

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
 Data File : BF135204.D
 Acq On : 13 Sep 2023 03:56
 Operator : CG\JU
 Sample : 04299-10
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-01

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: BF135204.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	22	26	37	rVB	40575	53671	1.89%	0.243%
2	2.840	123	128	136	rBV	37092	57873	2.03%	0.262%
3	4.363	383	387	397	rBV	926975	1126931	39.61%	5.093%
4	4.987	489	493	508	rVB	644186	716895	25.20%	3.240%
5	5.251	535	538	543	rVB	32726	31891	1.12%	0.144%
6	5.393	558	562	572	rBV	1463051	1269747	44.63%	5.739%
7	6.398	729	733	744	rVB	1310960	1178610	41.42%	5.327%
8	6.598	764	767	781	rVB	56666	72145	2.54%	0.326%
9	6.763	791	795	798	rBV	810385	680874	23.93%	3.077%
10	6.834	804	807	812	rBV2	23604	39680	1.39%	0.179%
11	7.328	886	891	894	rBV	1702057	1646170	57.86%	7.440%
12	7.422	901	907	914	rVB	32468	47980	1.69%	0.217%
13	7.781	962	968	975	rBV3	51501	71296	2.51%	0.322%
14	7.957	993	998	1006	rBV4	21865	41563	1.46%	0.188%
15	8.040	1006	1012	1015	rBV	1122770	929466	32.67%	4.201%
16	8.387	1068	1071	1077	rBV4	37341	42160	1.48%	0.191%
17	9.122	1191	1196	1199	rBV	3323858	2845235	100.00%	12.859%
18	9.798	1306	1311	1314	rBV	1246682	1029014	36.17%	4.651%
19	10.222	1378	1383	1388	rVB2	79505	88932	3.13%	0.402%
20	10.586	1441	1445	1450	rBV	1423314	1278328	44.93%	5.777%
21	11.286	1560	1564	1568	rBV	1200898	1108357	38.95%	5.009%
22	11.404	1581	1584	1590	rBV5	26151	37384	1.31%	0.169%
23	11.751	1640	1643	1648	rBV5	29992	40360	1.42%	0.182%
24	11.833	1652	1657	1669	rBV	1022734	1046954	36.80%	4.732%
25	12.392	1748	1752	1758	rVB2	43707	58658	2.06%	0.265%
26	12.545	1774	1778	1784	rVB2	64940	81821	2.88%	0.370%
27	12.616	1787	1790	1797	rVB	203309	189121	6.65%	0.855%
28	12.704	1802	1805	1809	rVV	59468	53084	1.87%	0.240%
29	12.763	1812	1815	1818	rBV	62699	49227	1.73%	0.222%
30	12.886	1832	1836	1839	rBV	2557142	2295466	80.68%	10.375%
31	13.122	1873	1876	1879	rBV	81311	73558	2.59%	0.332%
32	13.469	1932	1935	1938	rVB	76636	69933	2.46%	0.316%
33	13.798	1988	1991	1992	rBV	71102	53319	1.87%	0.241%
34	13.821	1992	1995	2009	rVB	174551	367853	12.93%	1.663%
35	13.939	2010	2015	2019	rBV	679832	713883	25.09%	3.226%
36	14.116	2042	2045	2049	rVB	54240	46991	1.65%	0.212%

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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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.421	2094	2097	2101	rVB	48343	47945	1.69%	0.217%
38	14.474	2101	2106	2110	rBV6	26708	52170	1.83%	0.236%
39	14.580	2121	2124	2127	rVB	69743	60073	2.11%	0.272%
40	14.627	2129	2132	2136	rBV3	29301	34254	1.20%	0.155%
41	14.727	2146	2149	2154	rVB2	36362	46240	1.63%	0.209%
42	14.804	2159	2162	2165	rVB	41172	44776	1.57%	0.202%
43	15.068	2204	2207	2210	rVB	31730	34292	1.21%	0.155%
44	15.339	2249	2253	2257	rVB	42307	56100	1.97%	0.254%
45	15.404	2259	2264	2269	rBV	512612	612479	21.53%	2.768%
46	15.892	2343	2347	2353	rVB4	37845	65482	2.30%	0.296%
47	16.021	2364	2369	2376	rVB9	27551	61526	2.16%	0.278%
48	16.127	2385	2387	2393	rVB7	25869	38497	1.35%	0.174%
49	16.533	2450	2456	2459	rBV5	21119	40422	1.42%	0.183%
50	16.715	2485	2487	2495	rVB8	19712	34726	1.22%	0.157%
51	16.921	2514	2522	2532	rBV2	538319	1123582	39.49%	5.078%
52	17.851	2674	2680	2689	rVB2	14901	46420	1.63%	0.210%
53	18.339	2755	2763	2774	rVB5	68677	192593	6.77%	0.870%

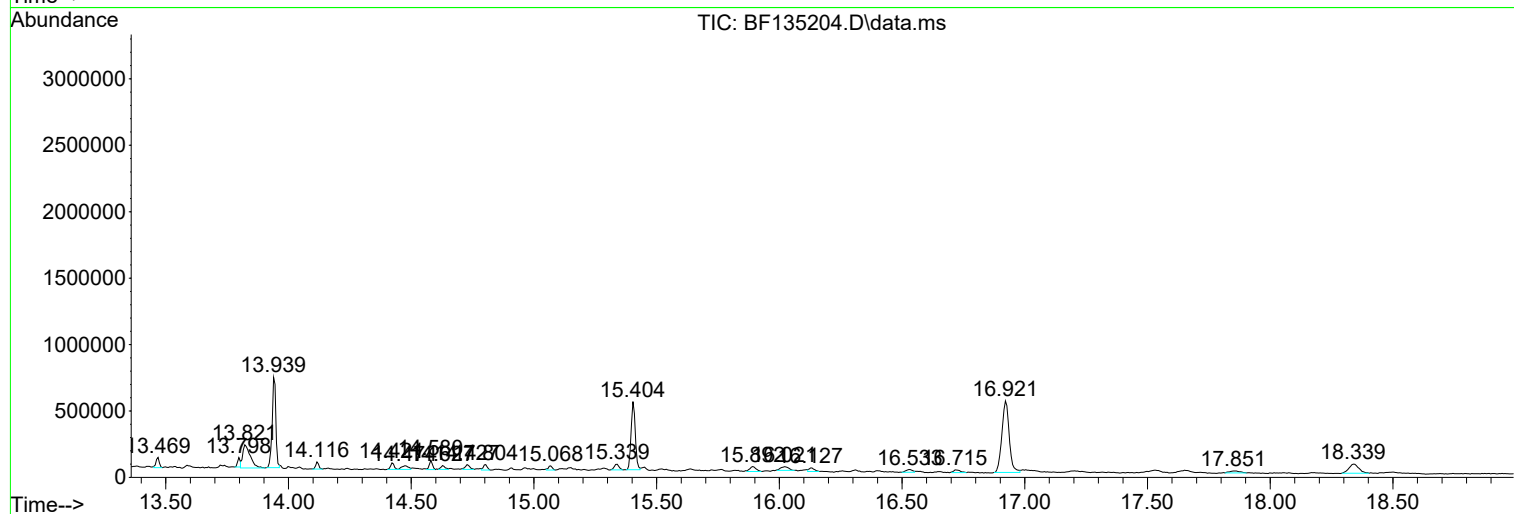
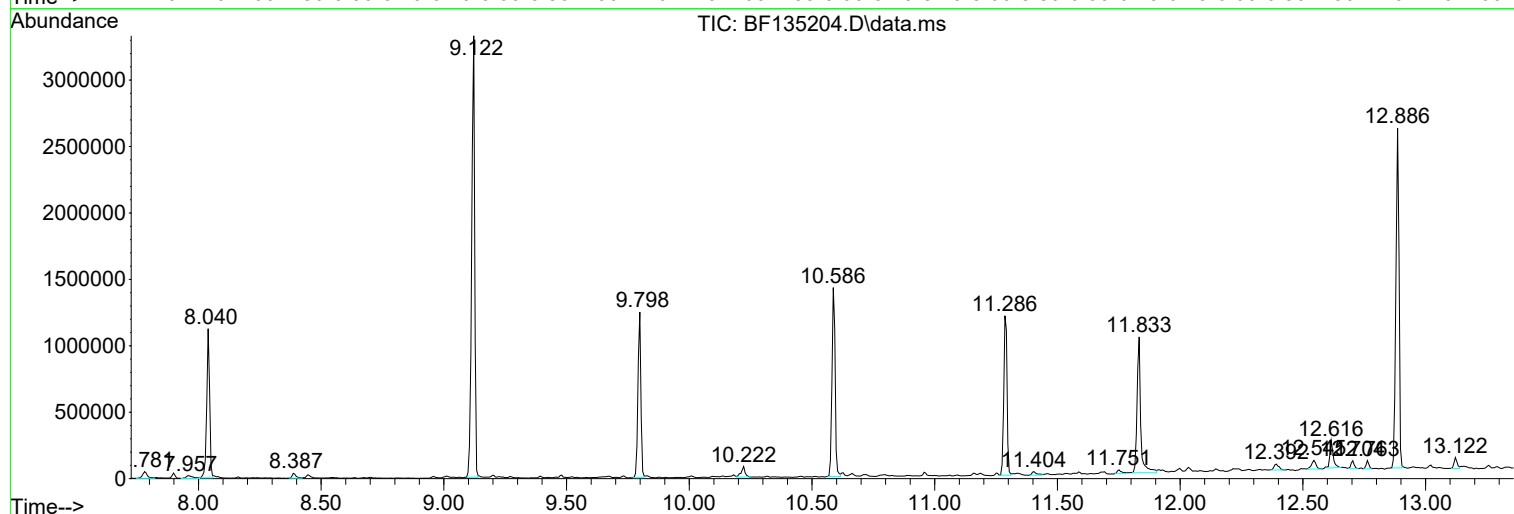
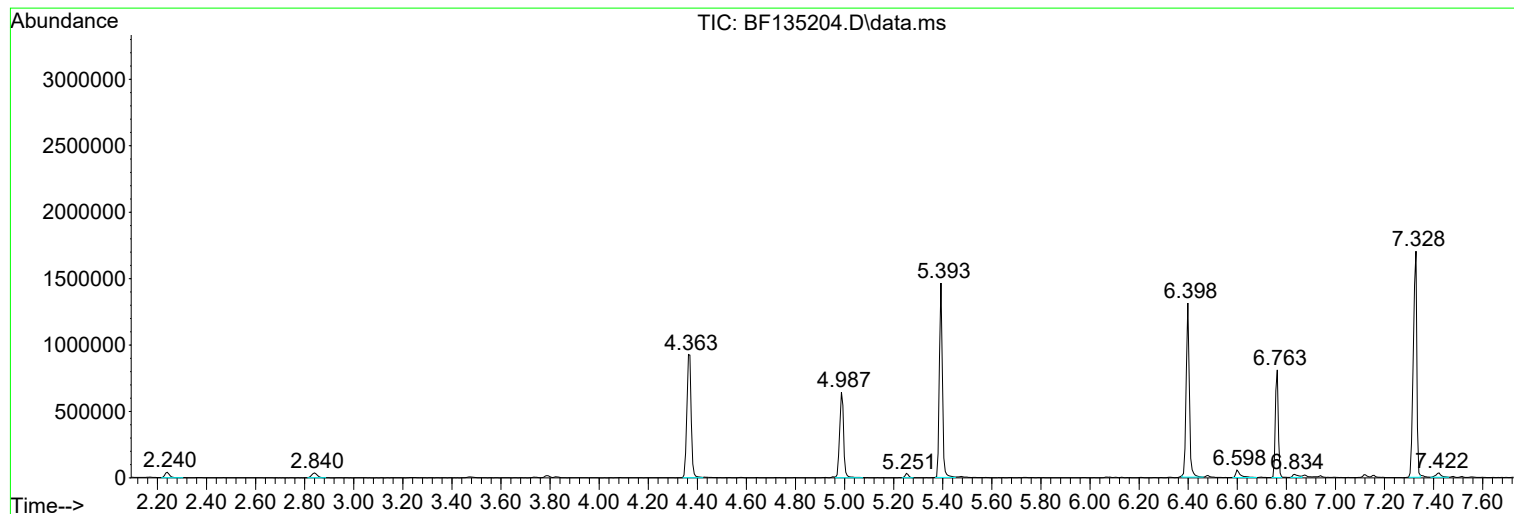
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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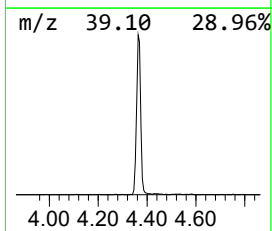
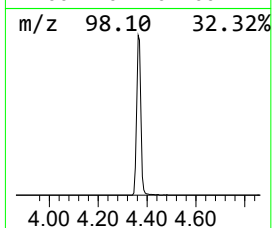
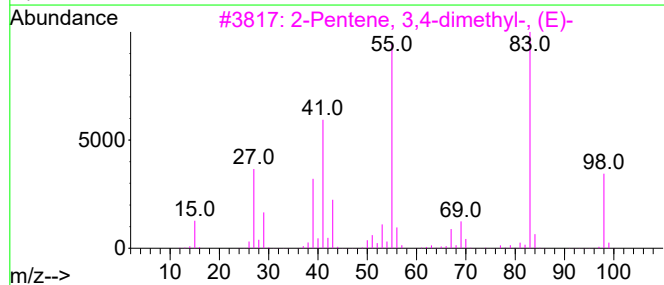
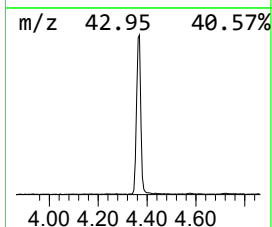
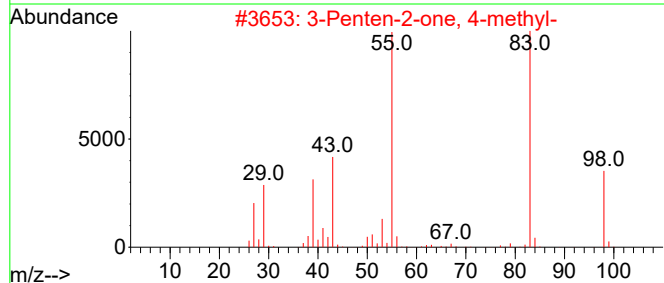
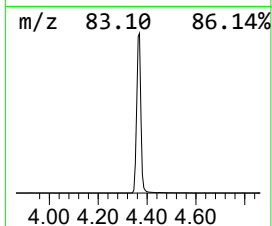
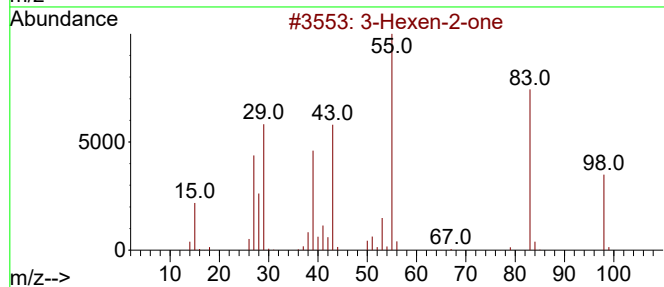
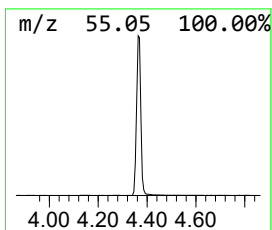
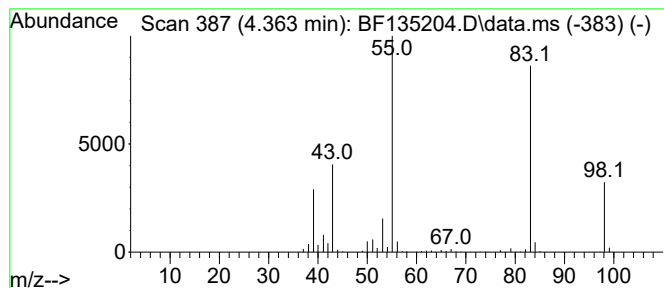
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.363	33.10 ng	1126930	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72



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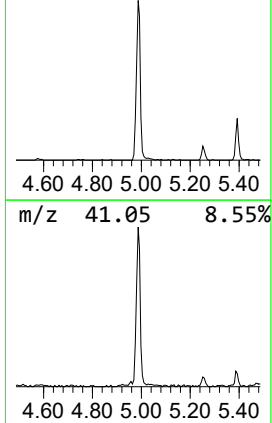
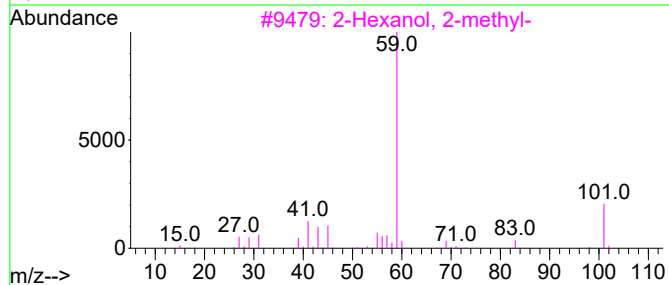
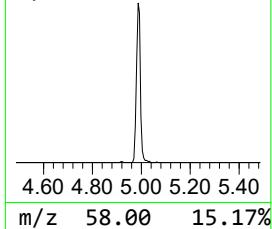
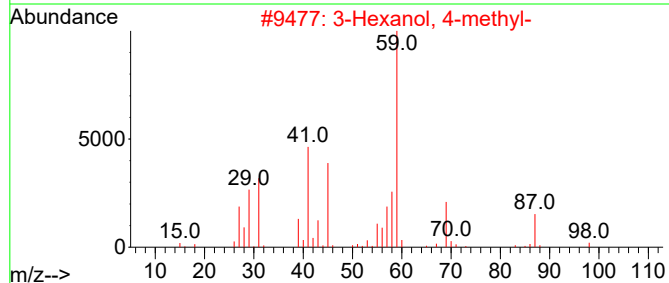
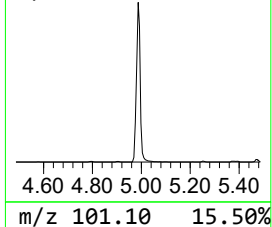
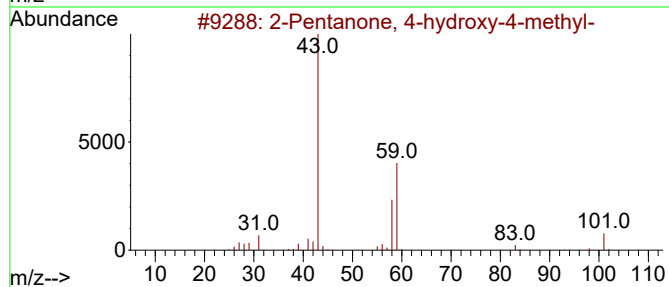
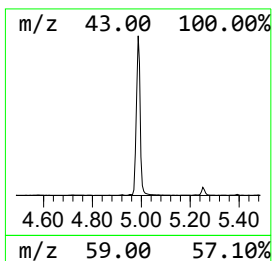
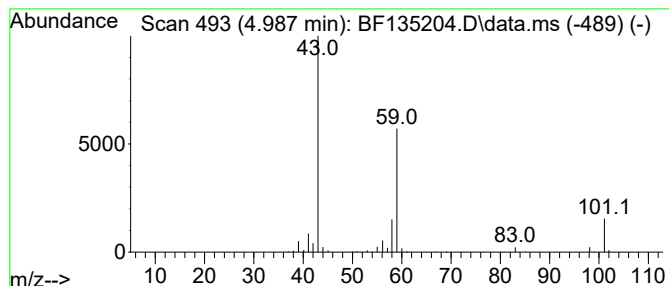
Instrument :
BNA_F
ClientSampleId :
TWP-01

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 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.987	21.06 ng	716895	1,4-Dichlorobenzene-d4			6.763
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10



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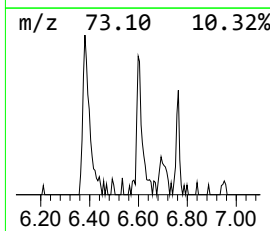
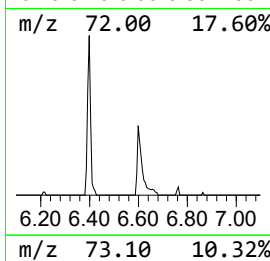
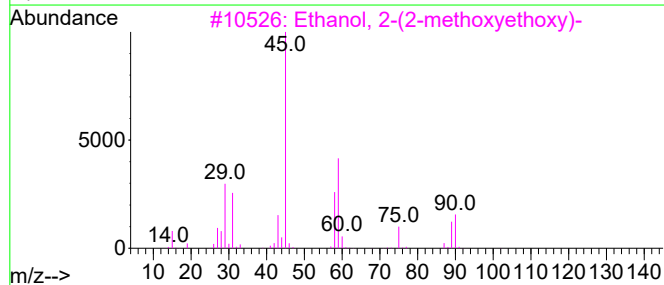
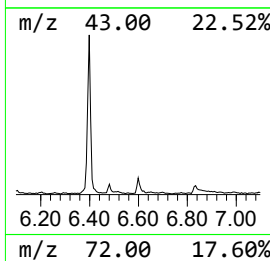
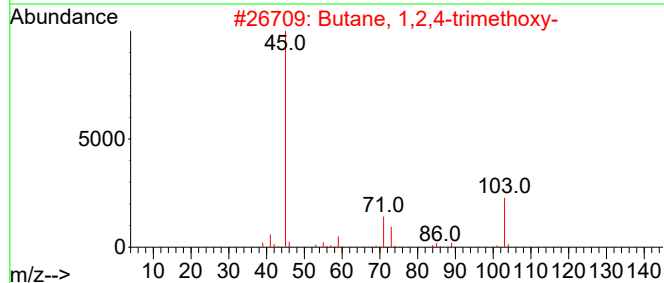
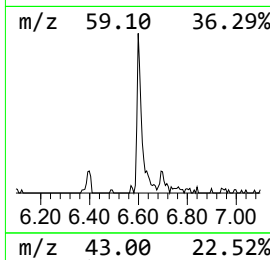
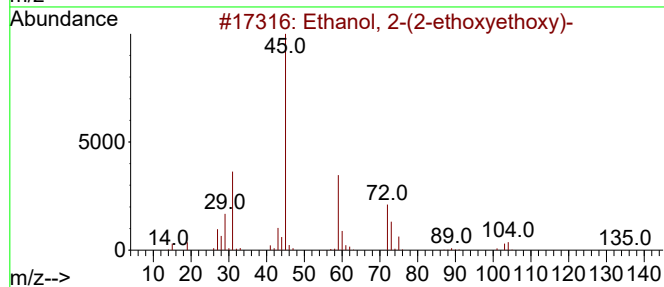
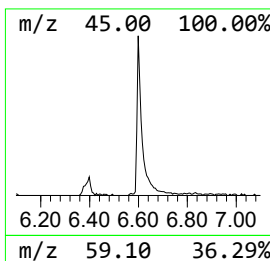
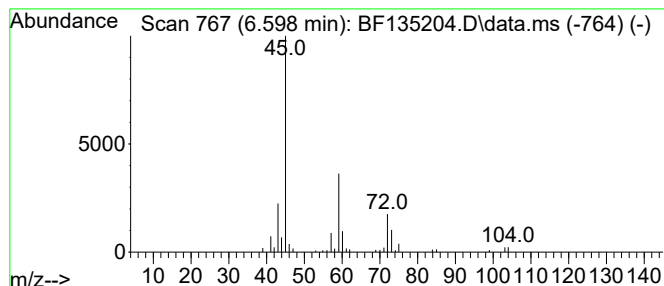
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.598 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	2.12 ng	72145	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	47
2			Butane, 1,2,4-trimethoxy-	148	C7H16O3	020637-48-3	42
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	39
4			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
5			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	38



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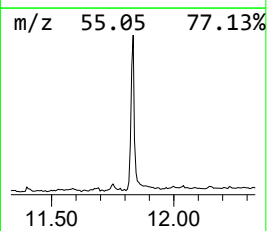
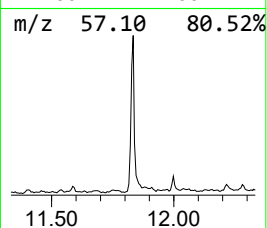
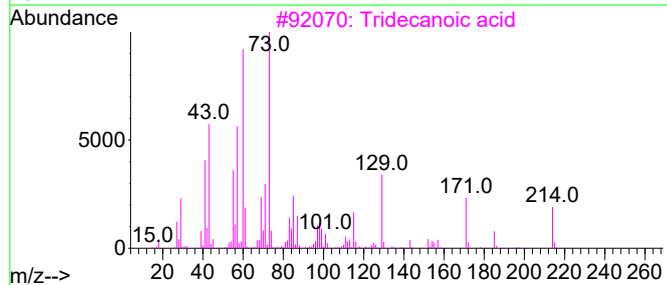
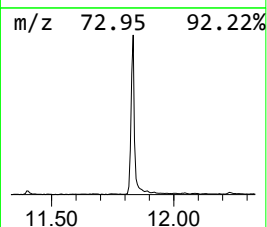
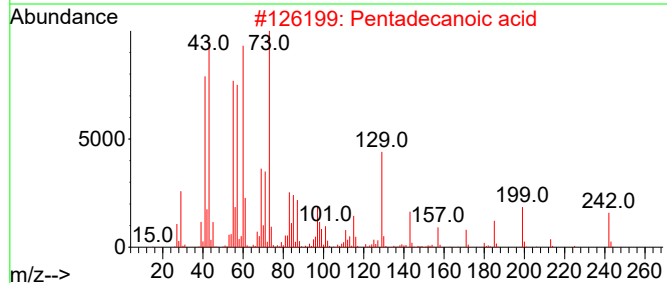
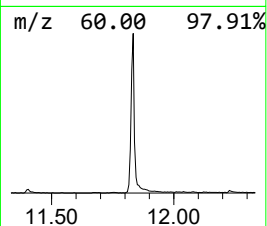
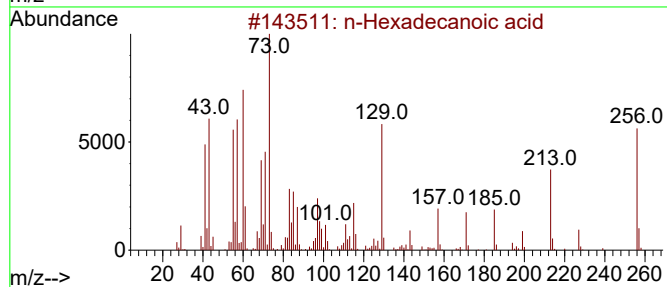
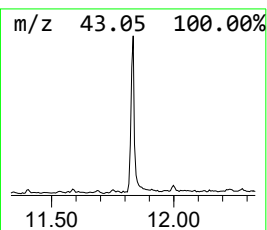
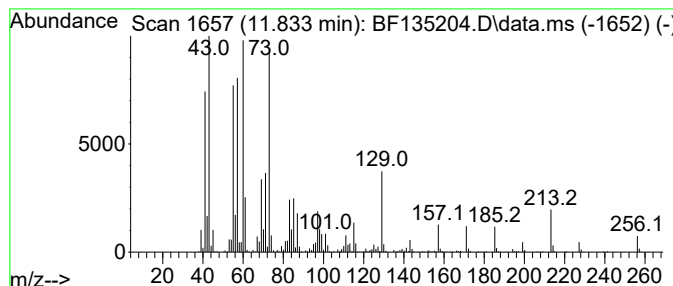
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	18.89 ng	1046950	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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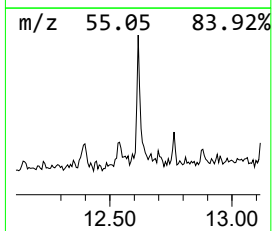
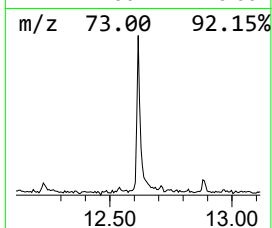
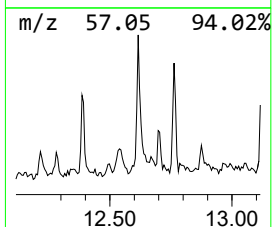
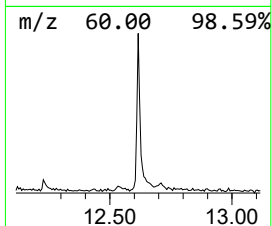
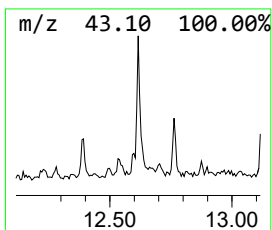
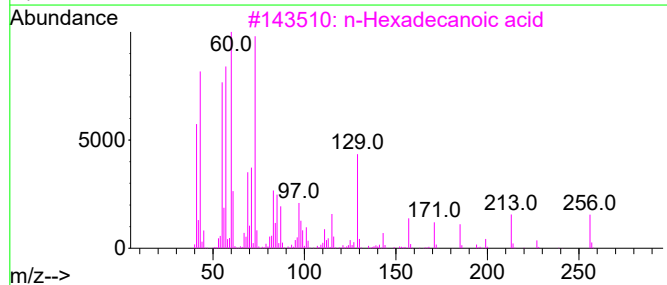
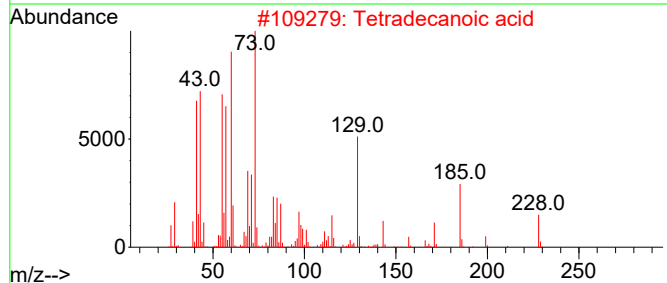
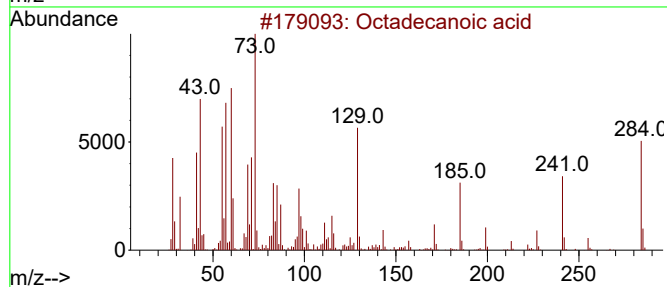
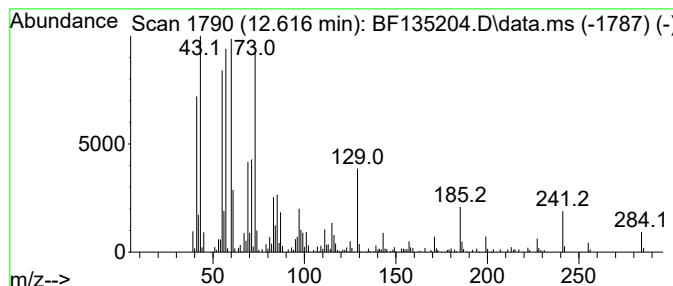
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	5.30 ng	189121	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
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Acq On : 13 Sep 2023 03:56
Operator : CG\JU
Sample : 04299-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

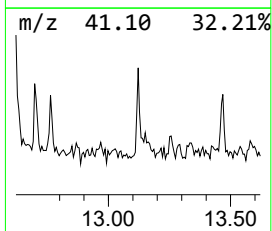
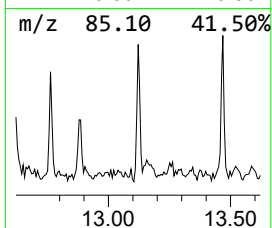
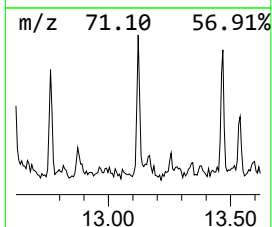
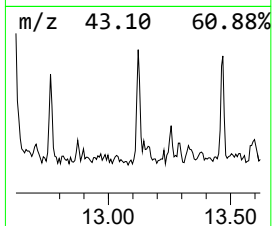
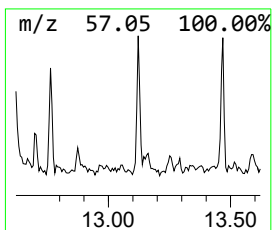
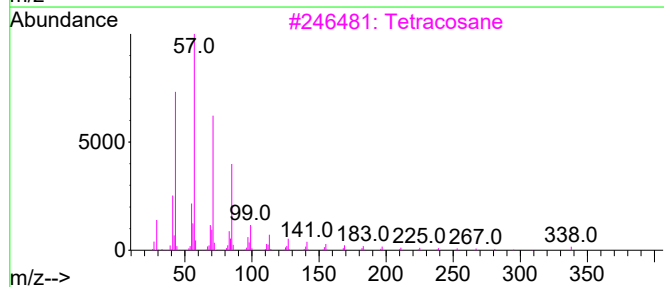
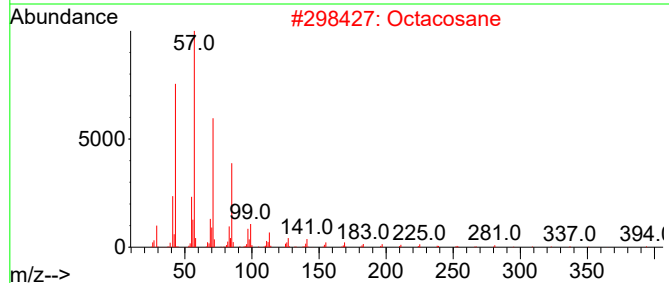
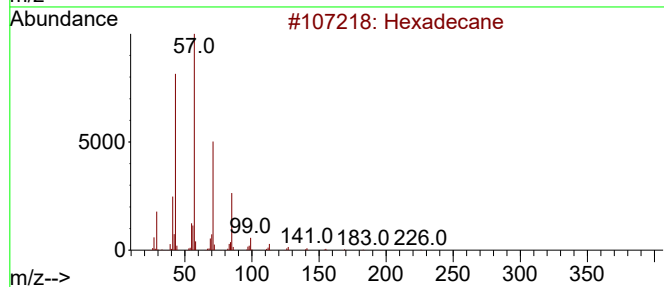
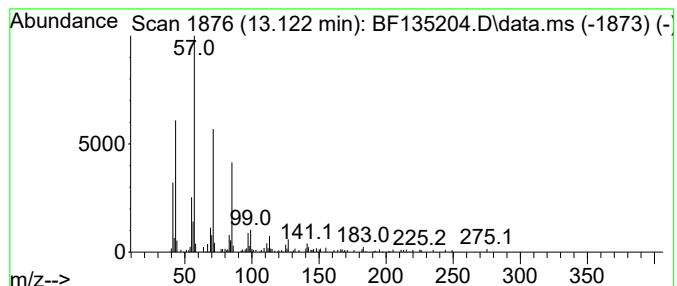
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.121	2.06 ng	73558	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Octacosane	394	C28H58	000630-02-4	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5	Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135204.D
Acq On : 13 Sep 2023 03:56
Operator : CG\JU
Sample : 04299-10
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Instrument :
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ClientSampleId :
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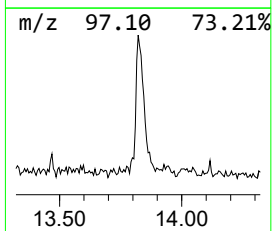
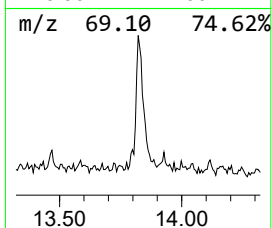
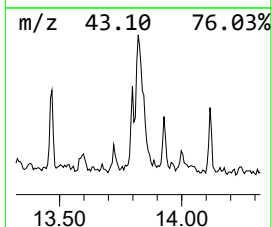
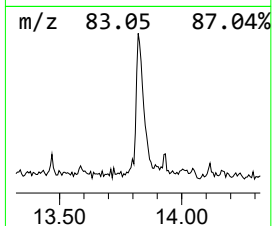
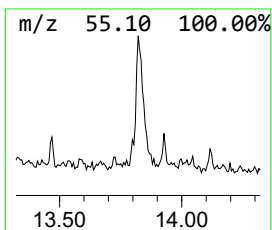
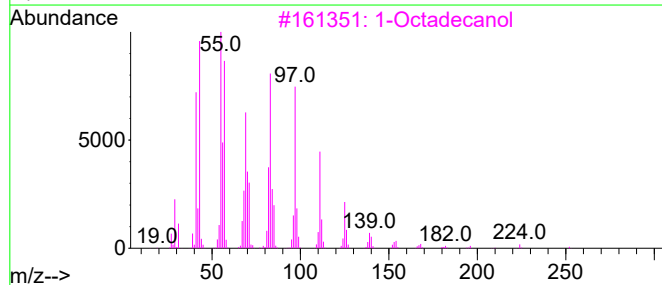
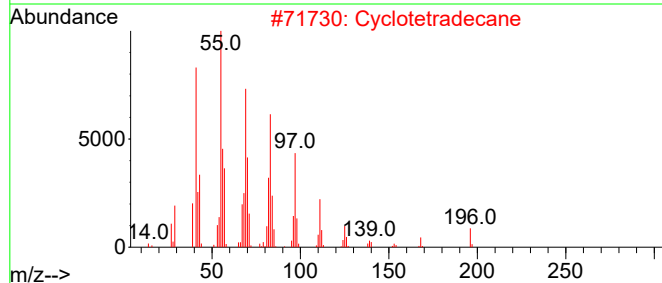
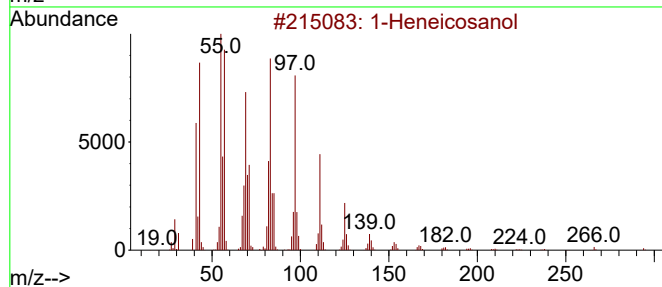
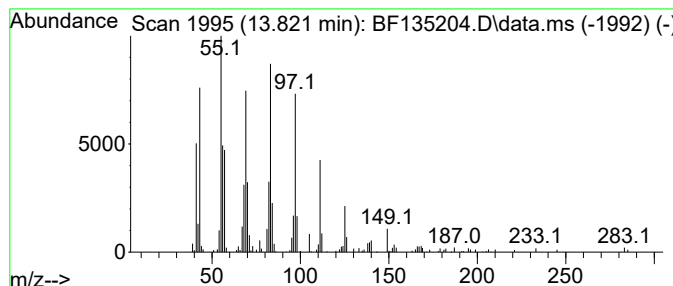
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	10.31 ng	367853	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	91
2			Cyclotetradecane	196	C14H28	000295-17-0	72
3			1-Octadecanol	270	C18H38O	000112-92-5	68
4			1-Hexacosanol	382	C26H54O	000506-52-5	64
5			1-Eicosanol	298	C20H42O	000629-96-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135204.D
Acq On : 13 Sep 2023 03:56
Operator : CG\JU
Sample : 04299-10
Misc :
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Instrument :
BNA_F
ClientSampleId :
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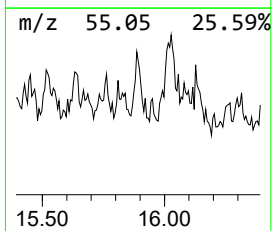
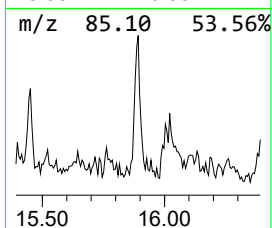
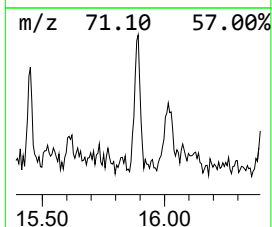
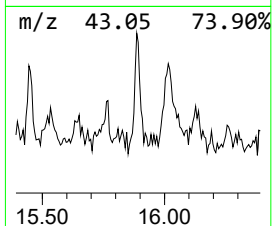
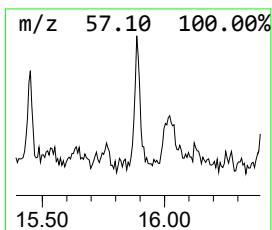
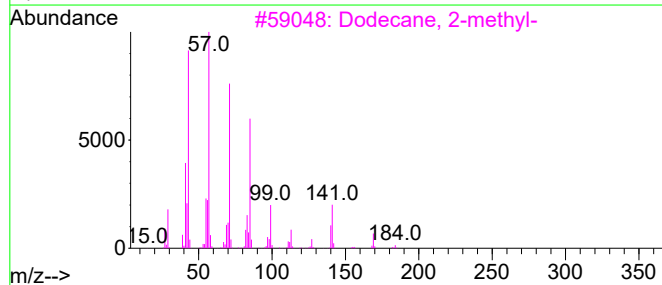
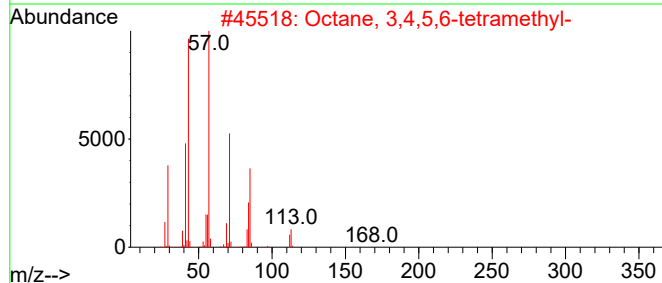
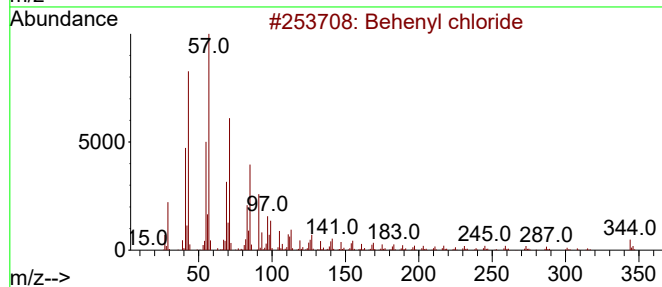
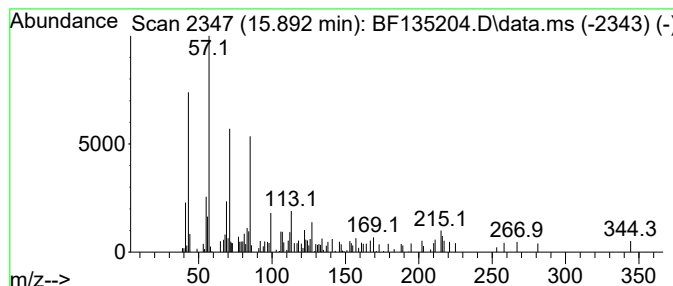
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenyl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	2.14 ng	65482	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenyl chloride	344	C22H45Cl	042217-03-8	64
2			Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	50
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	49
4			Octadecane	254	C18H38	000593-45-3	47
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
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Sample : 04299-10
Misc :
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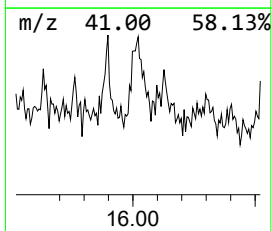
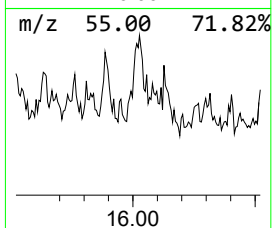
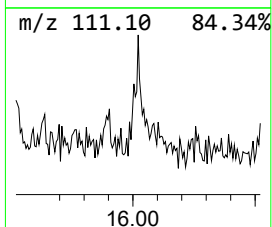
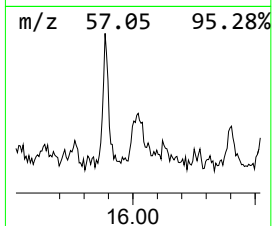
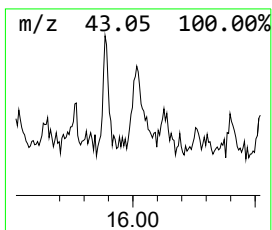
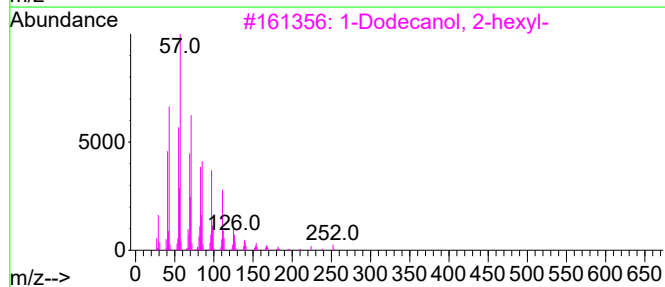
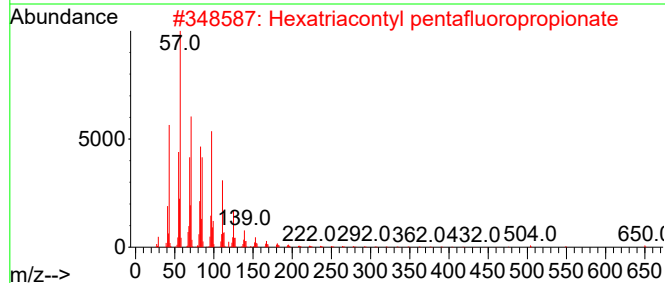
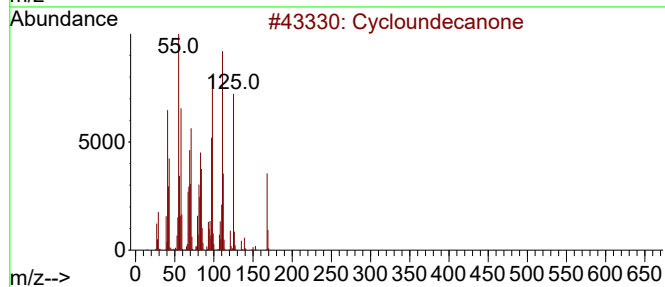
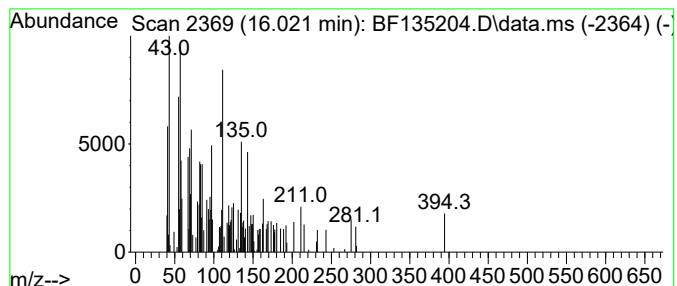
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.021 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.021	2.01 ng	61526	Perylene-d12	15.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloundecanone	168	C11H20O	000878-13-7	30
2	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	18
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	18
4	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	18
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135204.D
Acq On : 13 Sep 2023 03:56
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Misc :
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Instrument :
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ClientSampleId :
TWP-01

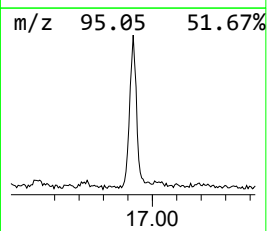
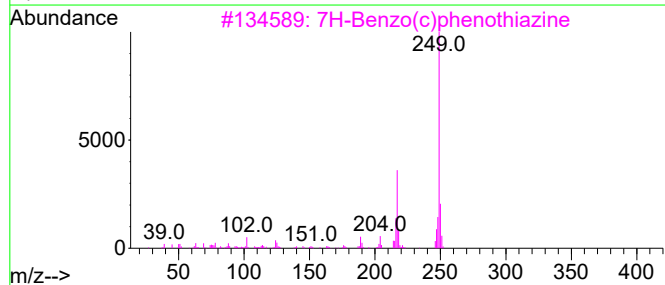
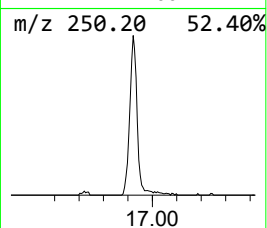
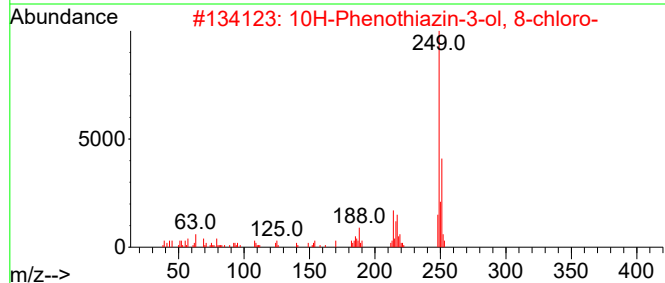
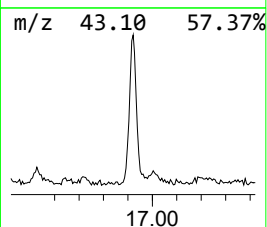
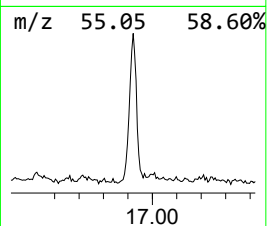
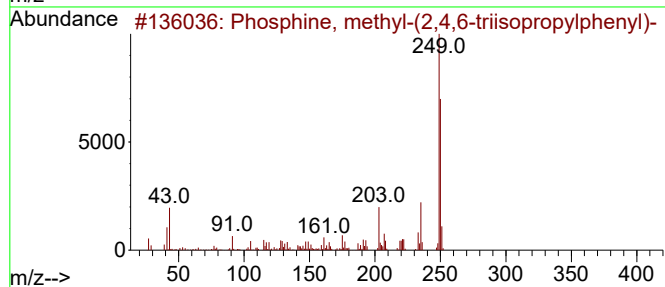
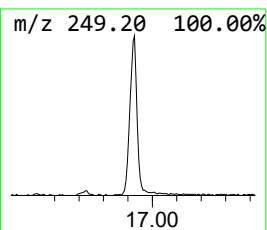
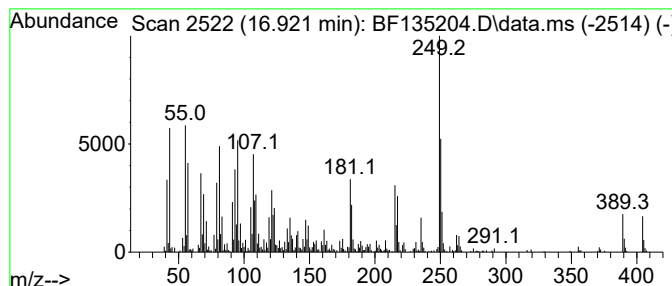
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.921 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.921	36.69 ng	1123580	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	43
2			10H-Phenothiazin-3-ol, 8-chloro-	249	C12H8ClNOS	002002-32-6	27
3			7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	27
4			2-Cyclopropyl-4-methyl-5-pyrimid...	250	C12H18N2O2Si	1000477-09-5	22
5			Benzene, 1-nitro-2-hydroxy-4-(p...	249	C12H8FN04	189214-56-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
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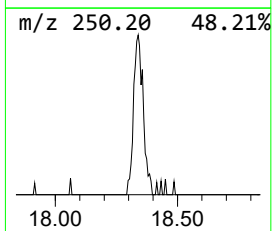
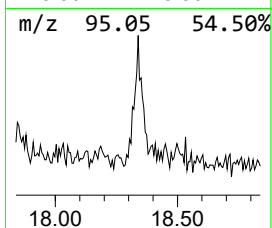
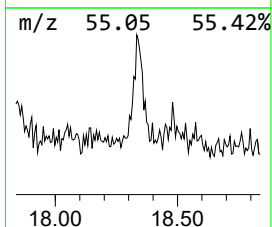
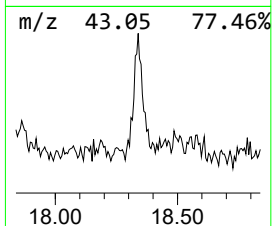
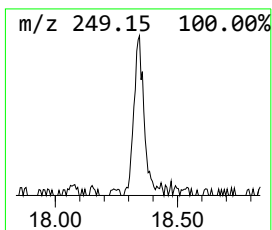
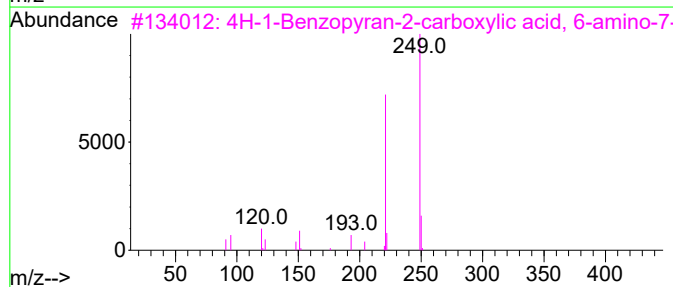
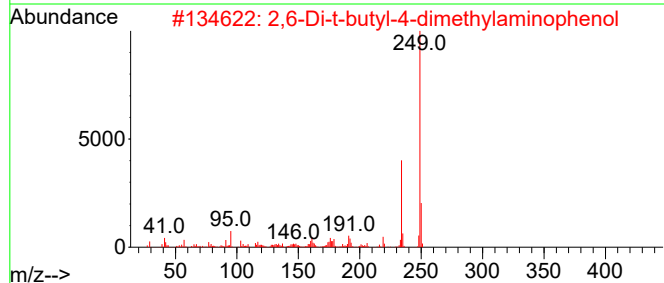
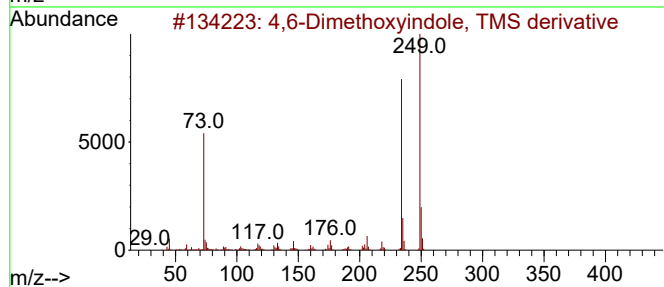
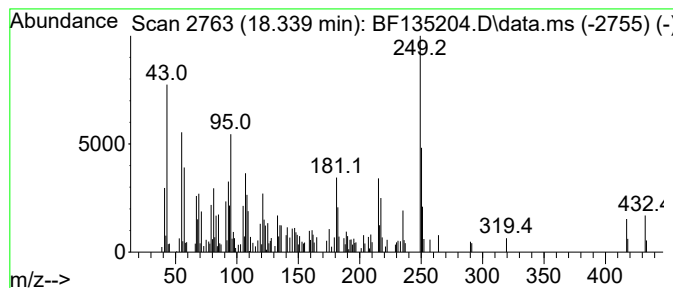
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown18.339 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.339	6.29 ng	192593	Perylene-d12	15.404

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4,6-Dimethoxyindole, TMS derivative	249	C13H19NO2Si	1782456-13-6	38
2		2,6-Di-t-butyl-4-dimethylaminoph...	249	C16H27NO	010437-44-2	35
3		4H-1-Benzopyran-2-carboxylic aci...	249	C12H11NO5	030192-11-1	35
4		7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	35
5		Phenothiazin-2-ol, 8-chloro-	249	C12H8ClNOS	005909-61-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135204.D
Acq On : 13 Sep 2023 03:56
Operator : CG\JU
Sample : 04299-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01

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
3-Hexen-2-one	4.363	33.1	ng	1126930	1	6.763	680874	20.0
2-Pentanone, 4-...	4.987	21.1	ng	716895	1	6.763	680874	20.0
unknown6.598	6.598	2.1	ng	72145	1	6.763	680874	20.0
n-Hexadecanoic ...	11.833	18.9	ng	1046950	4	11.286	1108360	20.0
Octadecanoic acid	12.616	5.3	ng	189121	5	13.939	713883	20.0
Hexadecane	13.121	2.1	ng	73558	5	13.939	713883	20.0
1-Heneicosanol	13.822	10.3	ng	367853	5	13.939	713883	20.0
Behenyl chloride	15.892	2.1	ng	65482	6	15.404	612479	20.0
unknown16.021	16.021	2.0	ng	61526	6	15.404	612479	20.0
unknown16.921	16.921	36.7	ng	1123580	6	15.404	612479	20.0
unknown18.339	18.339	6.3	ng	192593	6	15.404	612479	20.0