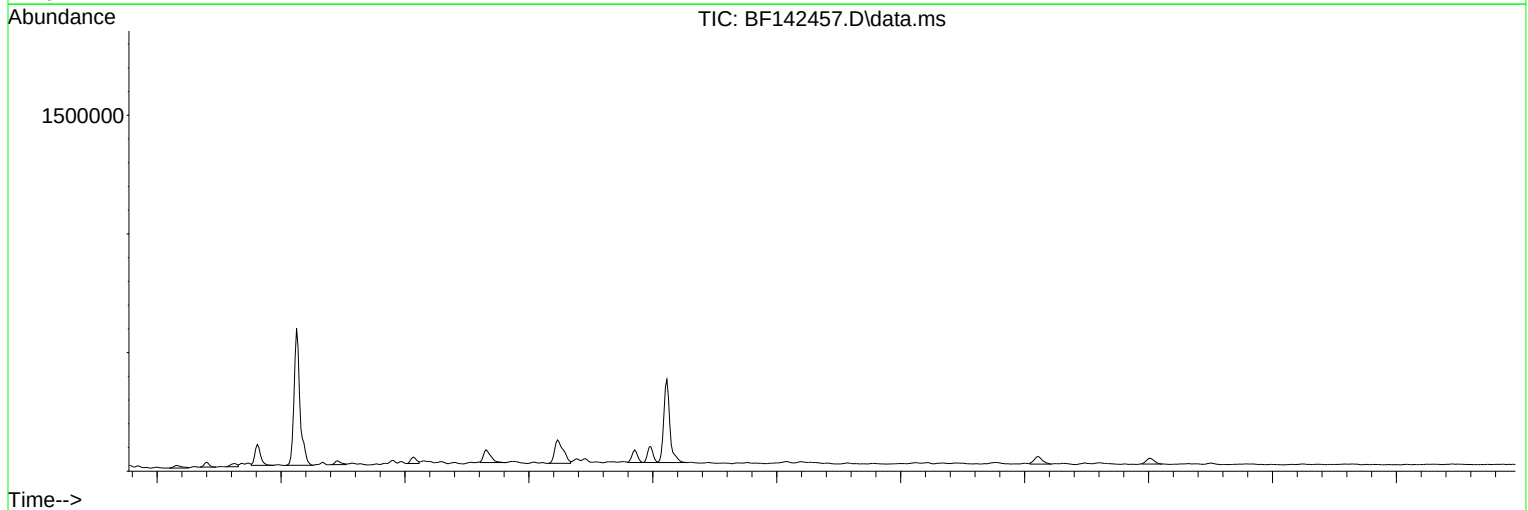
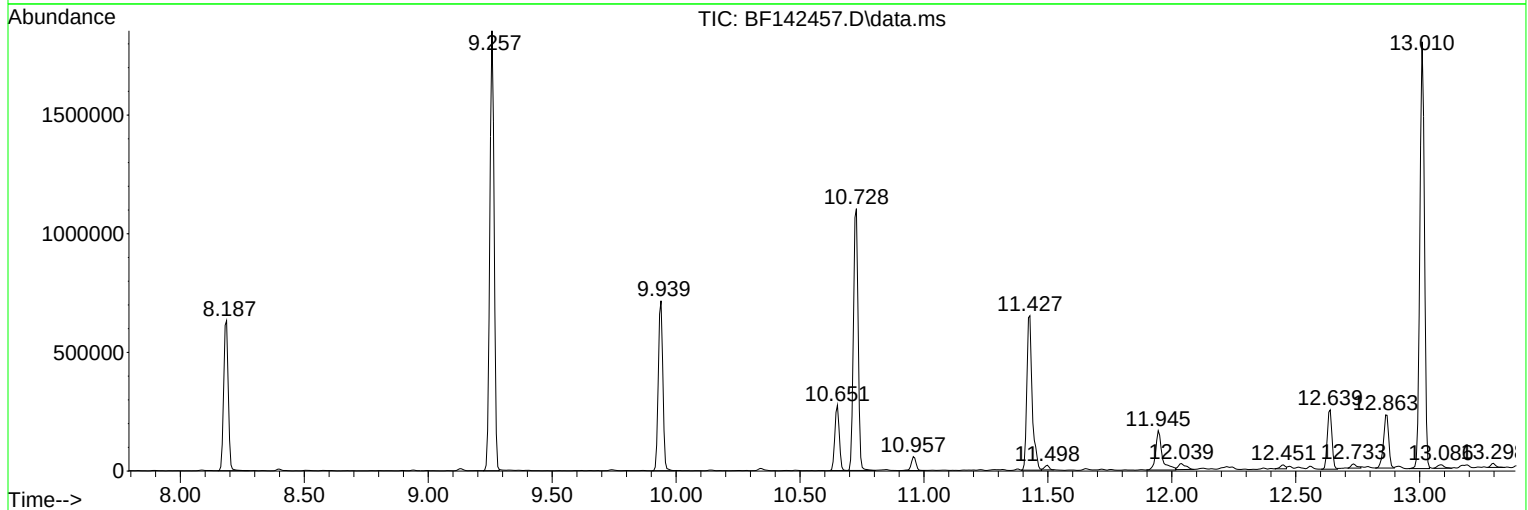
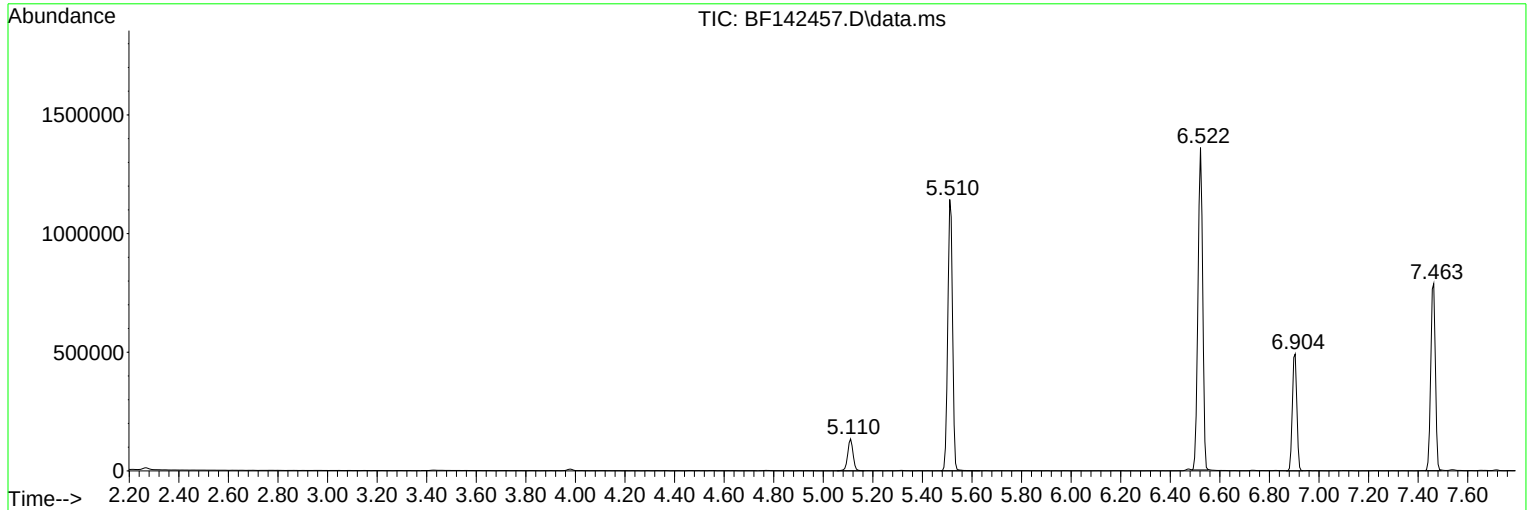
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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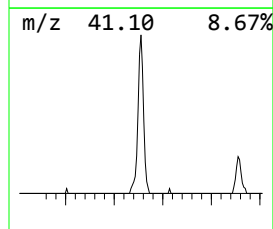
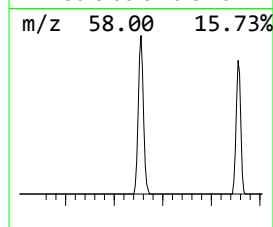
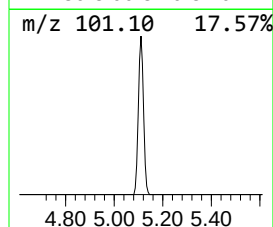
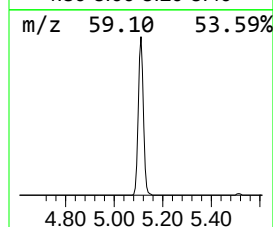
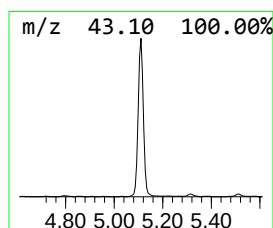
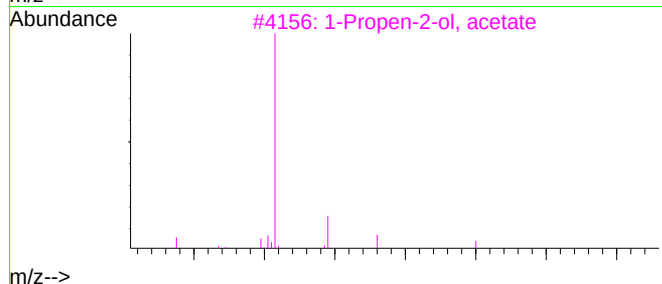
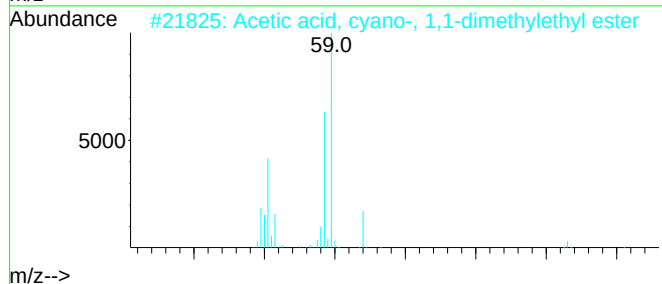
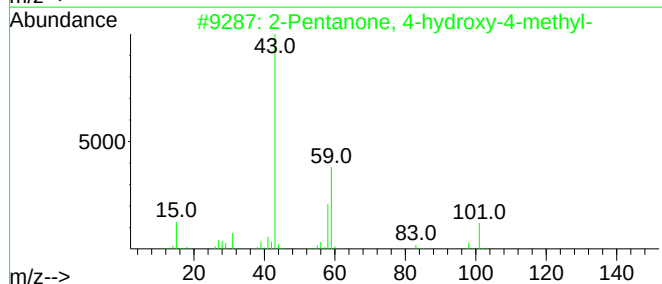
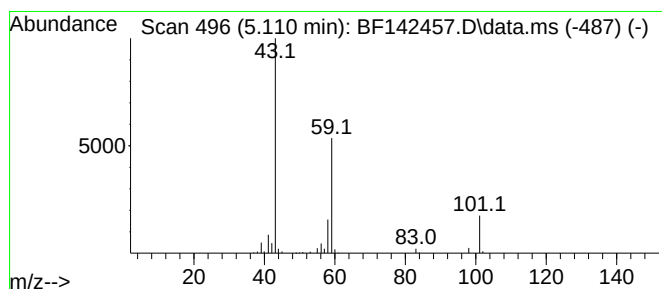
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.110	6.49 ng	199837	1,4-Dichlorobenzene-d4	6.904	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

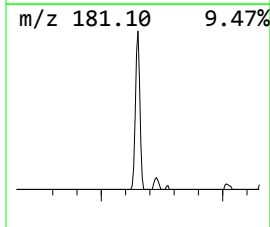
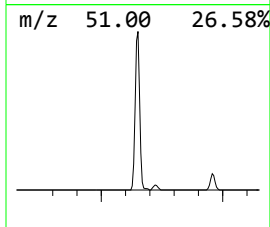
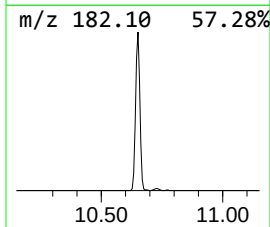
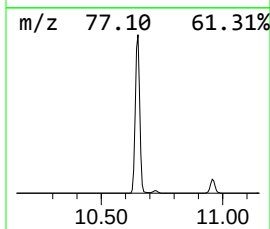
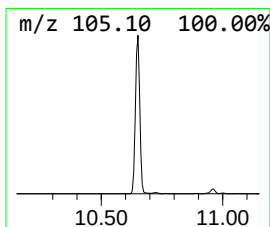
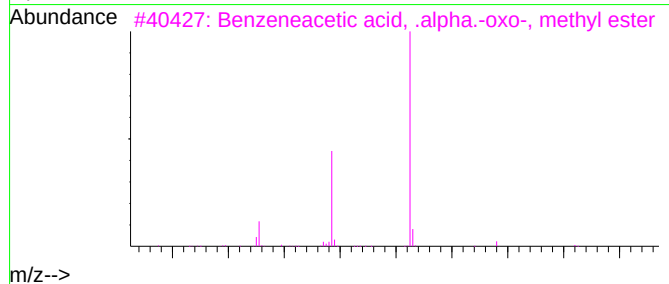
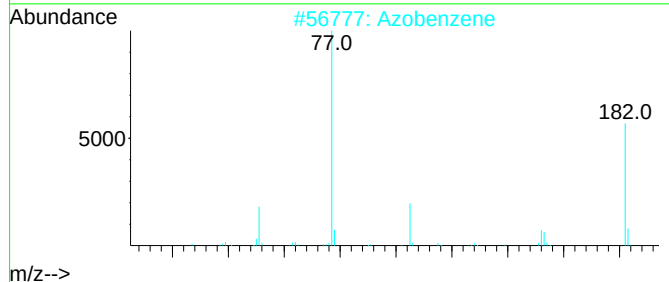
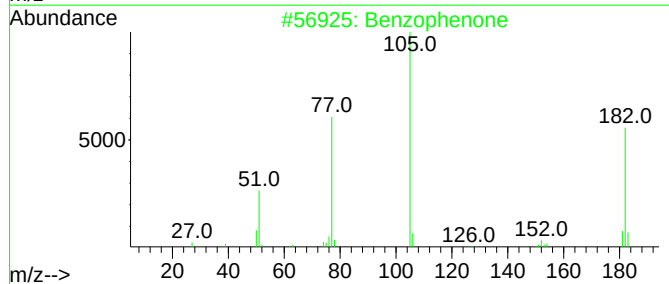
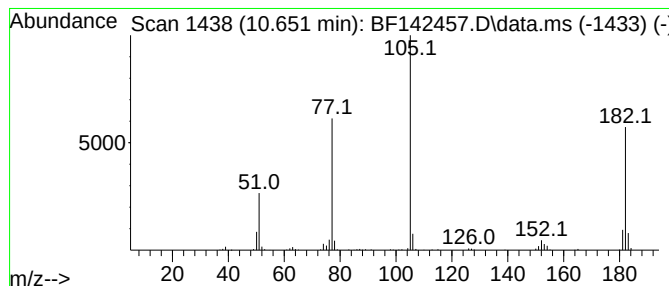
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	7.60 ng	342091	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49



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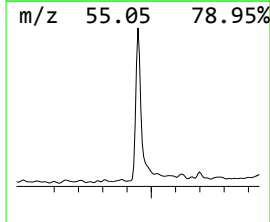
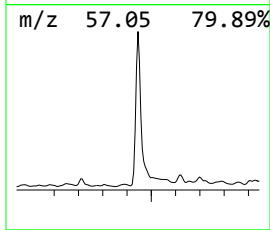
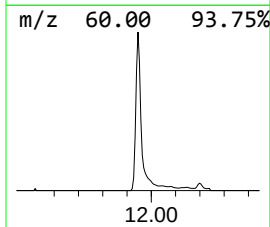
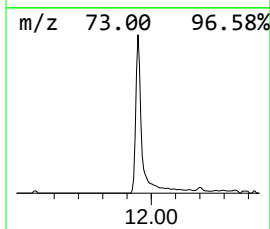
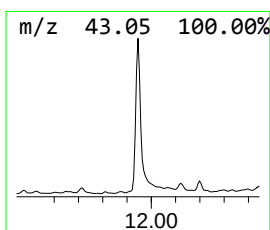
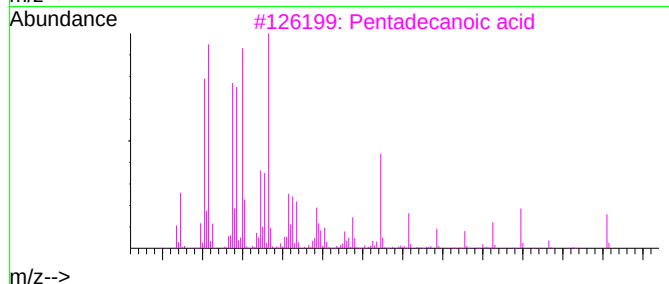
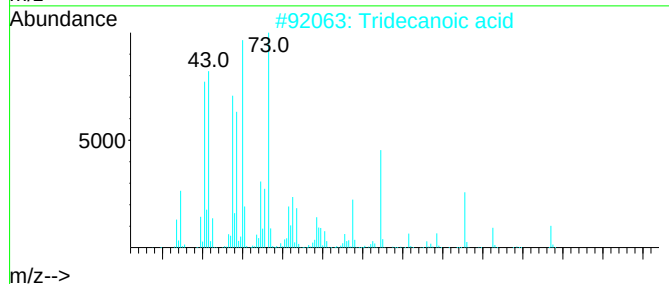
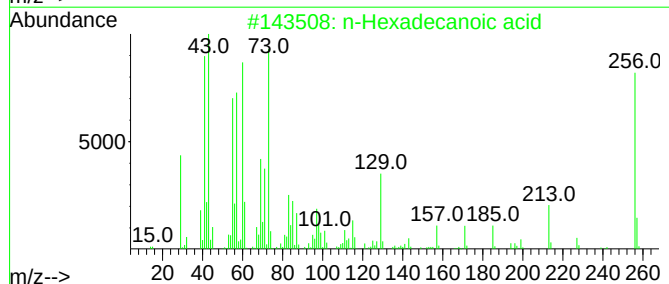
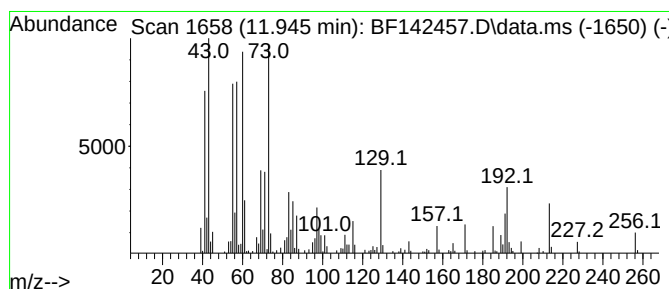
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.945	6.10 ng	297370	Phenanthrene-d10	11.428	
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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
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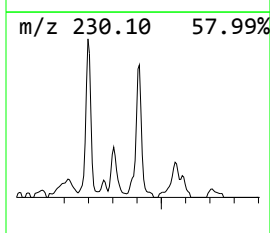
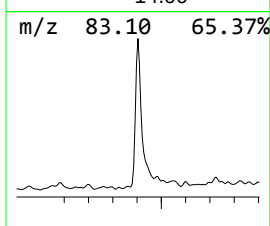
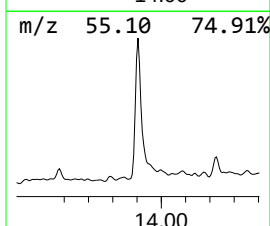
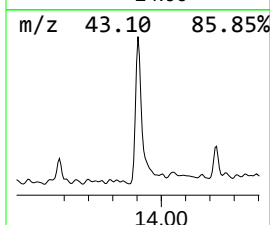
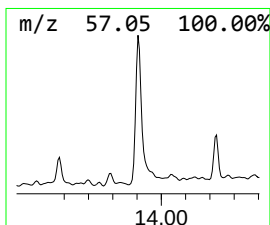
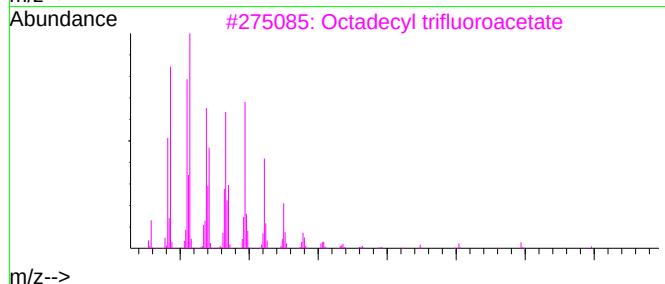
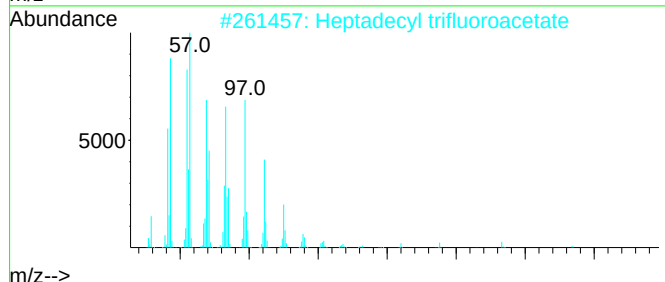
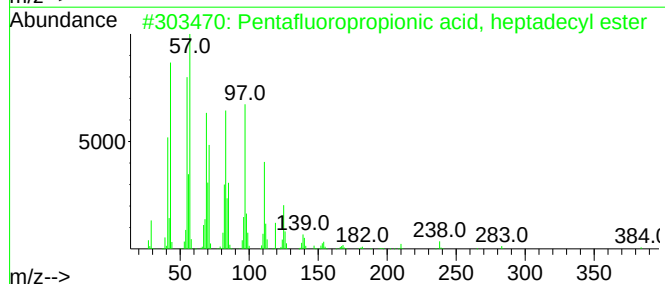
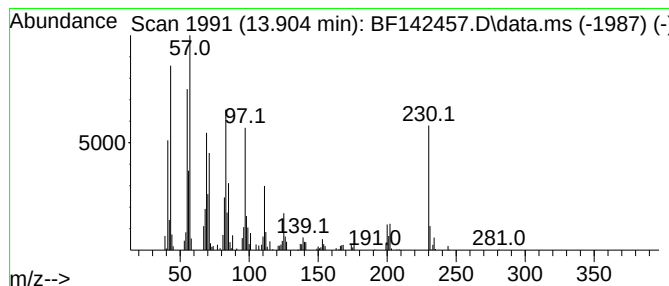
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.88 ng	137047	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83



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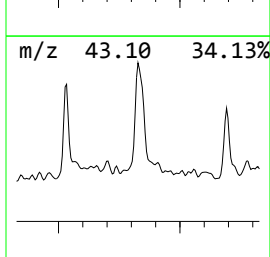
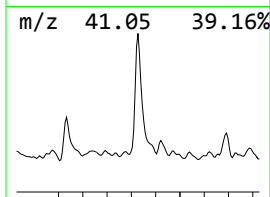
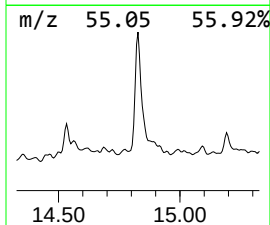
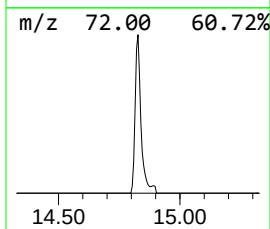
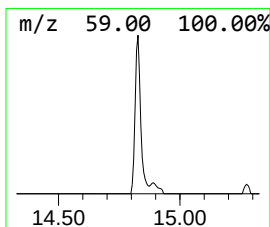
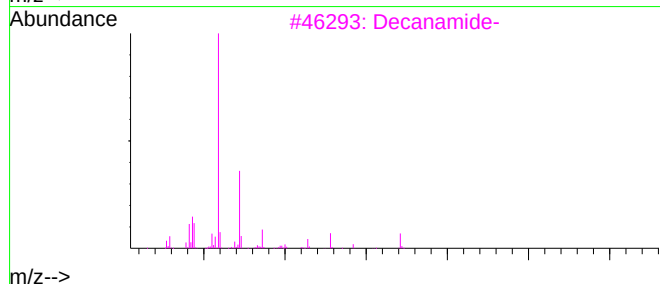
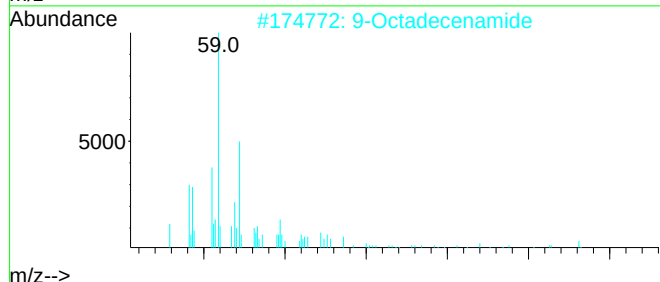
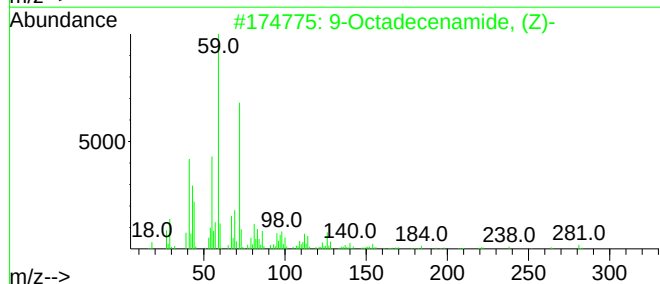
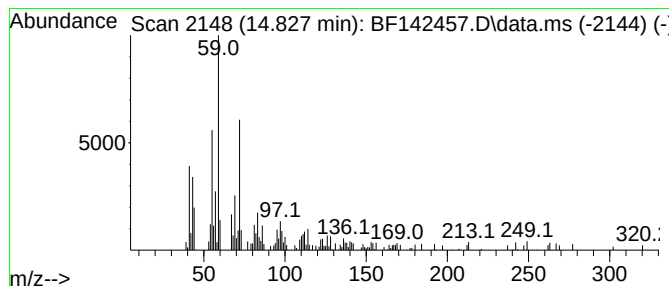
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.827	3.62 ng	107818	Perylene-d12	15.557	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	9-Octadecenamide	281	C18H35NO	003322-62-1	72
3	Decanamide-	171	C10H21NO	002319-29-1	59
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
5	Palmitoleamide	253	C16H31NO	106010-22-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142457.D
Acq On : 19 May 2025 17:58
Operator : RC/JU
Sample : Q2062-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L1-WC-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

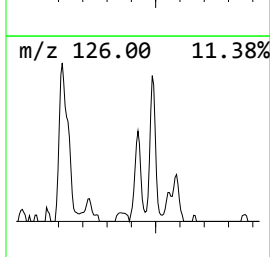
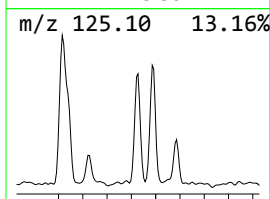
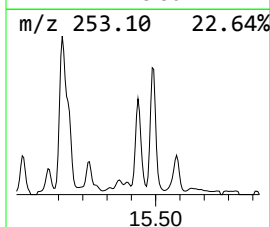
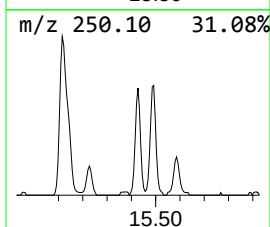
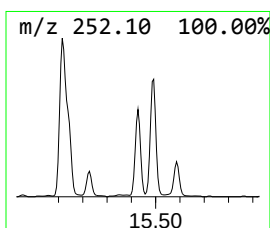
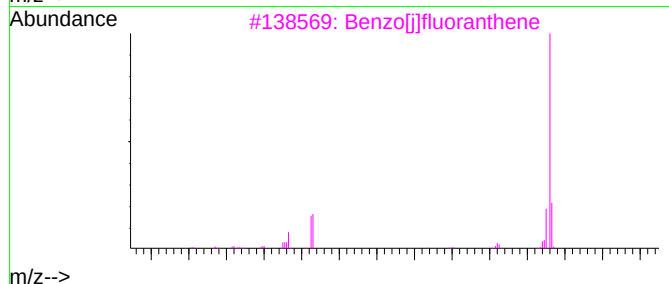
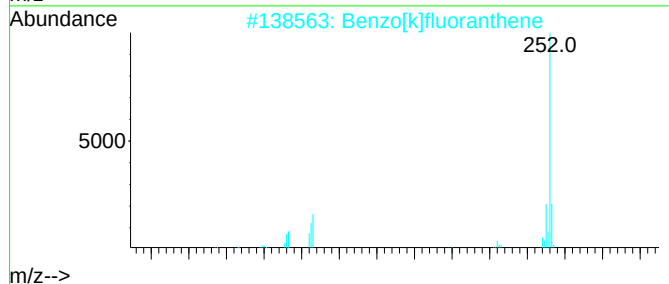
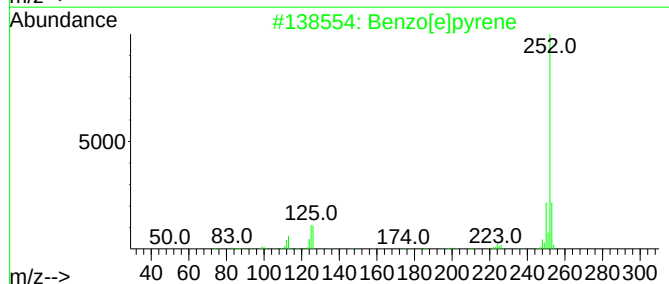
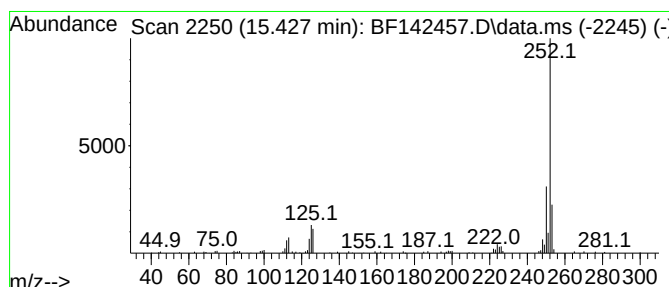
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	2.79 ng	83100	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142457.D
Acq On : 19 May 2025 17:58
Operator : RC/JU
Sample : Q2062-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L1-WC-3

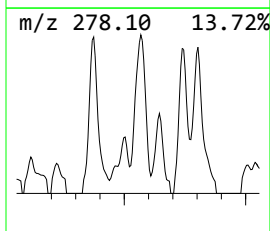
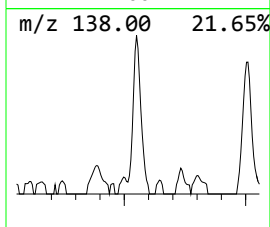
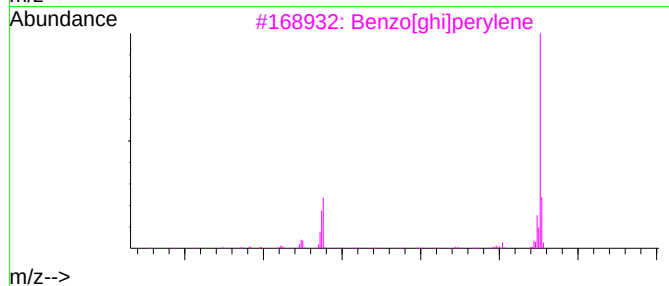
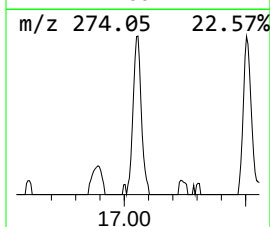
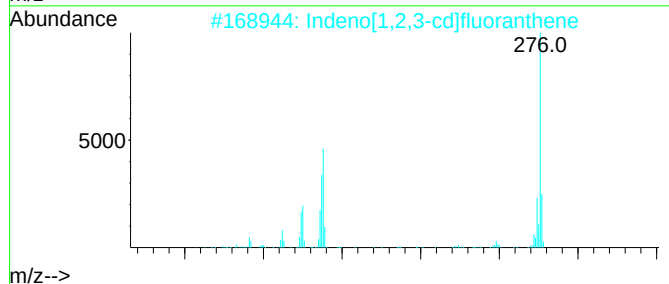
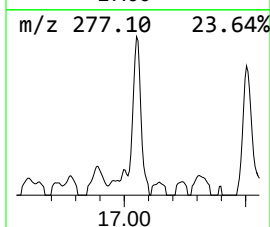
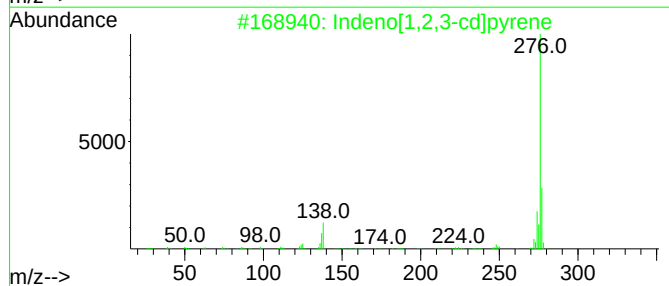
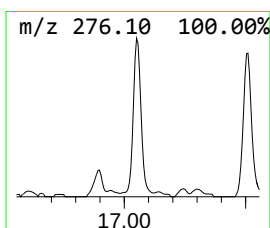
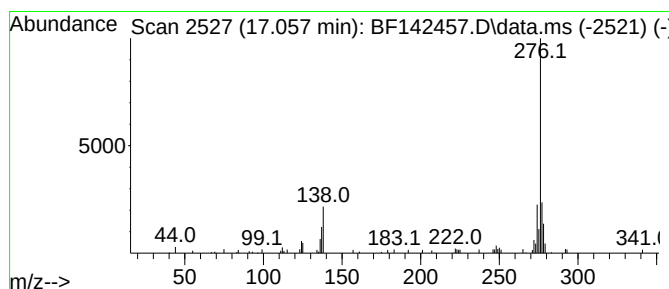
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Indeno[1,2,3-cd]fluoranthene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.057	2.44 ng	72861	Perylene-d12	15.557	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	97
2	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	93
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	93
4	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	76
5	2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142457.D
Acq On : 19 May 2025 17:58
Operator : RC/JU
Sample : Q2062-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L1-WC-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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
2-Pentanone, 4-...	5.110	6.5	ng	199837	1	6.904	616124	20.0
Benzophenone	10.651	7.6	ng	342091	3	9.939	900146	20.0
n-Hexadecanoic ...	11.945	6.1	ng	297370	4	11.428	975137	20.0
Pentafluoroprop...	13.904	2.9	ng	137047	5	14.063	950992	20.0
9-Octadecenamid...	14.827	3.6	ng	107818	6	15.557	596146	20.0
Benzo[e]pyrene	15.427	2.8	ng	83100	6	15.557	596146	20.0
Indeno[1,2,3-cd...	17.057	2.4	ng	72861	6	15.557	596146	20.0