

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
 Data File : BF135761.D
 Acq On : 13 Oct 2023 19:41
 Operator : CG\JU
 Sample : 04837-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-290

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	487	490	499	rBV	81712	122392	5.92%	0.670%
2	5.375	555	559	579	rBV	1718867	2067748	100.00%	11.323%
3	6.387	728	731	757	rBV	2010903	2056060	99.43%	11.259%
4	6.734	787	790	801	rVB	707487	641115	31.01%	3.511%
5	7.304	884	887	900	rBV	1474243	1305131	63.12%	7.147%
6	8.016	1005	1008	1024	rVB	878975	760357	36.77%	4.164%
7	9.092	1187	1191	1202	rBV	2369033	1925938	93.14%	10.546%
8	9.216	1208	1212	1222	rVB	945656	893924	43.23%	4.895%
9	9.775	1303	1307	1311	rBV	921496	782759	37.86%	4.286%
10	10.569	1438	1442	1451	rBV	1295936	1142746	55.27%	6.258%
11	10.704	1462	1465	1470	rVB2	28536	37158	1.80%	0.203%
12	10.751	1470	1473	1476	rBV	64576	75743	3.66%	0.415%
13	10.786	1476	1479	1482	rVV2	54168	71899	3.48%	0.394%
14	10.822	1482	1485	1487	rVV	45746	38776	1.88%	0.212%
15	10.886	1494	1496	1501	rVB2	21686	24526	1.19%	0.134%
16	10.933	1501	1504	1508	rVV3	64782	88232	4.27%	0.483%
17	10.975	1508	1511	1514	rVV	69580	79136	3.83%	0.433%
18	11.010	1516	1517	1528	rVB	40711	46051	2.23%	0.252%
19	11.157	1539	1542	1549	rVB4	12636	23211	1.12%	0.127%
20	11.269	1557	1561	1564	rBV	922193	779887	37.72%	4.271%
21	11.292	1564	1565	1570	rVB	119211	91546	4.43%	0.501%
22	11.380	1578	1580	1586	rBV7	14930	23061	1.12%	0.126%
23	11.663	1625	1628	1631	rBV	32001	25433	1.23%	0.139%
24	11.727	1637	1639	1645	rBV5	24161	41850	2.02%	0.229%
25	11.804	1649	1652	1659	rVV2	381770	390978	18.91%	2.141%
26	12.210	1718	1721	1726	rBV4	24322	30662	1.48%	0.168%
27	12.374	1743	1749	1753	rBV2	95193	104113	5.04%	0.570%
28	12.492	1766	1769	1772	rBV	209388	201310	9.74%	1.102%
29	12.592	1784	1786	1793	rBV2	81505	104804	5.07%	0.574%
30	12.645	1793	1795	1803	rVB5	19339	27078	1.31%	0.148%
31	12.721	1803	1808	1814	rBV	174709	199164	9.63%	1.091%
32	12.780	1816	1818	1826	rVB7	17992	24574	1.19%	0.135%
33	12.863	1828	1832	1836	rBV	1680514	1444354	69.85%	7.909%
34	12.945	1843	1846	1852	rVB6	15404	27181	1.31%	0.149%
35	13.163	1880	1883	1889	rVB3	21533	28862	1.40%	0.158%
36	13.439	1927	1930	1933	rBV3	26245	23098	1.12%	0.126%

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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-BF101323.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.845	1994	1999	2007	rBV9	27878	76405	3.70%	0.418%
38	13.933	2007	2014	2017	rVV	598312	619949	29.98%	3.395%
39	13.963	2017	2019	2023	rVB	90438	83423	4.03%	0.457%
40	14.092	2038	2041	2047	rBV4	17478	26275	1.27%	0.144%
41	14.398	2090	2093	2097	rBV3	43949	43902	2.12%	0.240%
42	14.557	2117	2120	2124	rBV	45426	43031	2.08%	0.236%
43	14.704	2142	2145	2149	rVB	38299	45192	2.19%	0.247%
44	14.774	2153	2157	2161	rVB	451803	459880	22.24%	2.518%
45	14.986	2190	2193	2196	rBV	76386	99903	4.83%	0.547%
46	15.033	2199	2201	2207	rVB	70820	77614	3.75%	0.425%
47	15.286	2242	2244	2249	rVB	41361	46496	2.25%	0.255%
48	15.357	2253	2256	2260	rVB	50867	57711	2.79%	0.316%
49	15.410	2260	2265	2275	rVB	494572	670254	32.41%	3.670%
50	15.851	2336	2340	2344	rVB2	54469	78403	3.79%	0.429%
51	18.915	2856	2861	2870	rVB7	29444	82182	3.97%	0.450%

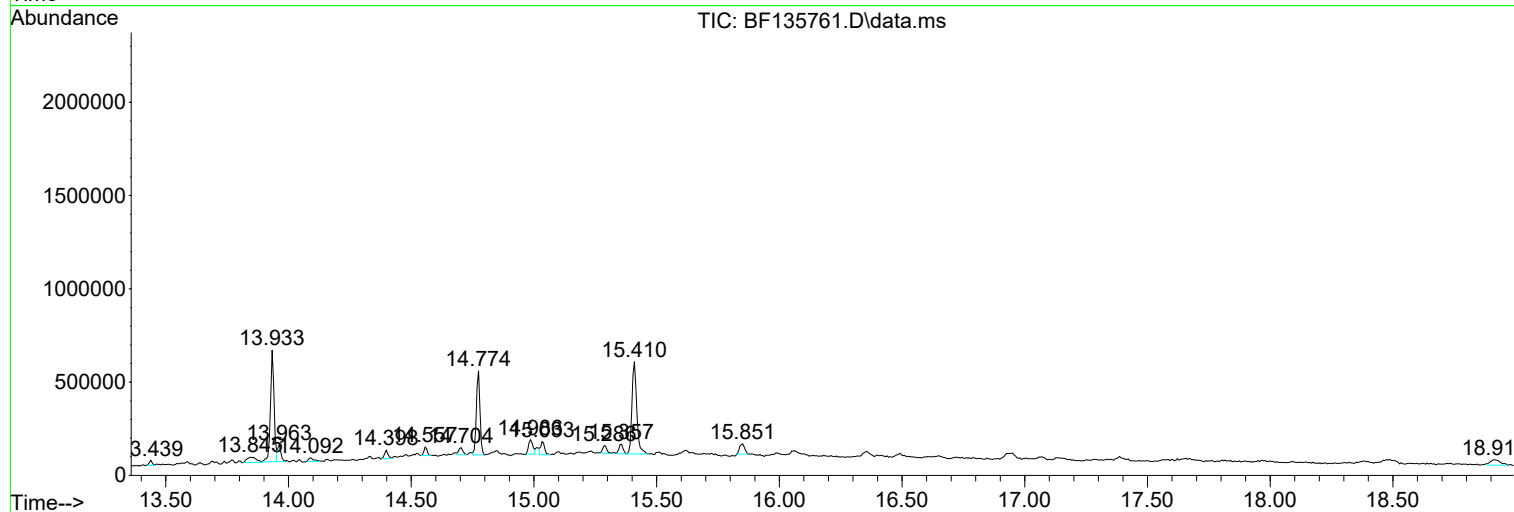
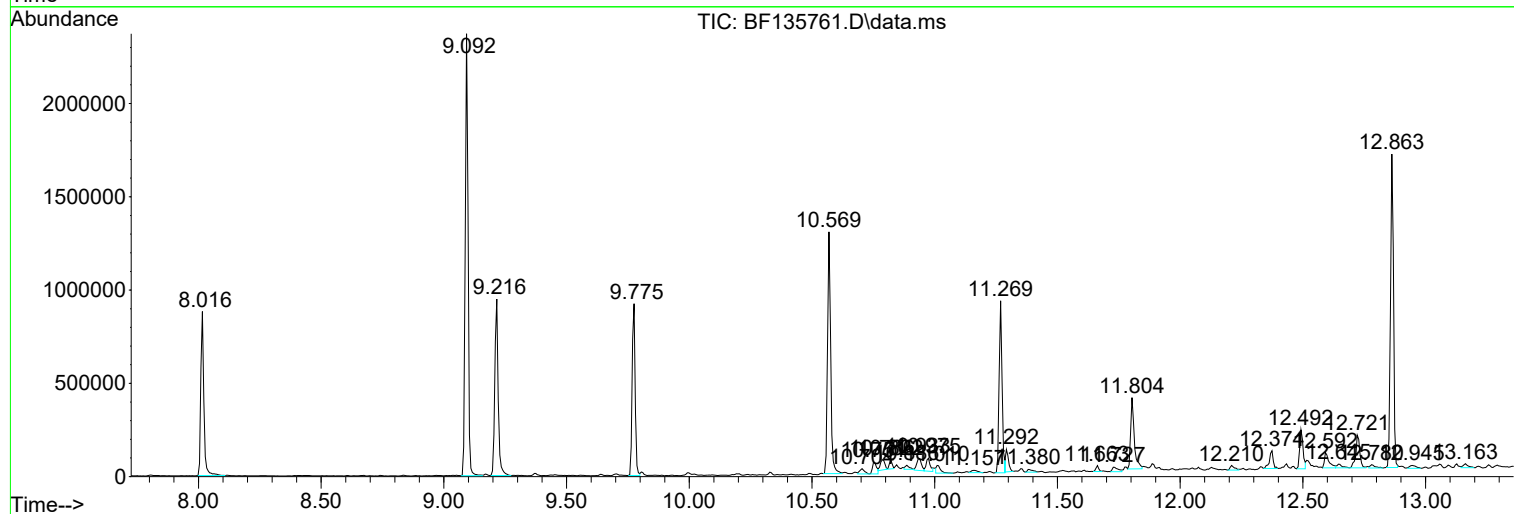
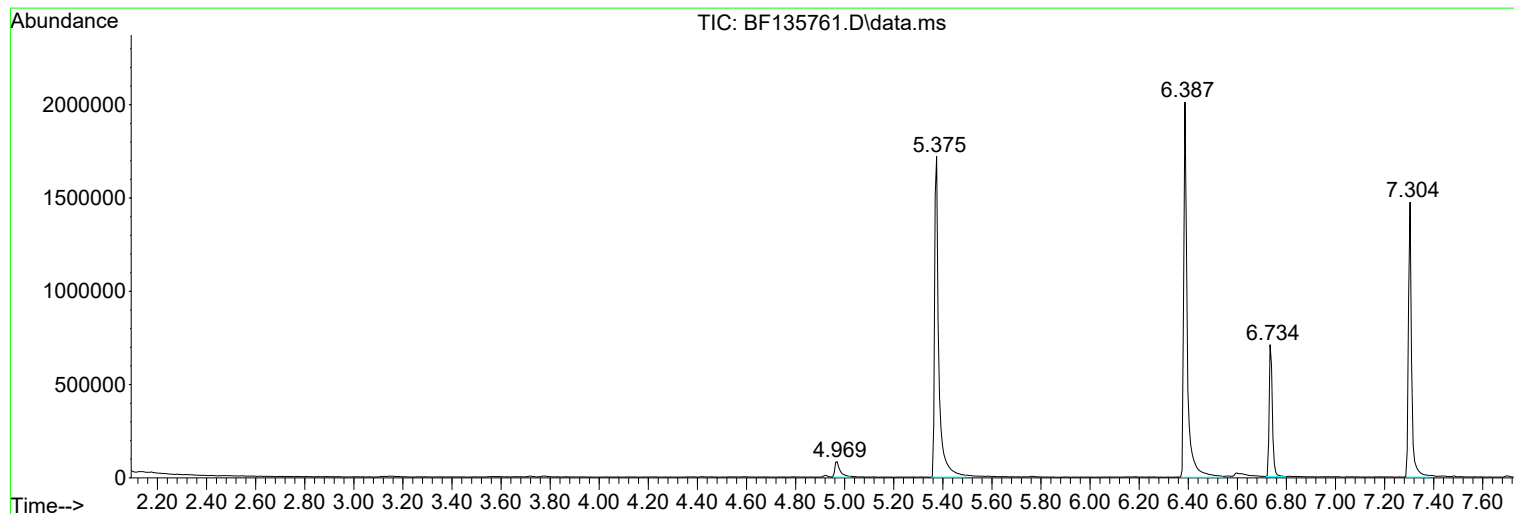
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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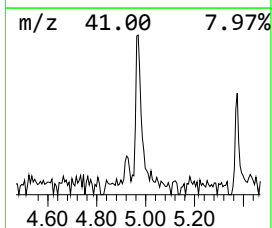
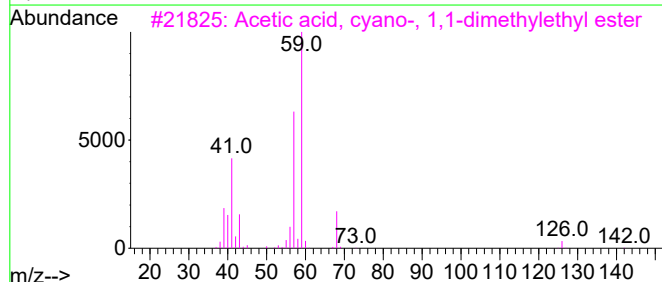
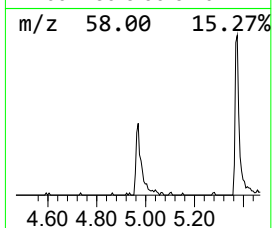
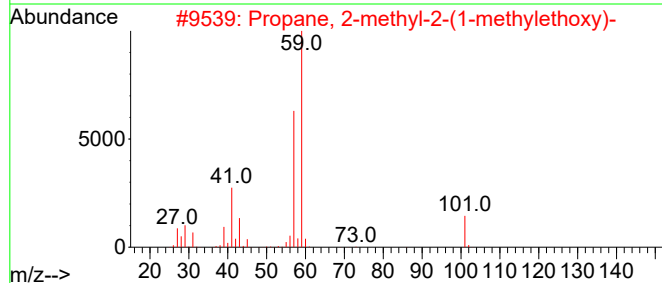
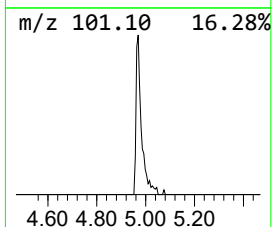
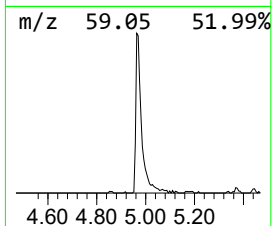
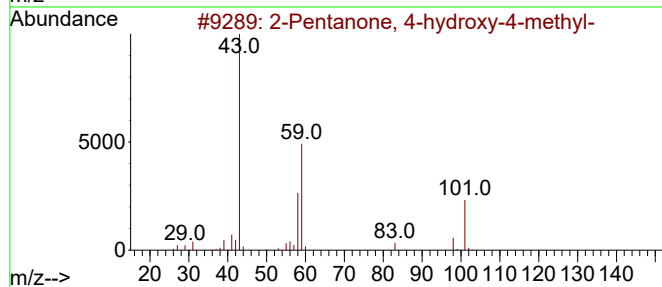
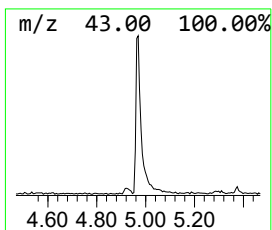
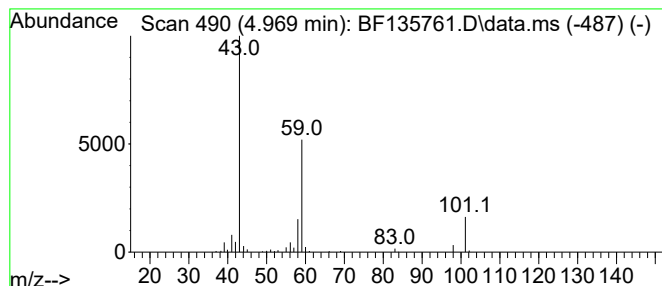
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	3.82 ng	122392	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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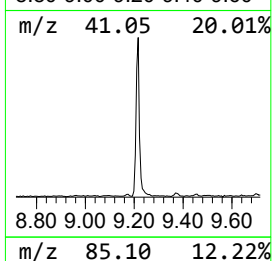
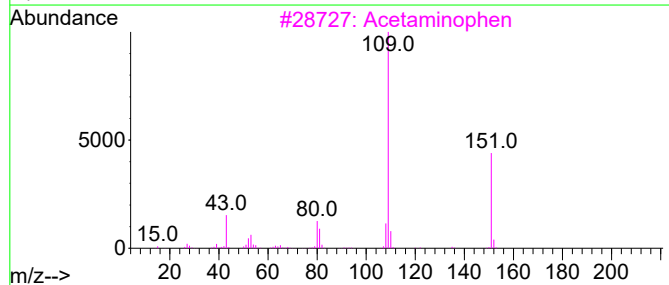
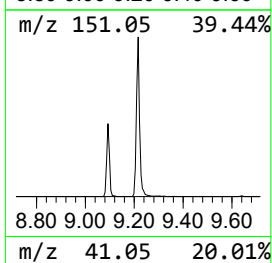
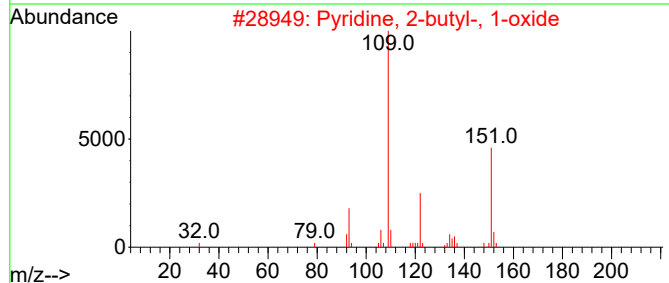
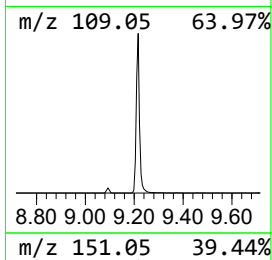
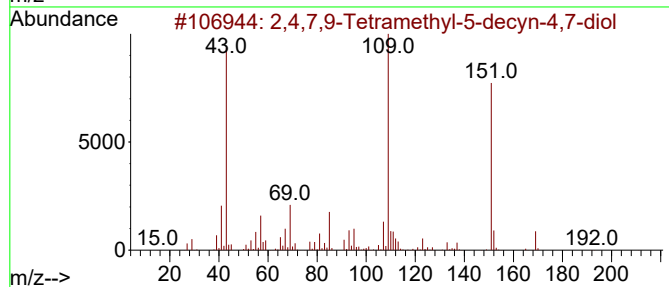
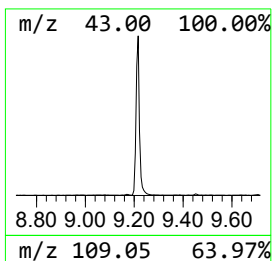
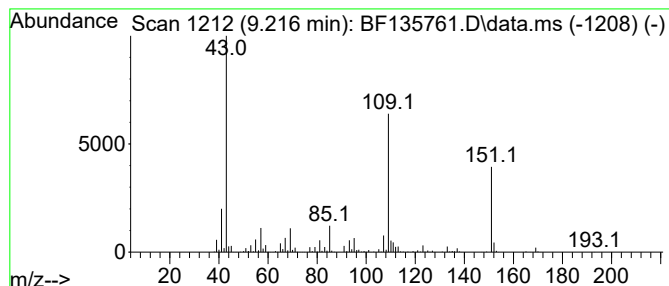
Instrument :
BNA_F
ClientSampleId :
ETGI-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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.
9.216	22.84 ng	893924	Acenaphthene-d10	9.775
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226 C14H26O2	000126-86-3	64
2	Pyridine, 2-butyl-, 1-oxide	151 C9H13NO	031396-32-4	59
3	Acetaminophen	151 C8H9NO2	000103-90-2	50
4	Metacetamol	151 C8H9NO2	000621-42-1	50
5	Butanamide, N-acetyl-N-(4-hydrox...	221 C12H15NO3	1000107-08-7	40



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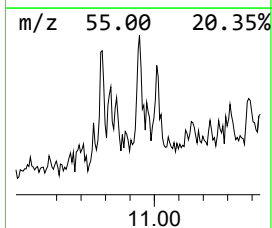
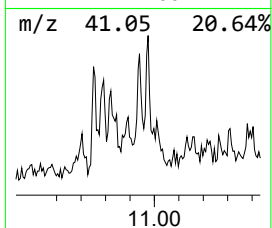
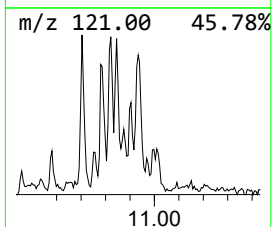
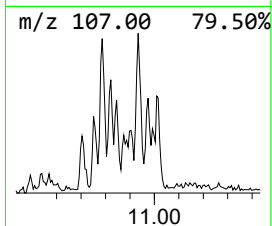
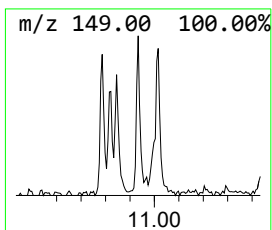
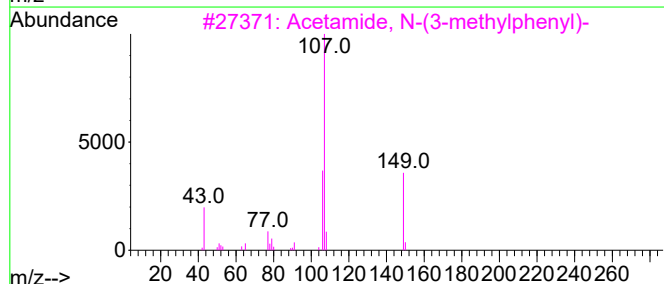
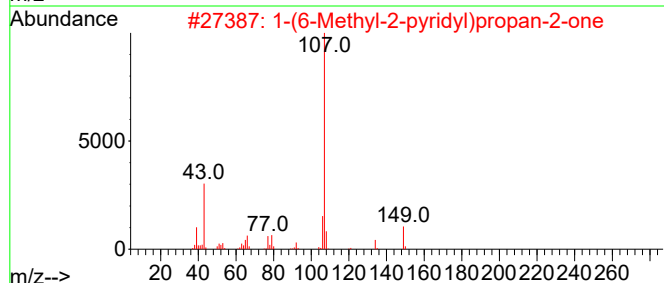
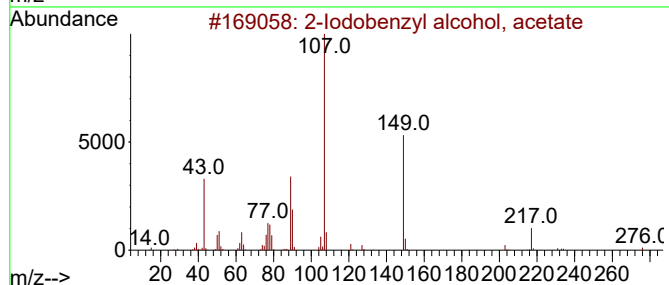
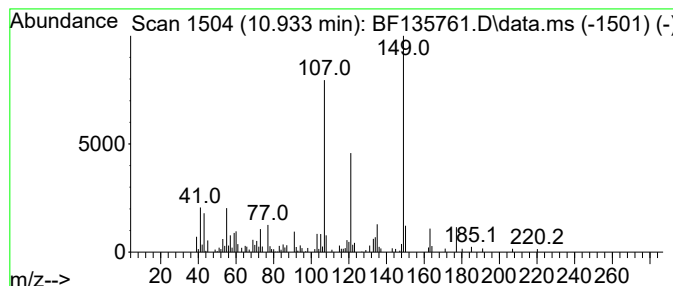
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Iodobenzyl alcohol, acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.933	2.26 ng	88232	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Iodobenzyl alcohol, acetate	276	C9H9IO2	1000364-47-1	59
2			1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	58
3			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	58
4			Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	53
5			Ethanone, 2-(1-methylethoxy)-1,2...	254	C17H18O2	006652-28-4	53



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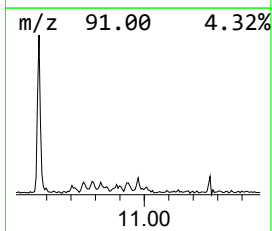
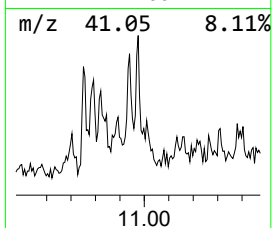
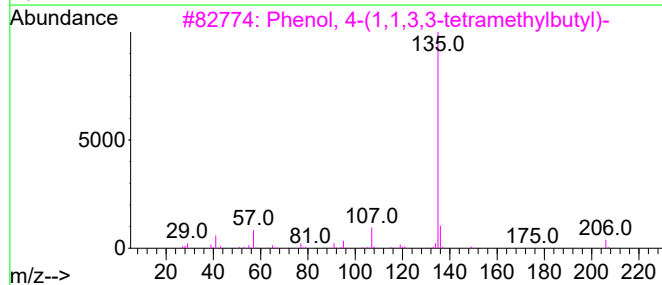
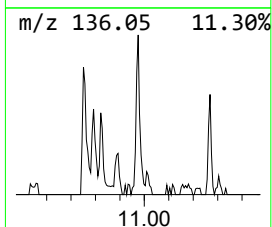
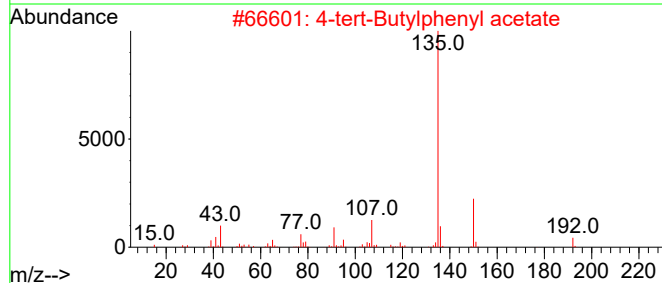
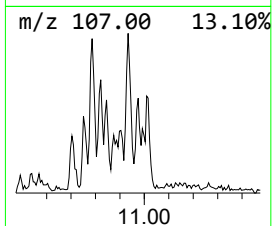
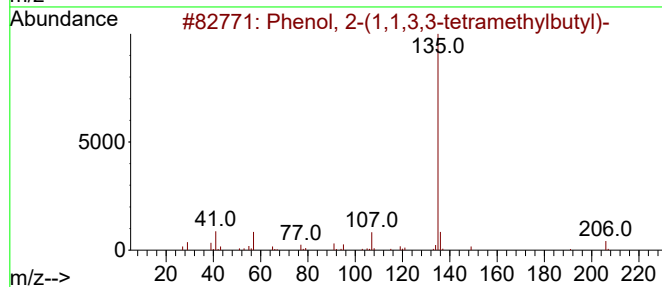
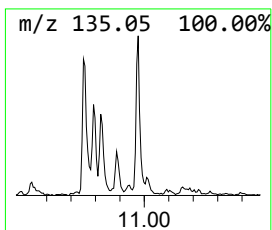
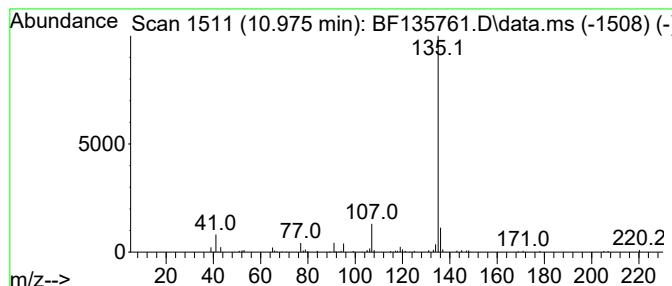
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenol, 2-(1,1,3,3-tetramet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.975	2.03 ng	79136	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
2	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78
3	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
4	4-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-25-4	78
5	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78



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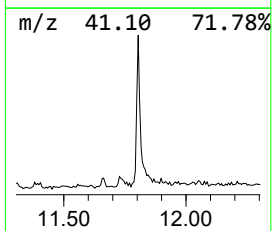
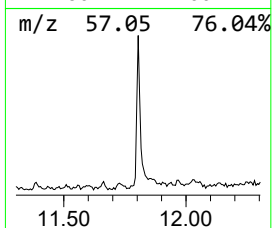
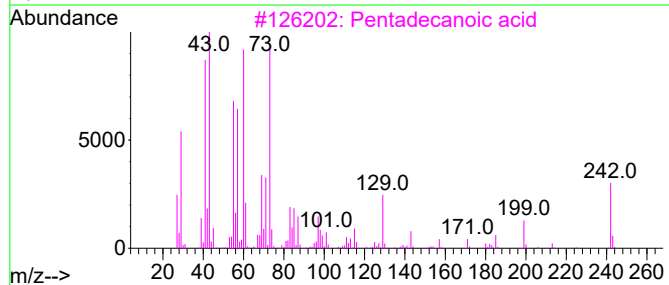
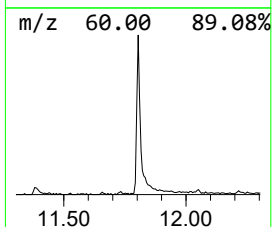
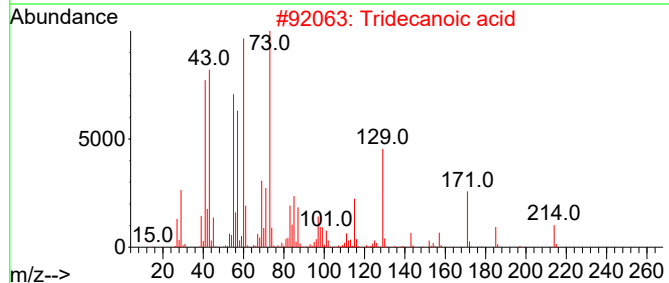
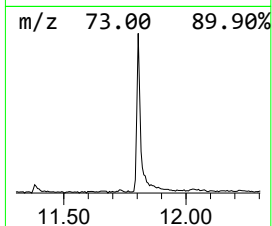
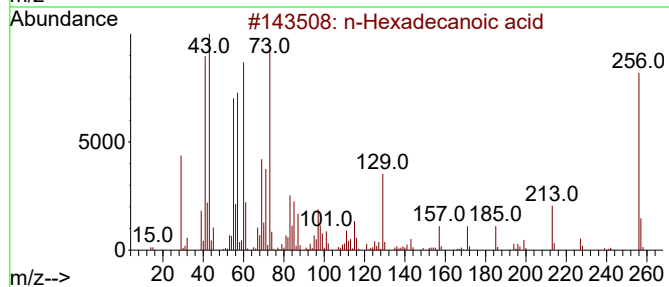
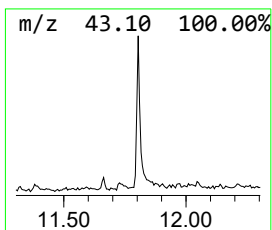
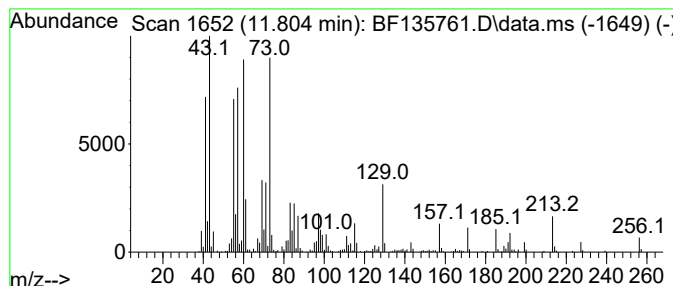
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
11.804	10.03 ng	390978	Phenanthrene-d10	11.269	
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	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135761.D
Acq On : 13 Oct 2023 19:41
Operator : CG\JU
Sample : 04837-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-290

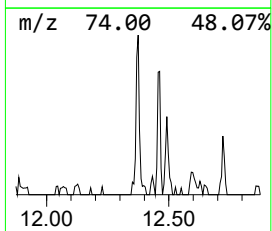
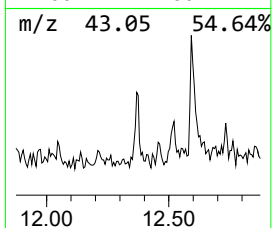
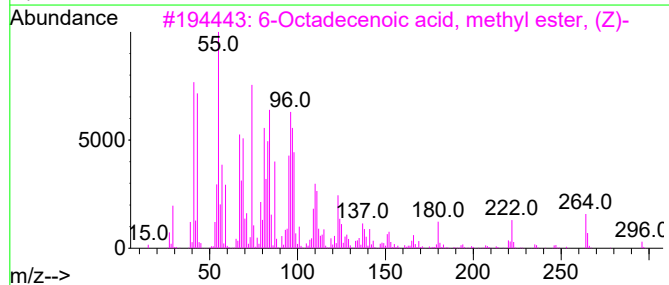
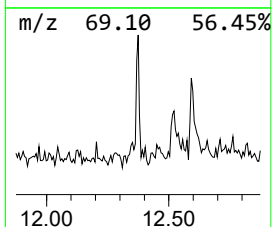
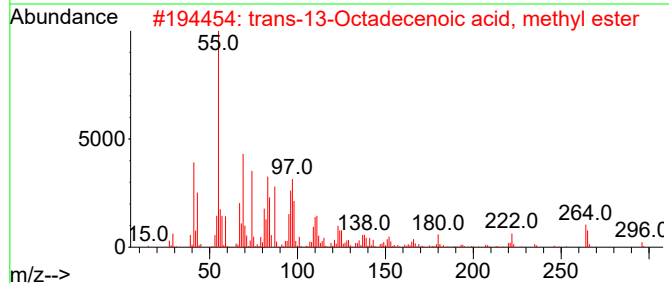
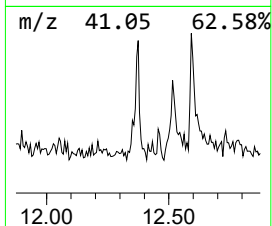
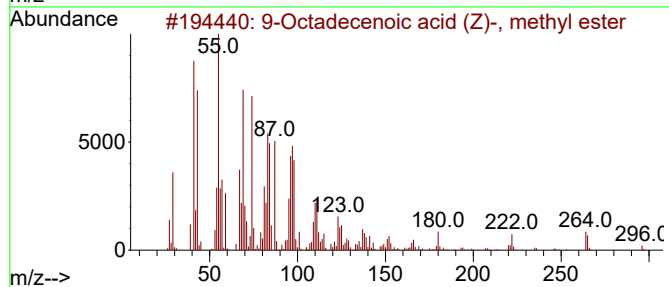
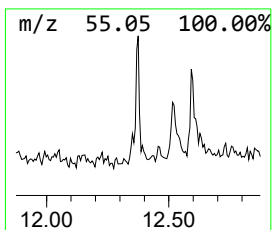
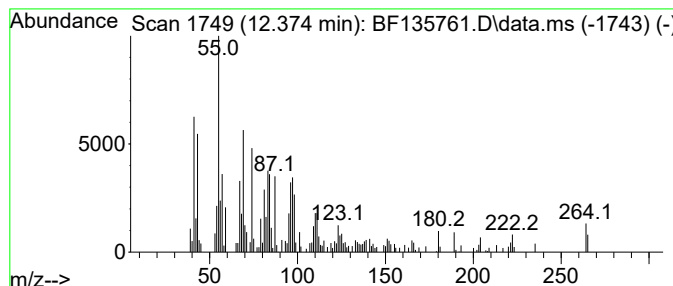
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	2.67 ng	104113	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
3			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	91
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
5			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135761.D
Acq On : 13 Oct 2023 19:41
Operator : CG\JU
Sample : 04837-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

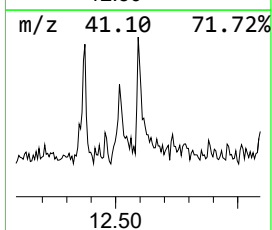
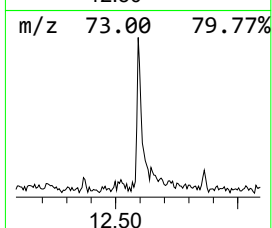
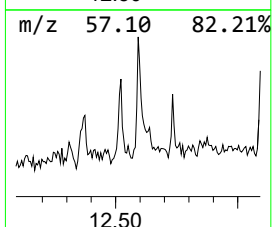
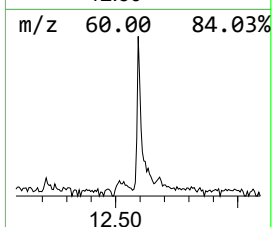
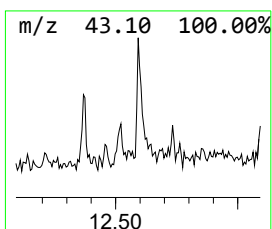
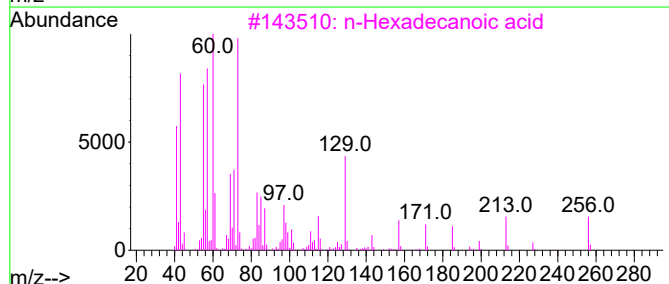
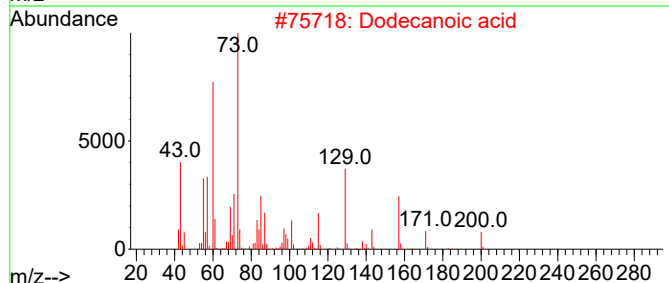
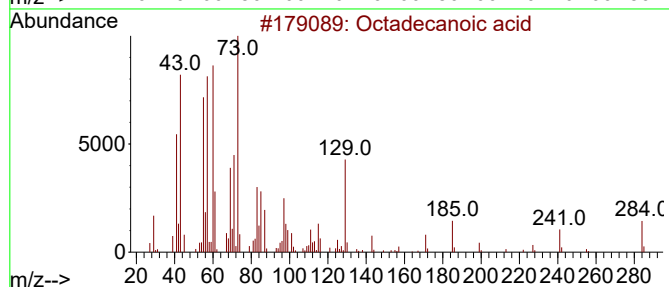
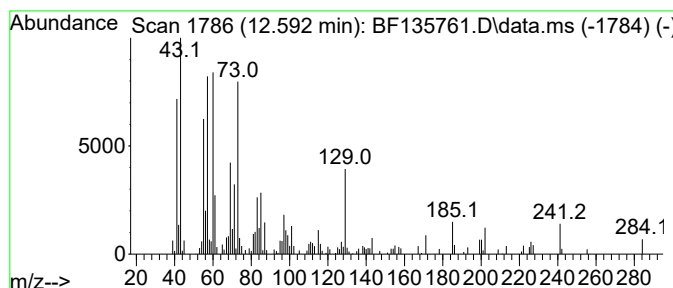
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.592	2.69 ng	104804	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	Dodecanoic acid	200	C12H24O2	000143-07-7	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
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Operator : CG\JU
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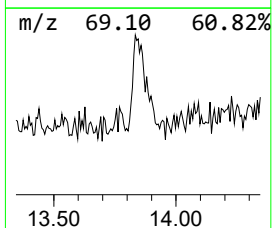
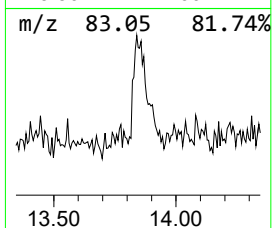
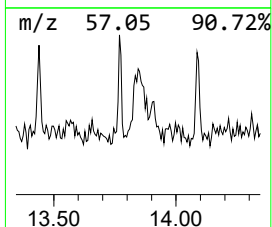
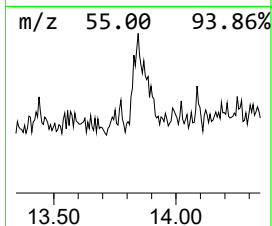
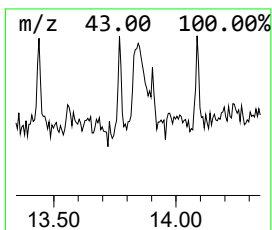
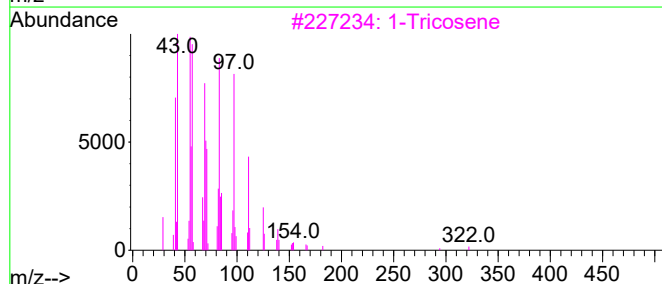
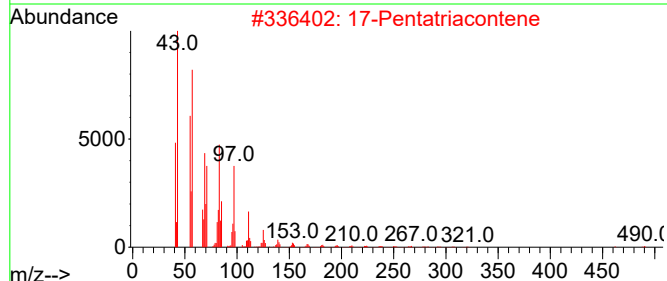
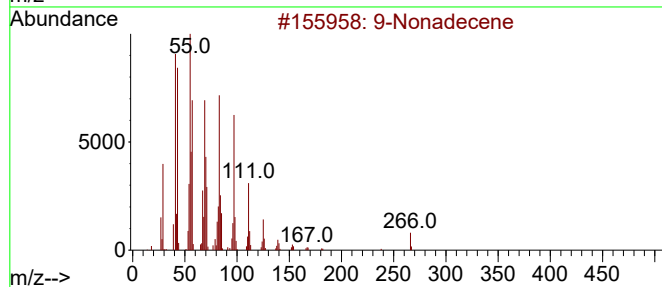
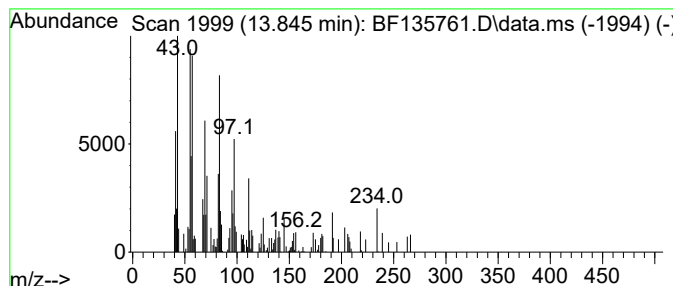
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.845	2.46 ng	76405	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Nonadecene	266	C19H38	031035-07-1	70
2	17-Pentatriacontene	491	C35H70	006971-40-0	68
3	1-Tricosene	322	C23H46	018835-32-0	58
4	1-Eicosanol	298	C20H42O	000629-96-9	58
5	1-Nonadecene	266	C19H38	018435-45-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135761.D
Acq On : 13 Oct 2023 19:41
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Sample : 04837-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ETGI-290

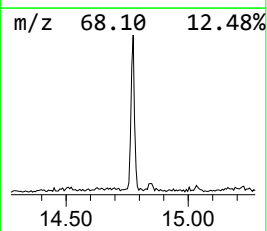
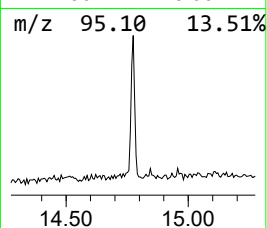
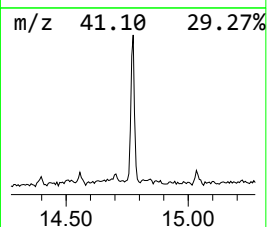
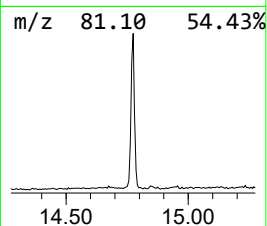
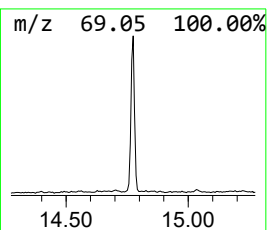
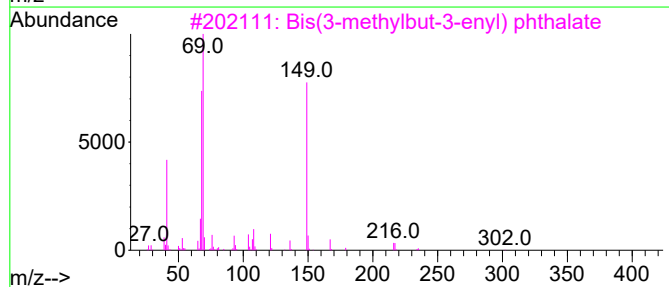
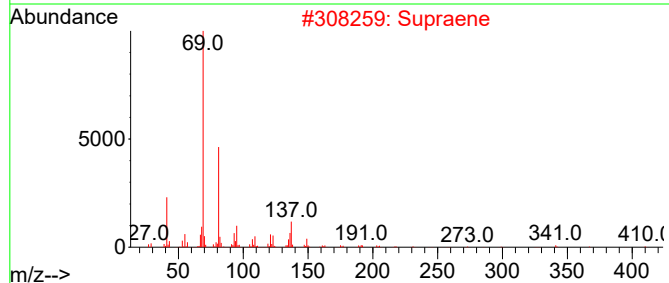
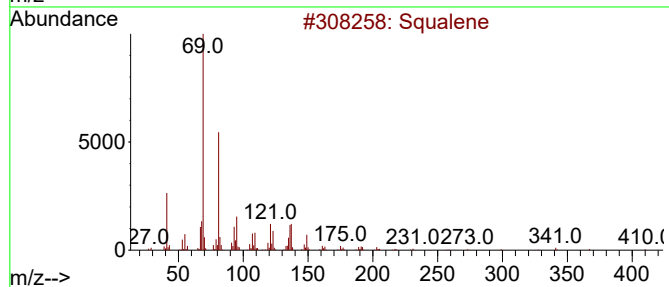
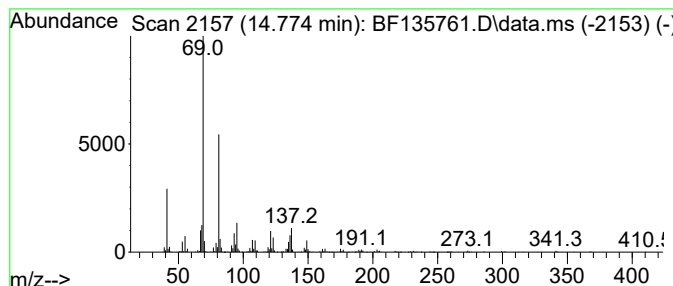
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	13.72 ng	459880	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	98
2			Supraene	410	C30H50	007683-64-9	91
3			Bis(3-methylbut-3-enyl) phthalate	302	C18H22O4	022711-53-1	53
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5			1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135761.D
Acq On : 13 Oct 2023 19:41
Operator : CG\JU
Sample : 04837-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-290

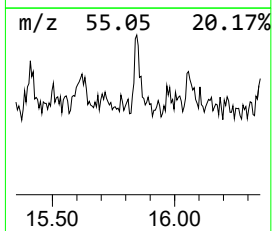
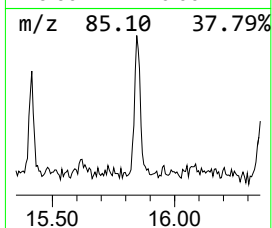
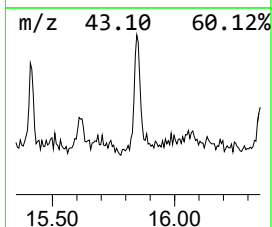
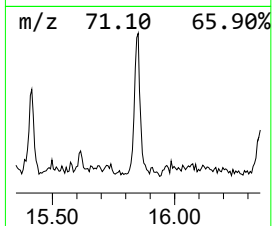
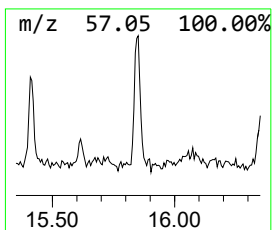
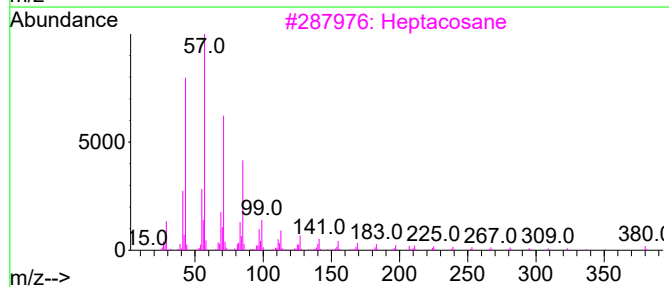
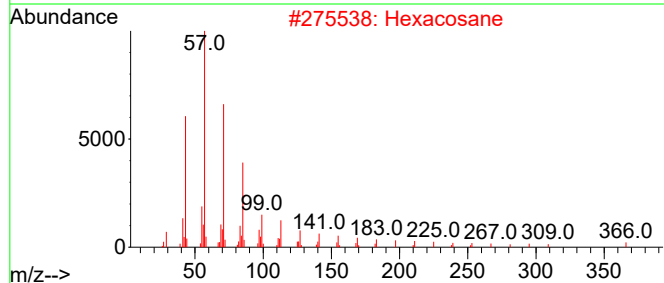
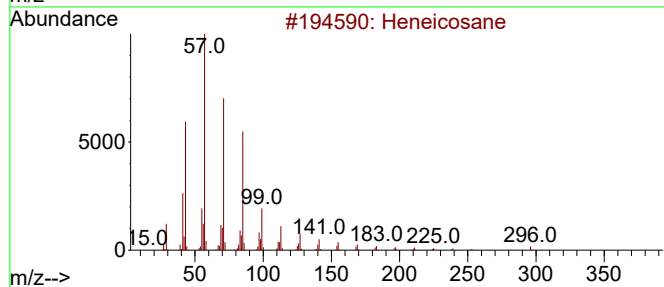
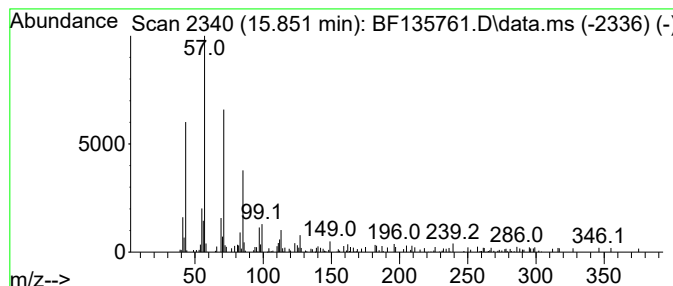
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	2.34 ng	78403	Perylene-d12	15.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	93
2		Hexacosane	366	C26H54	000630-01-3	86
3		Heptacosane	380	C27H56	000593-49-7	86
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135761.D
Acq On : 13 Oct 2023 19:41
Operator : CG\JU
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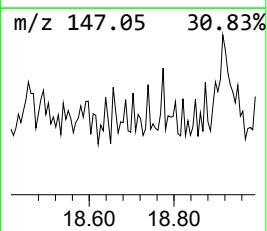
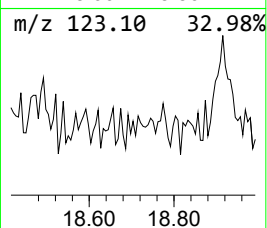
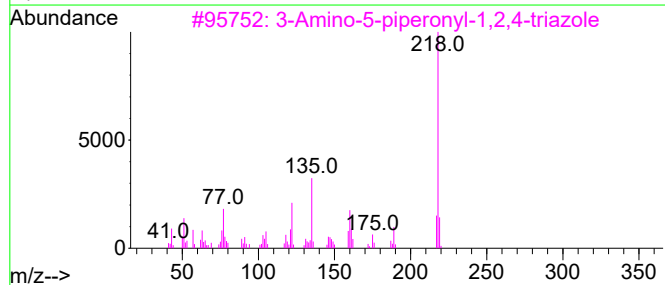
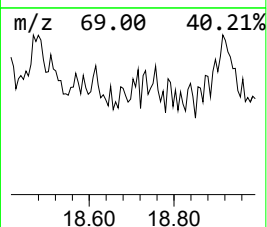
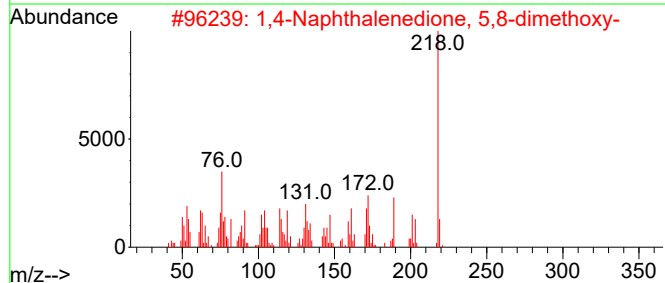
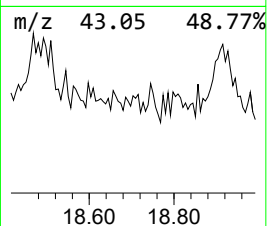
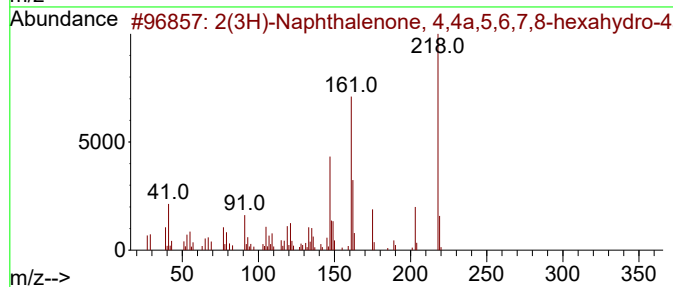
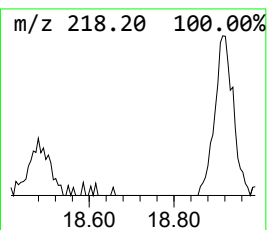
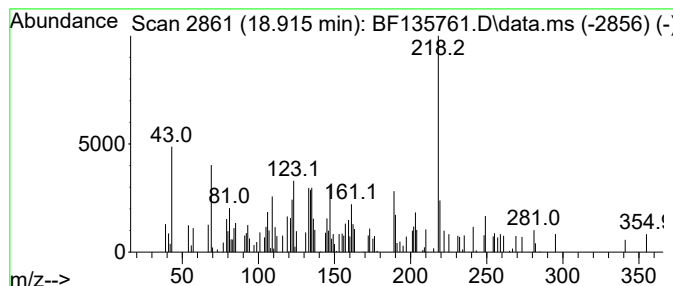
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2(3H)-Naphthalenone, 4,4a,5... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.915	2.45 ng	82182	Perylene-d12	15.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	60
2	1,4-Naphthalenedione, 5,8-dimeth...	218	C12H10O4	015013-16-8	49
3	3-Amino-5-piperonyl-1,2,4-triazole	218	C10H10N4O2	014730-92-8	49
4	.alpha.-Amyrin, TMS derivative	498	C33H58OSi	1000374-76-6	47
5	1H-Pyrrolo[3,4-c]quinoline-1,3,4...	218	C11H10N2O3	181021-85-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135761.D
Acq On : 13 Oct 2023 19:41
Operator : CG\JU
Sample : 04837-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ETGI-290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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
2-Pentanone, 4-...	4.969	3.8	ng	122392	1	6.734	641115	20.0
2,4,7,9-Tetrame...	9.216	22.8	ng	893924	3	9.775	782759	20.0
2-Iodobenzyl al...	10.933	2.3	ng	88232	4	11.269	779887	20.0
Phenol, 2-(1,1,...	10.975	2.0	ng	79136	4	11.269	779887	20.0
n-Hexadecanoic ...	11.804	10.0	ng	390978	4	11.269	779887	20.0
9-Octadecenoic ...	12.374	2.7	ng	104113	4	11.269	779887	20.0
Octadecanoic acid	12.592	2.7	ng	104804	4	11.269	779887	20.0
9-Nonadecene	13.845	2.5	ng	76405	5	13.933	619949	20.0
Squalene	14.774	13.7	ng	459880	6	15.410	670254	20.0
Heneicosane	15.851	2.3	ng	78403	6	15.410	670254	20.0
2(3H)-Naphthale...	18.915	2.5	ng	82182	6	15.410	670254	20.0