

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135281.D
 Acq On : 15 Sep 2023 16:11
 Operator : CG\JU
 Sample : 04409-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2(0-2)COMP

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB	39927	50565	1.92%	0.223%
2	4.993	490	494	502	rVB	86969	109265	4.15%	0.481%
3	5.392	557	562	565	rBV	2584976	2443806	92.87%	10.766%
4	6.398	728	733	736	rBV	2262679	2363142	89.80%	10.410%
5	6.592	762	766	780	rBV	81736	94766	3.60%	0.417%
6	6.757	790	794	799	rBV	800049	638981	24.28%	2.815%
7	7.322	885	890	893	rBV	1668552	1509337	57.36%	6.649%
8	8.034	1007	1011	1015	rBV	973528	896132	34.05%	3.948%
9	9.057	1183	1185	1190	rVB	37380	34666	1.32%	0.153%
10	9.116	1190	1195	1198	rBV	2999895	2631431	100.00%	11.592%
11	9.192	1204	1208	1211	rBV3	25361	36744	1.40%	0.162%
12	9.239	1211	1216	1219	rBV	1453444	1413233	53.71%	6.226%
13	9.386	1237	1241	1244	rBV4	43054	42652	1.62%	0.188%
14	9.498	1254	1260	1261	rBV3	25788	29242	1.11%	0.129%
15	9.516	1261	1263	1266	rVB	55716	44097	1.68%	0.194%
16	9.657	1284	1287	1292	rBV5	21588	30594	1.16%	0.135%
17	9.792	1304	1310	1313	rBV	1060880	909159	34.55%	4.005%
18	9.992	1341	1344	1350	rVB5	25642	36770	1.40%	0.162%
19	10.451	1417	1422	1428	rBV	62434	77455	2.94%	0.341%
20	10.586	1441	1445	1448	rBV	1803367	1555617	59.12%	6.853%
21	10.716	1462	1467	1472	rBV	126745	156710	5.96%	0.690%
22	10.757	1472	1474	1480	rVV2	24767	36851	1.40%	0.162%
23	10.869	1490	1493	1500	rBV	38991	53366	2.03%	0.235%
24	10.933	1501	1504	1508	rVV2	34966	34977	1.33%	0.154%
25	11.157	1540	1542	1544	rBV	41458	32115	1.22%	0.141%
26	11.186	1544	1547	1554	rVB	71675	80416	3.06%	0.354%
27	11.286	1560	1564	1566	rBV	1083420	907351	34.48%	3.997%
28	11.310	1566	1568	1571	rVV	194852	149343	5.68%	0.658%
29	11.357	1573	1576	1580	rVB	53459	54578	2.07%	0.240%
30	11.586	1612	1615	1617	rVB	40306	35524	1.35%	0.156%
31	11.686	1629	1632	1638	rVB2	36947	34869	1.33%	0.154%
32	11.821	1651	1655	1661	rBV	454108	442398	16.81%	1.949%
33	11.904	1666	1669	1672	rVB	40297	37398	1.42%	0.165%
34	12.398	1747	1753	1756	rBV2	105632	129269	4.91%	0.569%
35	12.504	1768	1771	1775	rVV	302282	231343	8.79%	1.019%
36	12.545	1775	1778	1781	rVB2	72405	60800	2.31%	0.268%

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Start Thrs: 0.2

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37	12.610	1786	1789	1795	rBV	123363	152276	5.79%	0.671%
38	12.733	1804	1810	1813	rBV	236055	253774	9.64%	1.118%
39	12.886	1831	1836	1839	rBV	2174593	1969504	74.85%	8.676%
40	13.068	1864	1867	1871	rVB	35620	36187	1.38%	0.159%
41	13.121	1872	1876	1877	rBV	31394	34746	1.32%	0.153%
42	13.374	1913	1919	1927	rVB	409995	427568	16.25%	1.884%
43	13.463	1930	1934	1937	rBV2	22753	29511	1.12%	0.130%
44	13.804	1987	1992	2006	rVB4	109292	257713	9.79%	1.135%
45	13.945	2008	2016	2018	rBV2	661399	733104	27.86%	3.230%
46	13.968	2018	2020	2023	rVB	97079	77559	2.95%	0.342%
47	14.421	2094	2097	2100	rBV2	39182	42248	1.61%	0.186%
48	14.727	2146	2149	2152	rBV2	41591	45138	1.72%	0.199%
49	14.980	2188	2192	2196	rBV	97745	146430	5.56%	0.645%
50	15.068	2203	2207	2209	rBV	41056	46825	1.78%	0.206%
51	15.286	2240	2244	2249	rVB	55194	71738	2.73%	0.316%
52	15.345	2250	2254	2259	rVB	85944	107421	4.08%	0.473%
53	15.409	2260	2265	2269	rBV	539073	664740	25.26%	2.928%
54	15.886	2342	2346	2351	rBV3	28878	43519	1.65%	0.192%
55	16.880	2510	2515	2523	rBV2	39236	85844	3.26%	0.378%
56	17.333	2587	2592	2597	rVB2	25861	49252	1.87%	0.217%

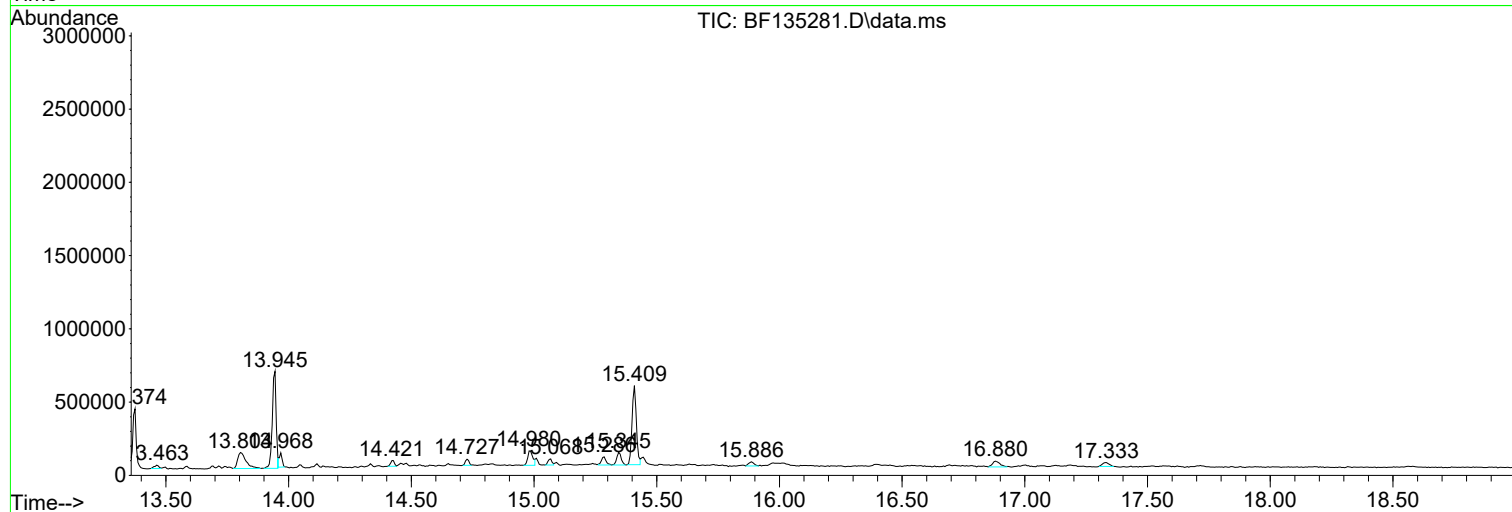
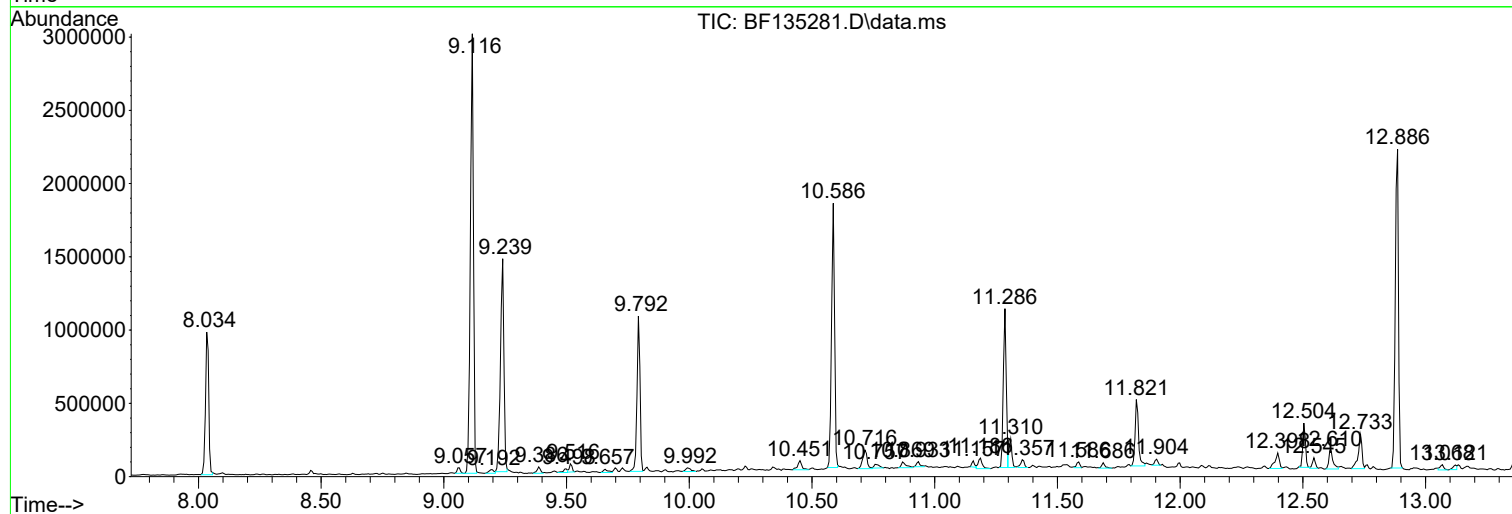
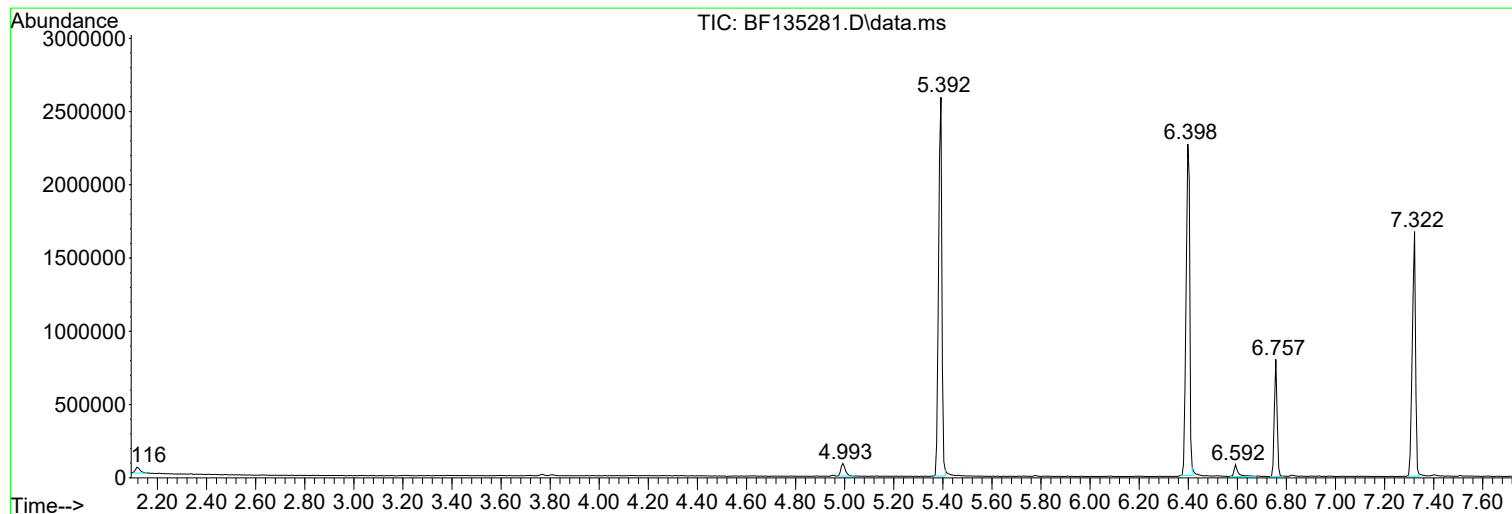
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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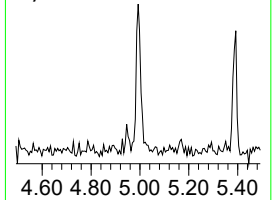
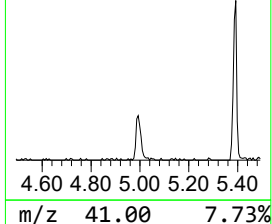
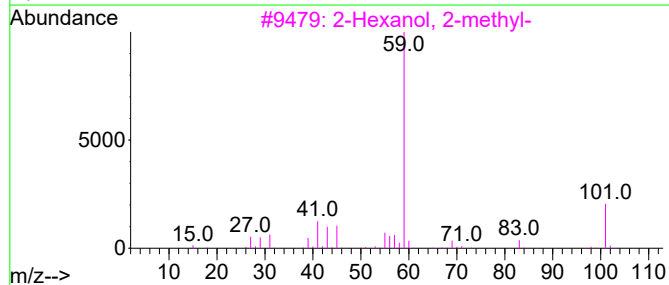
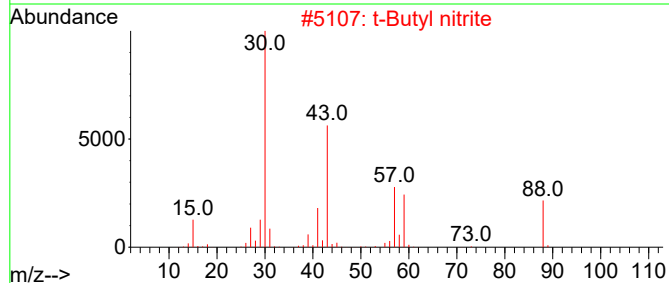
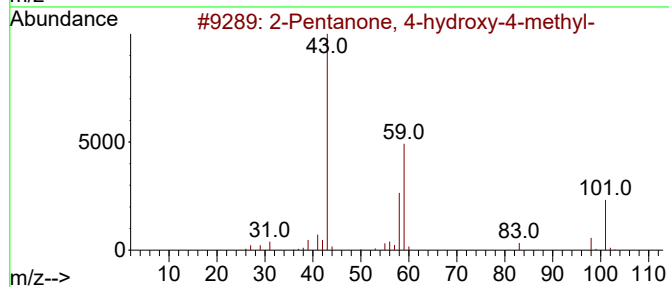
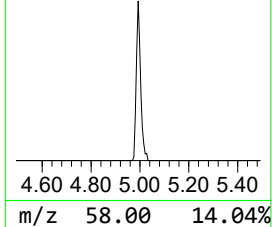
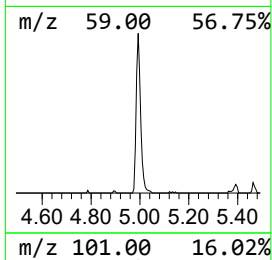
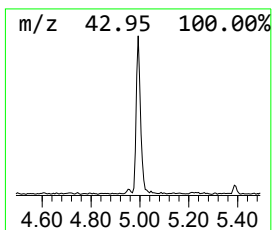
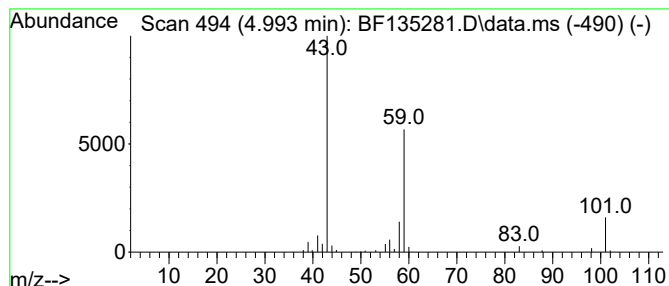
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	3.42 ng	109265	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	56		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		



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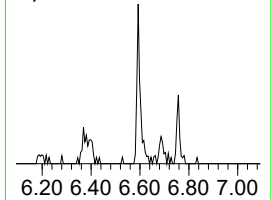
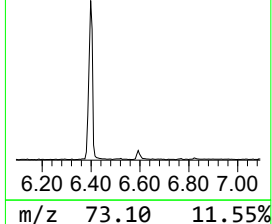
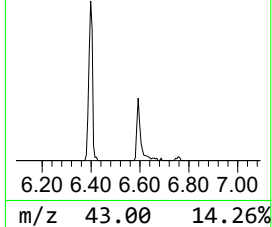
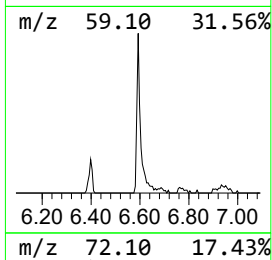
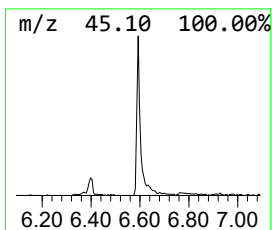
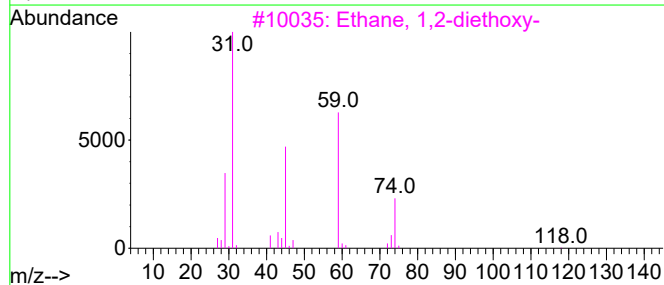
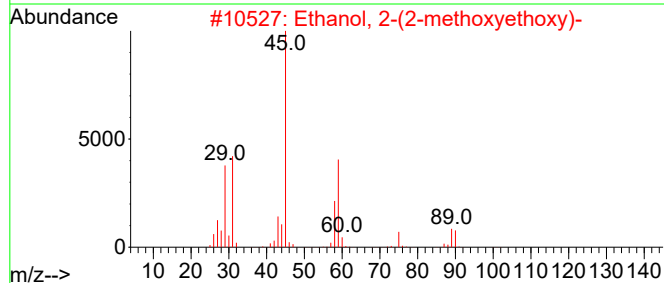
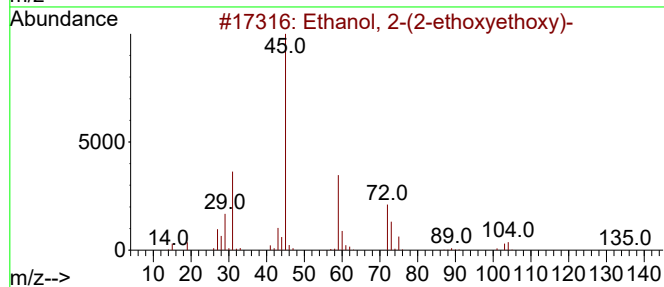
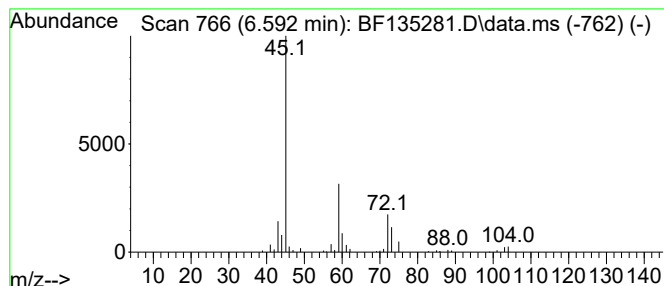
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	2.97 ng	94766	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	59
3			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	45
4			Ethanol, 2-[2-(2-propenyloxy)eth...]	146	C7H14O3	015075-50-0	42
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38



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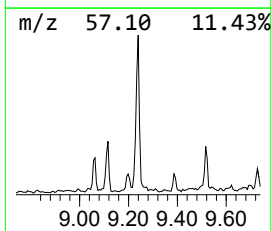
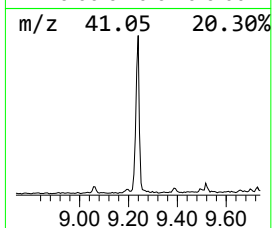
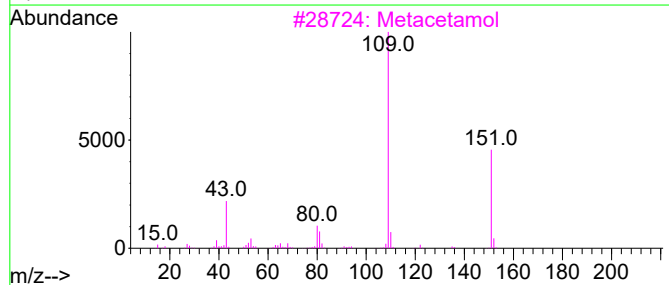
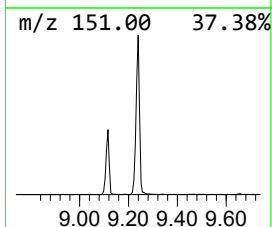
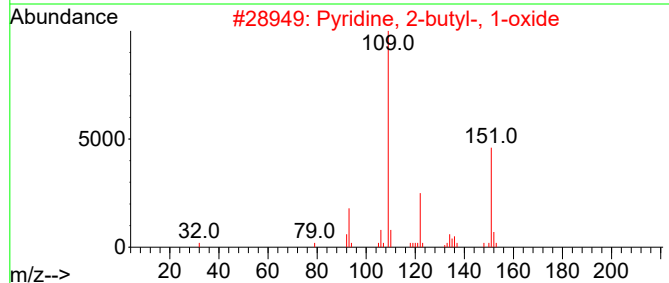
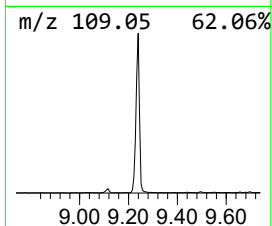
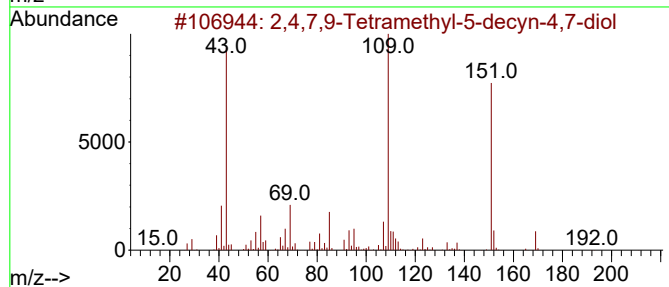
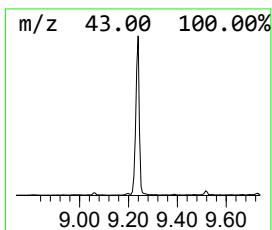
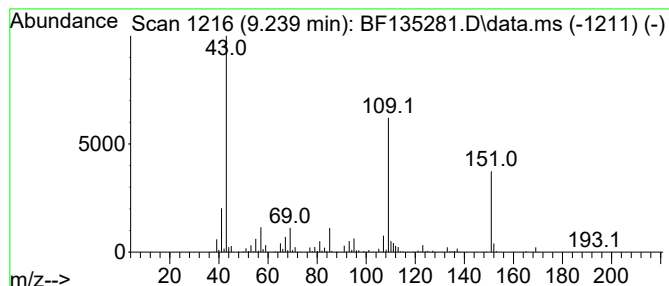
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.239	31.09 ng	1413230	Acenaphthene-d10			9.792
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	53
3	Metacetamol		151	C8H9NO2	000621-42-1	47
4	Acetaminophen		151	C8H9NO2	000103-90-2	47
5	m-Isopropoxyaniline		151	C9H13NO	041406-00-2	47



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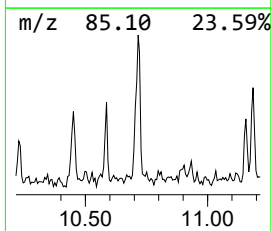
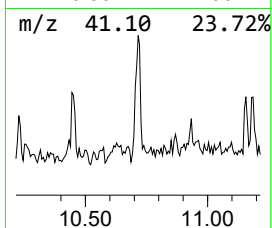
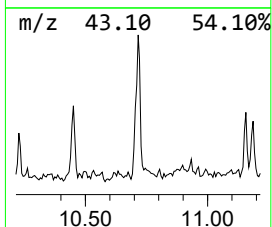
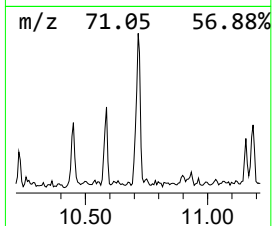
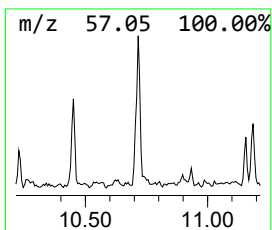
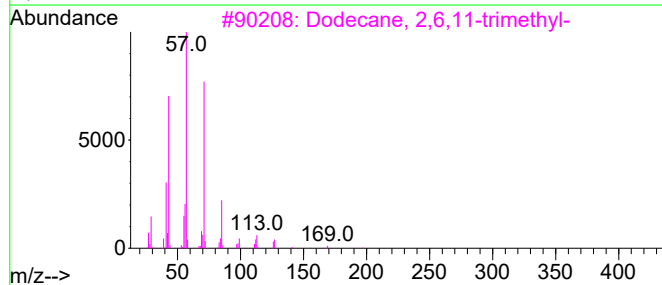
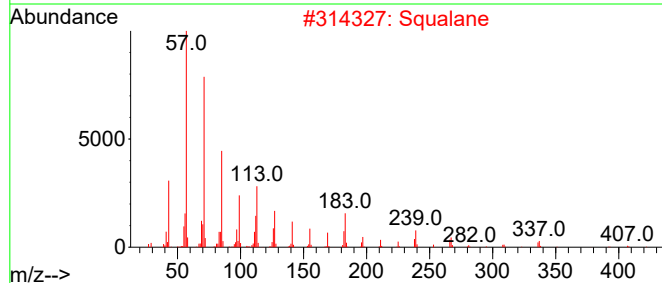
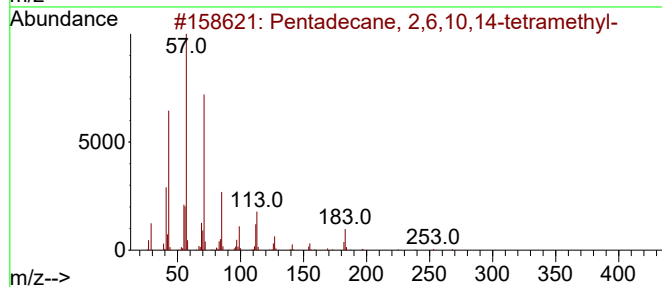
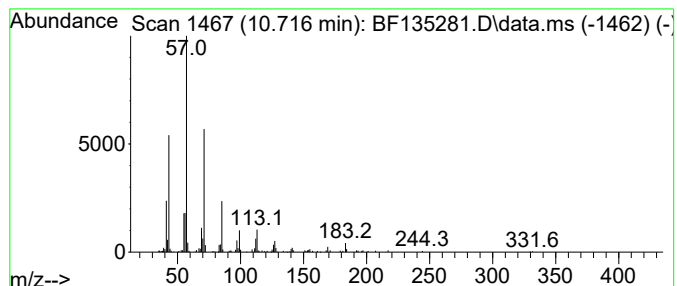
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecane, 2,6,10,14-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.716	3.45 ng	156710	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	83
2			Squalane	422	C30H62	000111-01-3	78
3			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
4			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64
5			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64



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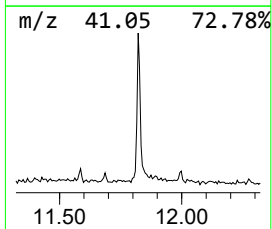
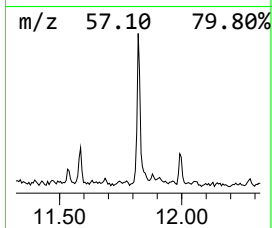
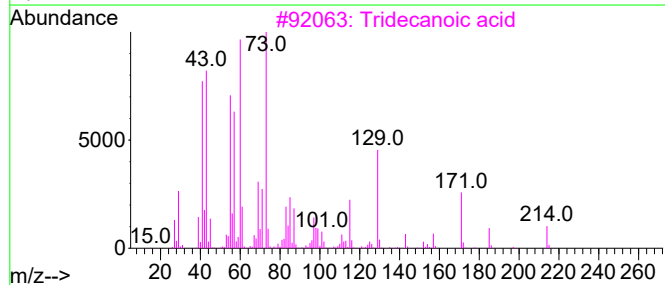
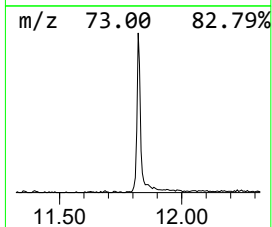
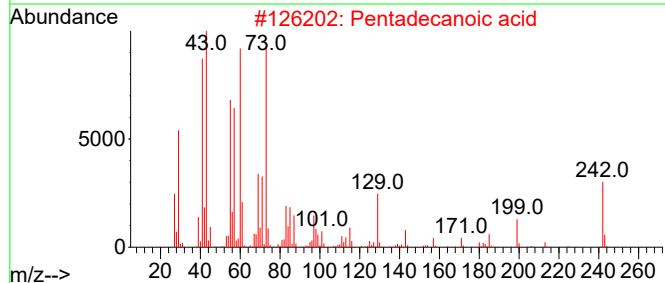
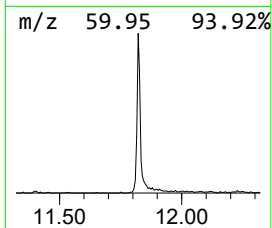
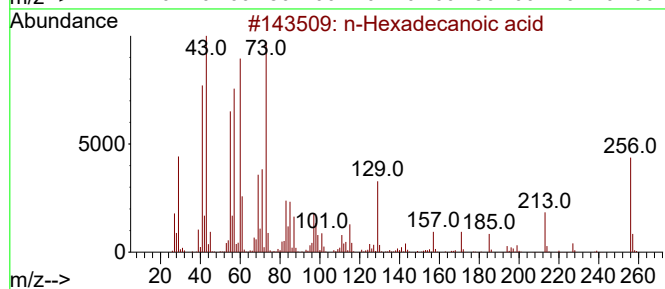
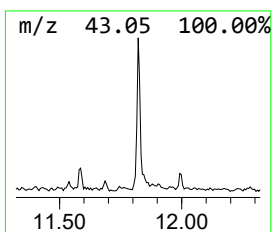
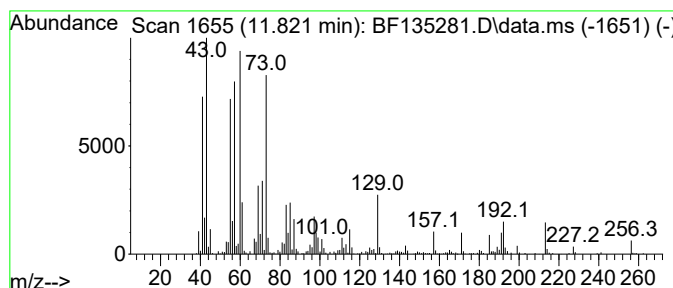
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	9.75 ng	442398	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Isopropyl palmitate	298	C19H38O2	000142-91-6	58
5			Octanoic acid	144	C8H16O2	000124-07-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135281.D
Acq On : 15 Sep 2023 16:11
Operator : CG\JU
Sample : 04409-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

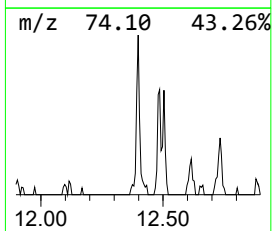
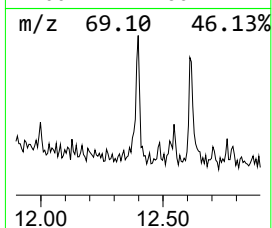
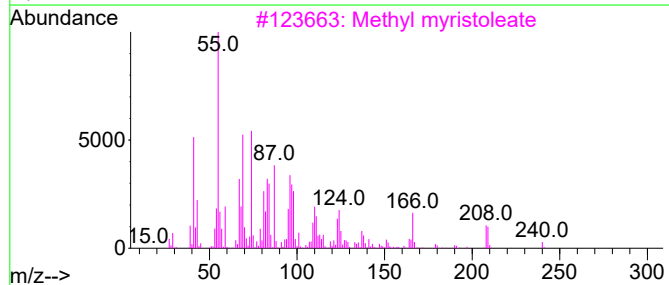
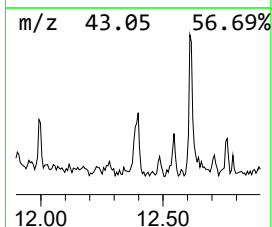
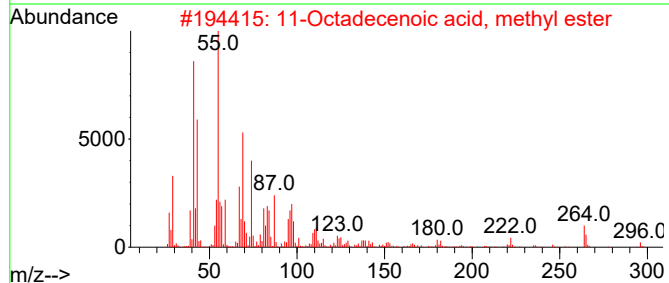
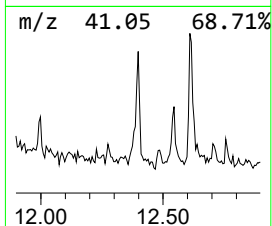
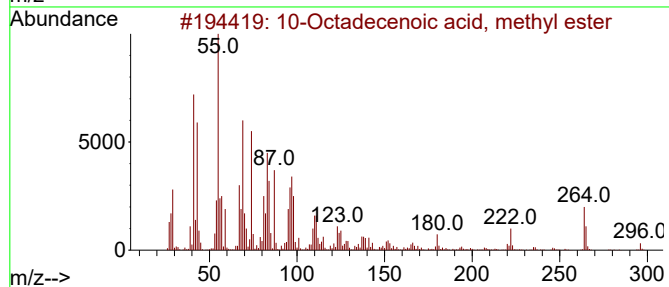
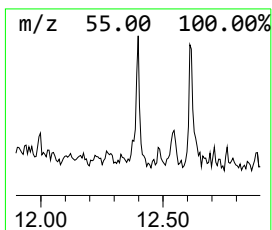
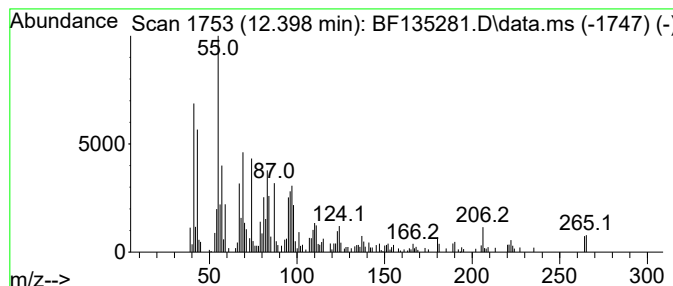
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WC-2(0-2)COMP

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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 10-Octadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.398	2.85 ng	129269	Phenanthrene-d10	11.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87
3	Methyl myristoleate	240	C15H28O2	056219-06-8	87
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
5	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135281.D
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Sample : 04409-04
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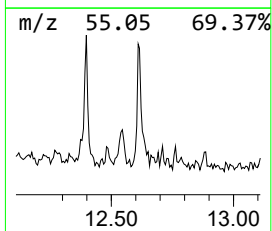
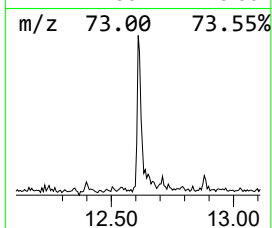
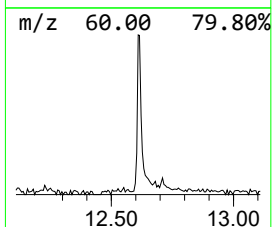
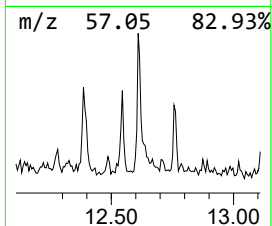
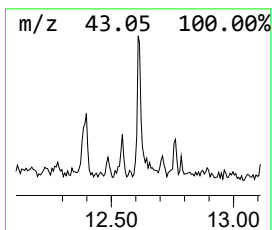
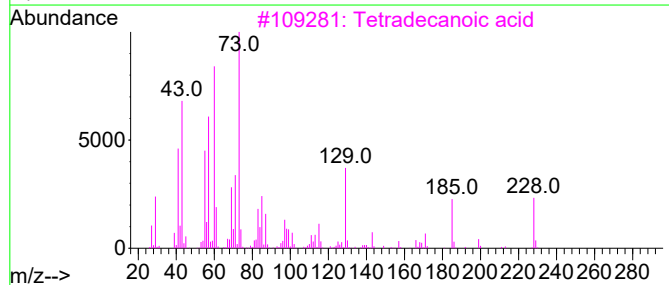
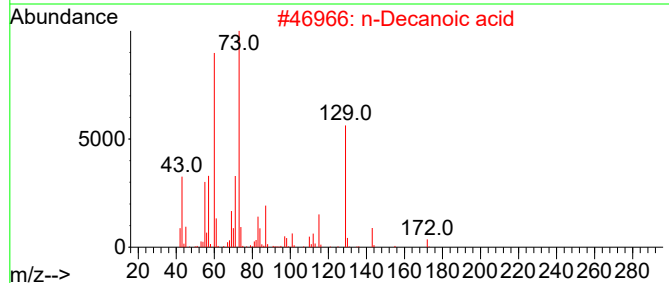
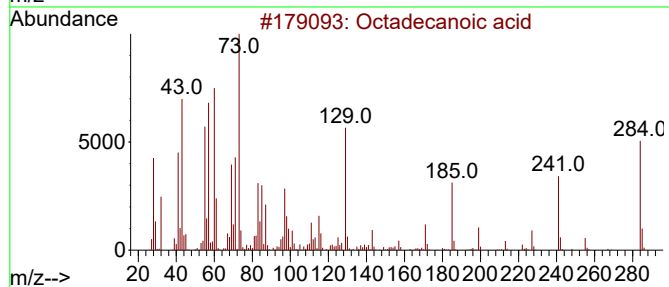
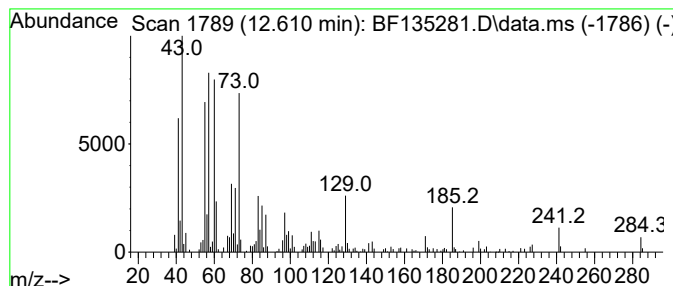
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.610	3.36 ng	152276	Phenanthrene-d10		11.286	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	98
2	n-Decanoic acid		172	C10H20O2	000334-48-5	78
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	72
5	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135281.D
Acq On : 15 Sep 2023 16:11
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Sample : 04409-04
Misc :
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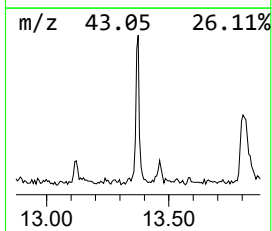
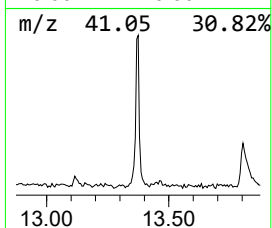
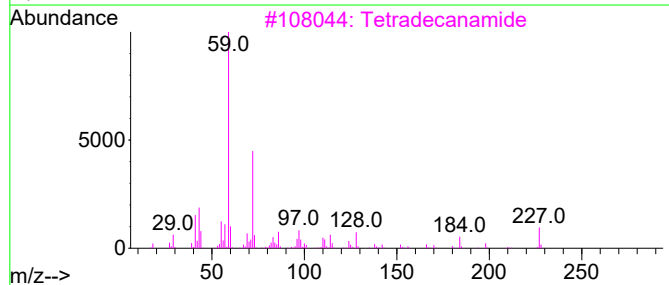
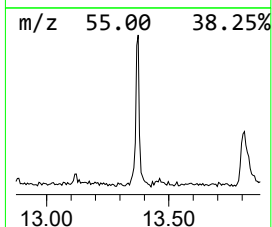
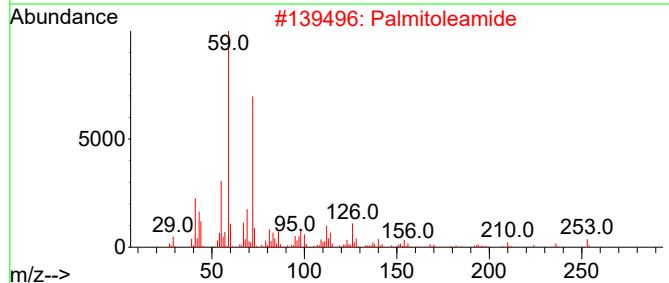
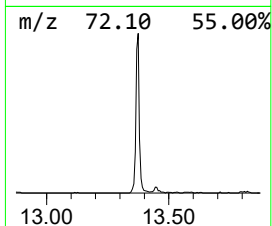
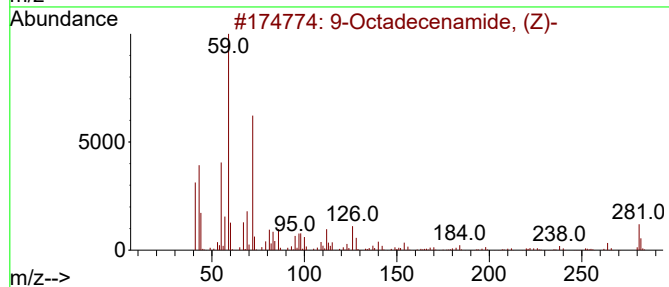
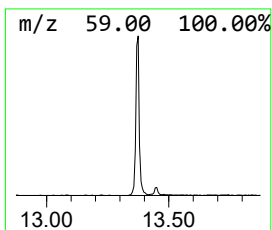
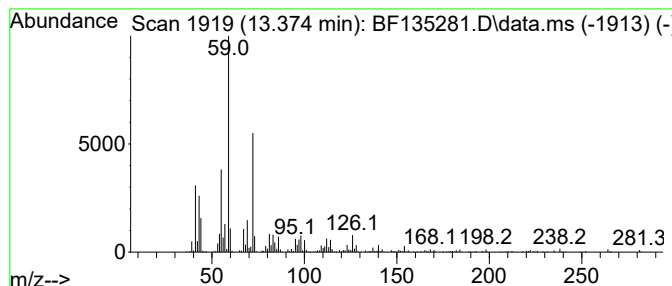
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.374	11.66 ng	427568	Chrysene-d12		13.945	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	94
2	Palmitoleamide		253	C16H31NO	106010-22-4	78
3	Tetradecanamide		227	C14H29NO	000638-58-4	72
4	Hexadecanamide		255	C16H33NO	000629-54-9	59
5	2,2-Dimethyl-tetrahydro-[1,3]dio...		190	C8H14O5	1000194-40-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135281.D
Acq On : 15 Sep 2023 16:11
Operator : CG\JU
Sample : 04409-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2(0-2)COMP

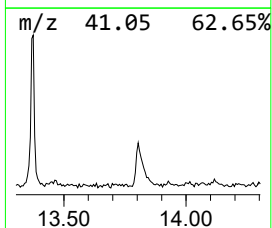
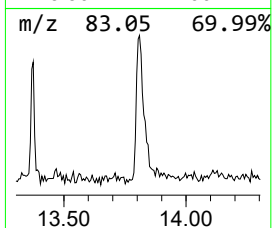
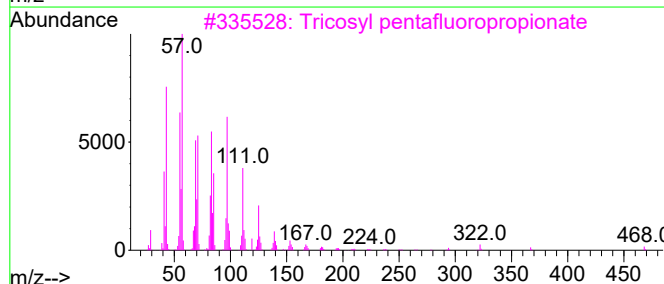
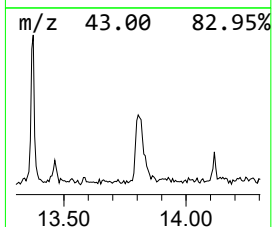
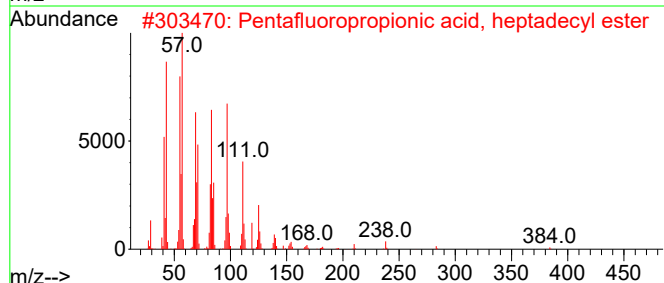
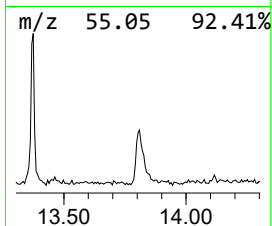
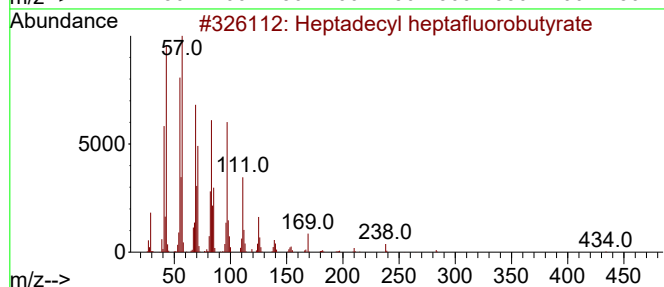
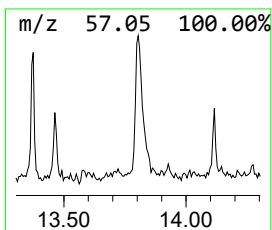
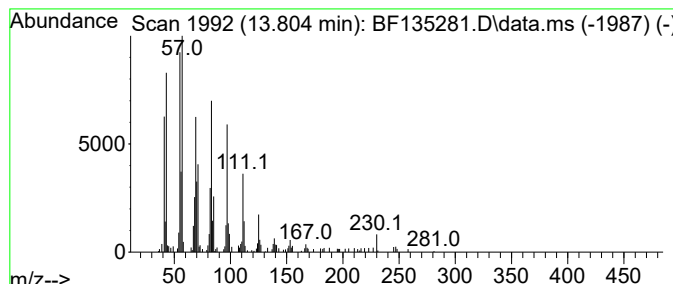
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	7.03 ng	257713	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135281.D
Acq On : 15 Sep 2023 16:11
Operator : CG\JU
Sample : 04409-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2(0-2)COMP

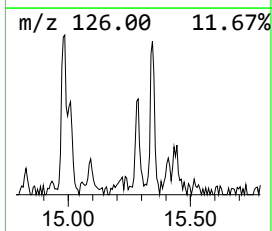
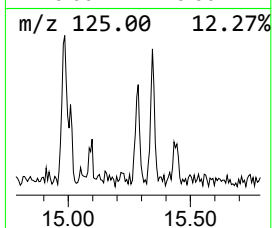
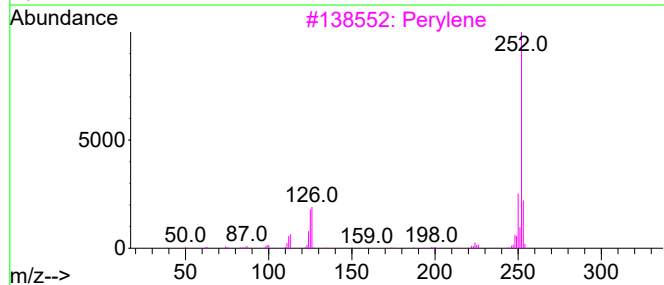
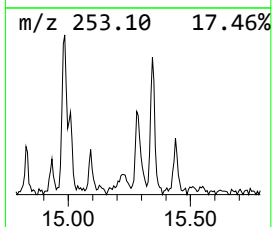
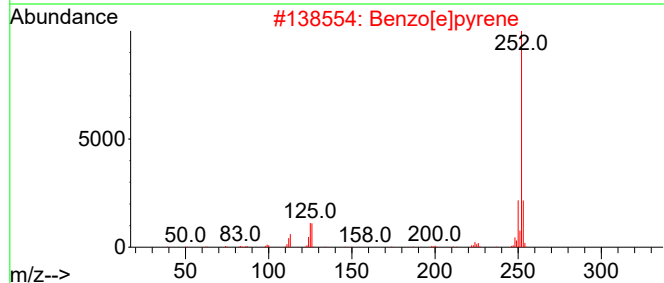
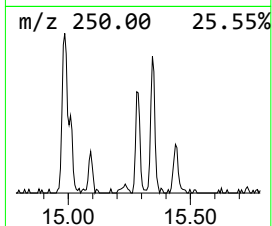
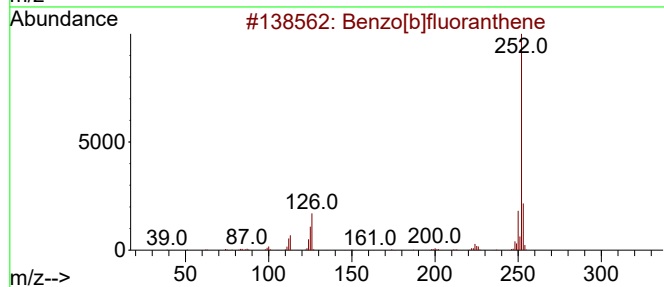
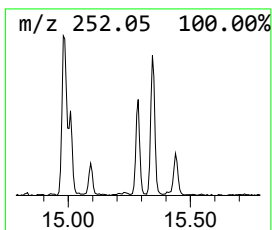
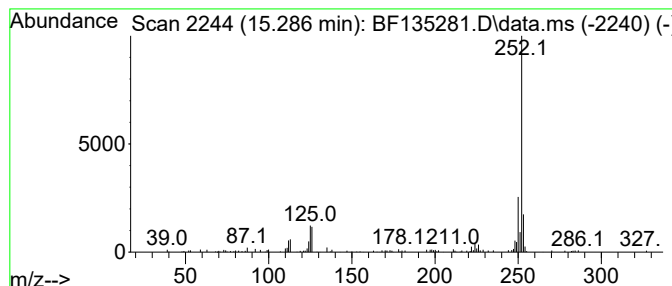
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	2.16 ng	71738	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
2			Benzo[e]pyrene	252	C20H12	000192-97-2	97
3			Perylene	252	C20H12	000198-55-0	96
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135281.D
Acq On : 15 Sep 2023 16:11
Operator : CG\JU
Sample : 04409-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2(0-2)COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
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Ethanol, 2-(2-e...	6.592	3.0	ng	94766	1	6.757	638981	20.0
2,4,7,9-Tetrame...	9.239	31.1	ng	1413230	3	9.792	909159	20.0
Pentadecane, 2,...	10.716	3.5	ng	156710	4	11.286	907351	20.0
n-Hexadecanoic ...	11.822	9.8	ng	442398	4	11.286	907351	20.0
10-Octadecenoic...	12.398	2.9	ng	129269	4	11.286	907351	20.0
Octadecanoic acid	12.610	3.4	ng	152276	4	11.286	907351	20.0
9-Octadecenamid...	13.374	11.7	ng	427568	5	13.945	733104	20.0
Heptadecyl hept...	13.804	7.0	ng	257713	5	13.945	733104	20.0
Benzo[e]pyrene	15.286	2.2	ng	71738	6	15.410	664740	20.0