

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
 Data File : BF140619.D
 Acq On : 25 Nov 2024 22:29
 Operator : RC/JU
 Sample : P4860-10
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PH2-BOT-005

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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	503	508	522	rVB	13193	19880	1.50%	0.218%
2	5.493	573	578	596	rBV	724593	966056	72.77%	10.588%
3	6.504	744	750	771	rBV	760428	1025884	77.27%	11.244%
4	6.869	807	812	821	rBV	260321	319371	24.06%	3.500%
5	7.428	902	907	925	rBV	503817	660566	49.76%	7.240%
6	8.151	1025	1030	1045	rBV	297119	393975	29.68%	4.318%
7	9.222	1207	1212	1222	rBV	1020392	1284468	96.75%	14.078%
8	9.904	1323	1328	1339	rBV	342168	439751	33.12%	4.820%
9	10.616	1444	1449	1458	rBV	165730	212183	15.98%	2.326%
10	10.698	1458	1463	1478	rVV	471092	662853	49.93%	7.265%
11	10.928	1497	1502	1512	rBV	25471	34510	2.60%	0.378%
12	11.392	1576	1581	1590	rBV	362243	475821	35.84%	5.215%
13	11.916	1666	1670	1685	rBV	42236	78683	5.93%	0.862%
14	12.645	1785	1794	1799	rBV	36213	50540	3.81%	0.554%
15	12.980	1845	1851	1860	rVB	1041433	1327600	100.00%	14.551%
16	13.545	1942	1947	1952	rBV	15410	20402	1.54%	0.224%
17	13.874	1998	2003	2006	rBV	23124	36381	2.74%	0.399%
18	14.010	2022	2026	2027	rBV	16378	18058	1.36%	0.198%
19	14.039	2027	2031	2044	rVB	254250	353128	26.60%	3.870%
20	14.192	2052	2057	2067	rBV	24765	34122	2.57%	0.374%
21	14.498	2104	2109	2115	rBV	34195	45458	3.42%	0.498%
22	14.810	2157	2162	2169	rVV	24600	36825	2.77%	0.404%
23	14.886	2171	2175	2181	rVB	9685	14717	1.11%	0.161%
24	15.151	2215	2220	2228	rVB	36145	53415	4.02%	0.585%
25	15.527	2278	2284	2299	rVB	208068	345241	26.00%	3.784%
26	15.974	2355	2360	2368	rBV	16408	28613	2.16%	0.314%
27	16.274	2405	2411	2431	rVB	12628	58265	4.39%	0.639%
28	16.433	2432	2438	2444	rVV3	50999	90580	6.82%	0.993%
29	17.427	2602	2607	2615	rBV9	8762	16560	1.25%	0.182%
30	17.909	2684	2689	2696	rVB8	8507	19926	1.50%	0.218%

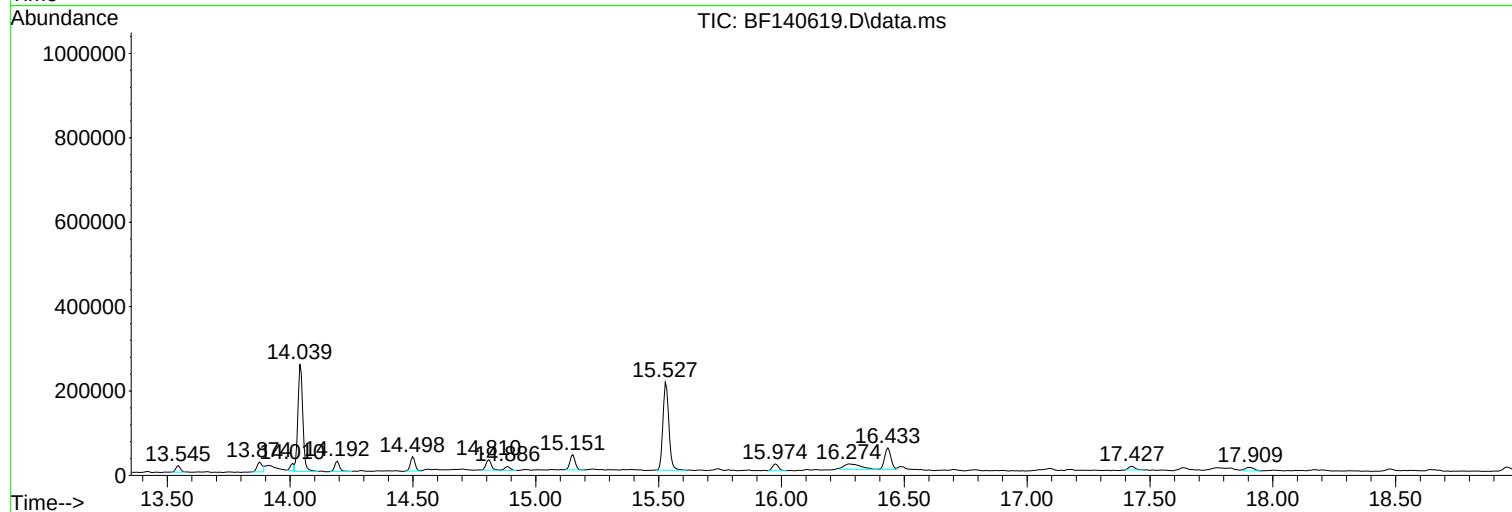
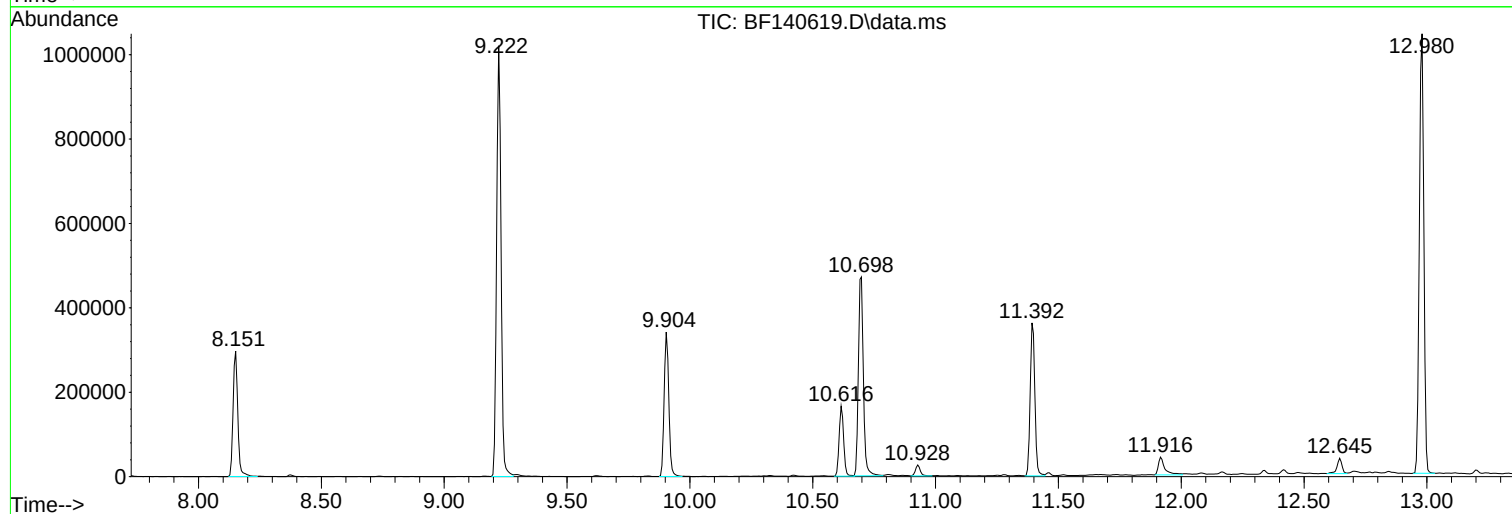
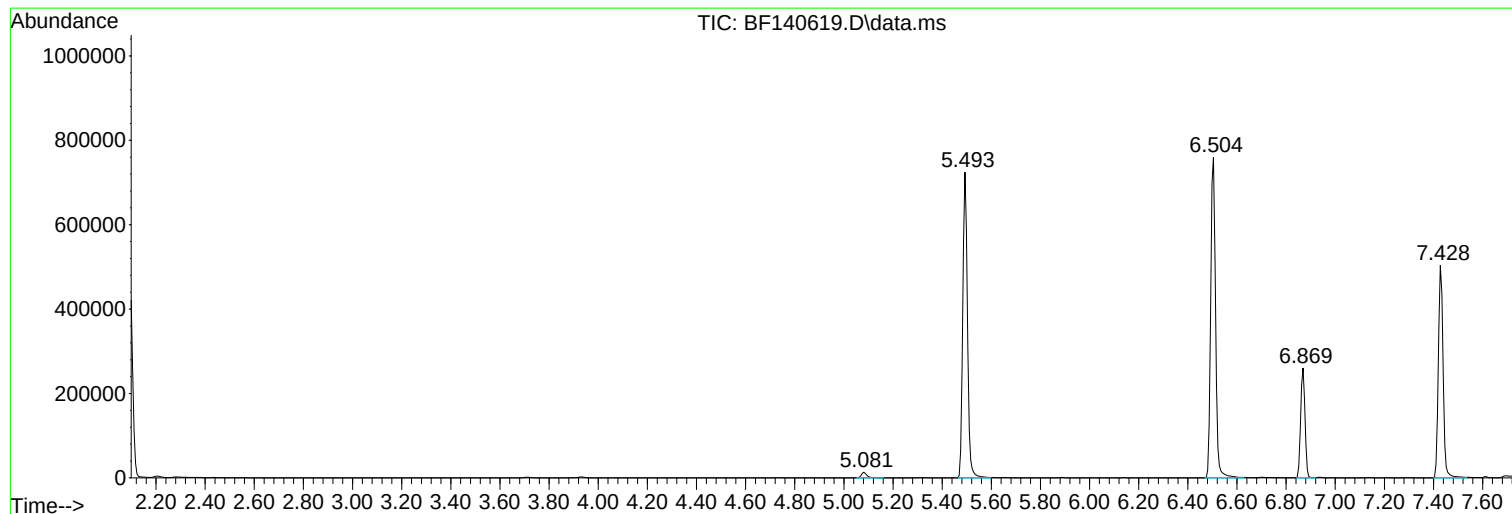
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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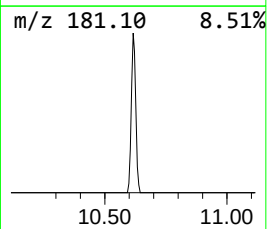
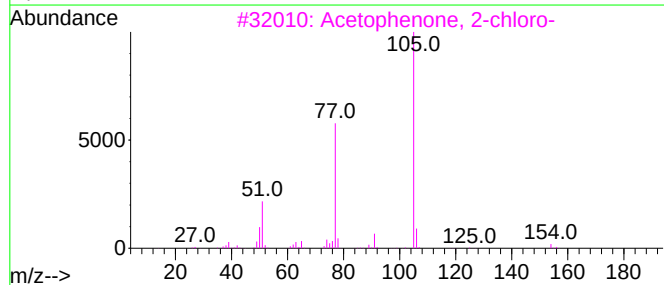
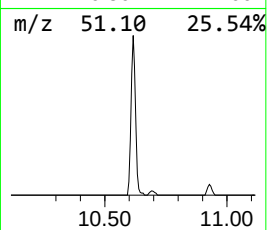
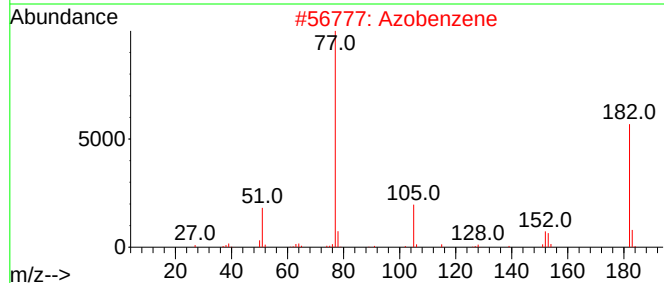
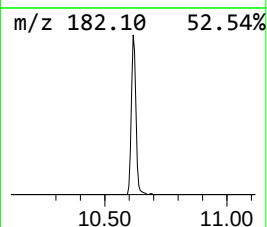
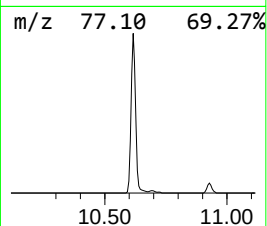
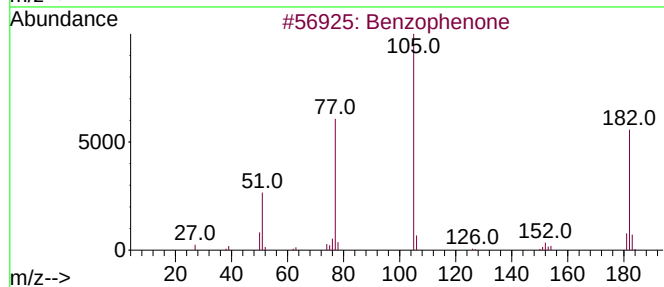
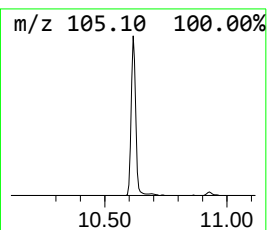
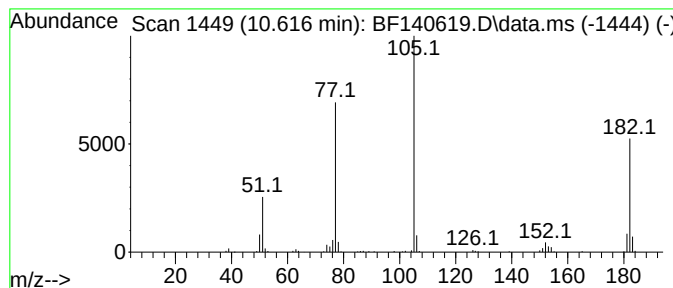
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	9.65 ng	212183	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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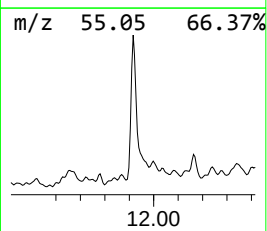
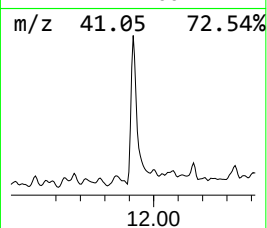
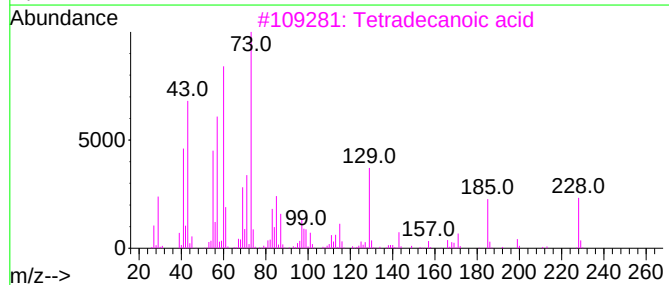
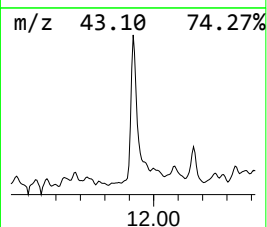
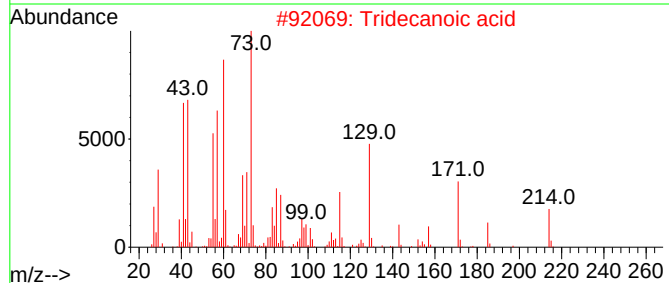
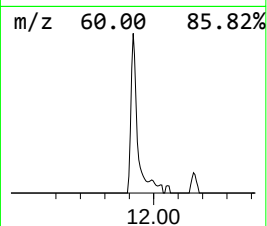
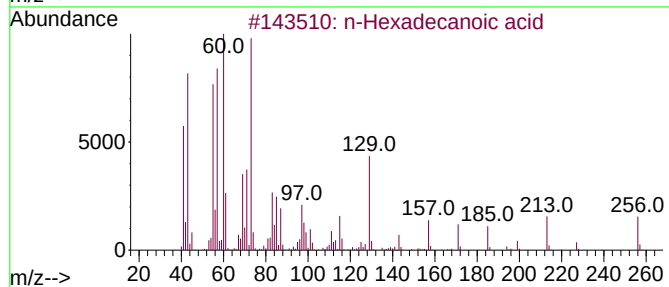
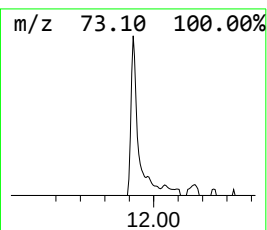
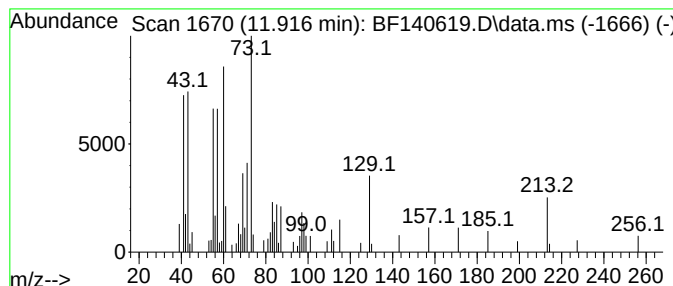
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.31 ng	78683	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59



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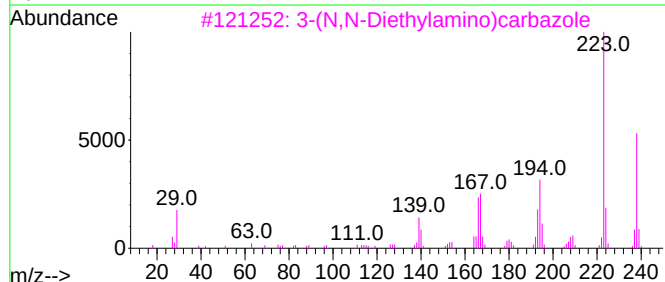
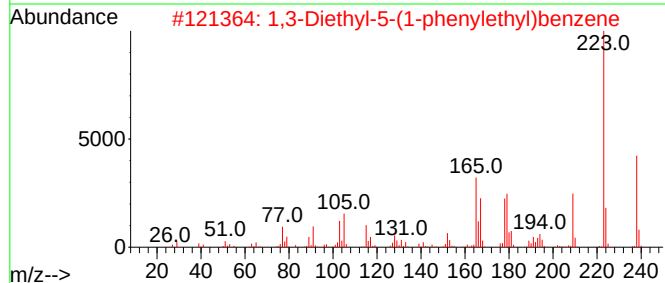
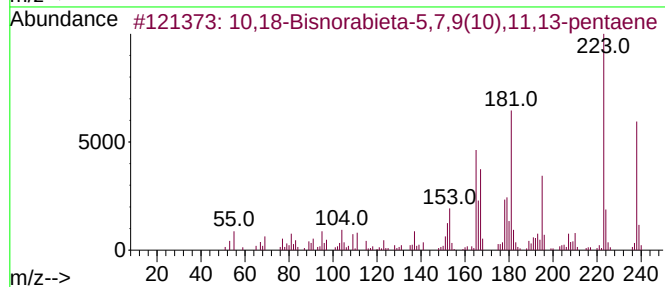
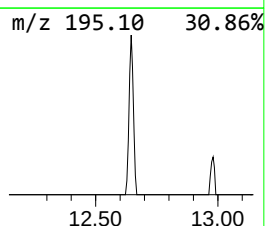
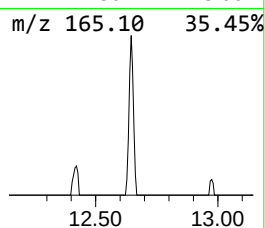
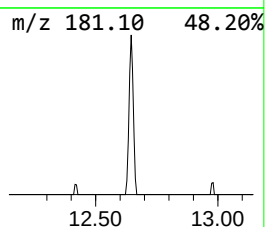
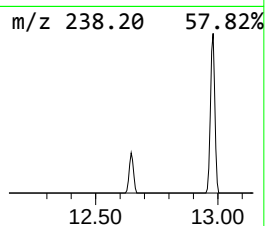
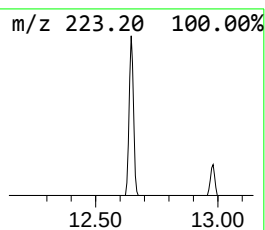
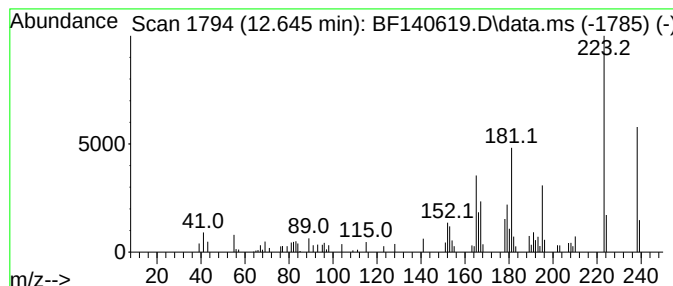
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Peak Number 3 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.12 ng	50540	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	96		
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	81		
3	3-(N,N-Diethylamino)carbazole	238	C16H18N2	054994-31-9	53		
4	Anthracene, 9,10-dimethoxy-	238	C16H14O2	002395-97-3	49		
5	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	49		



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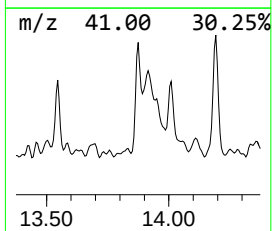
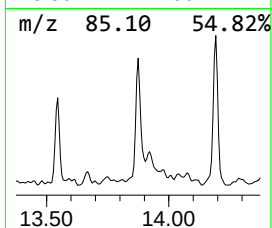
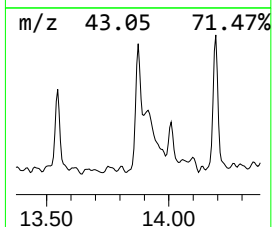
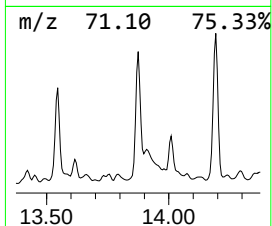
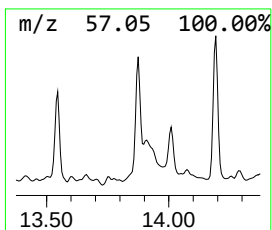
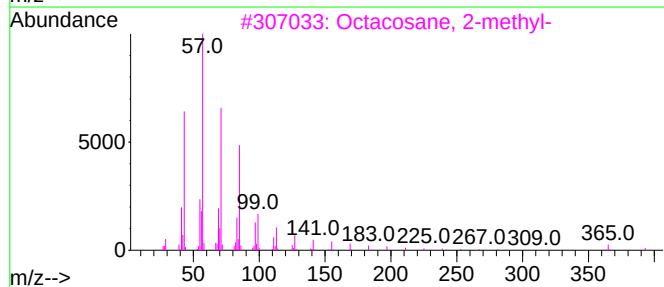
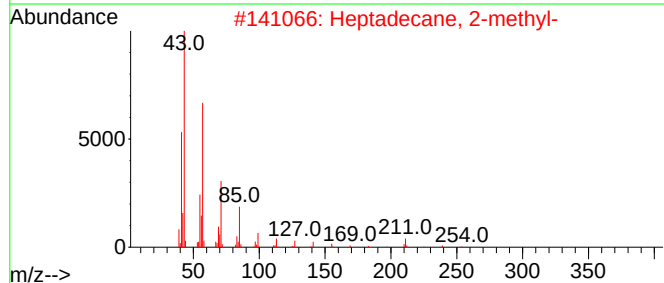
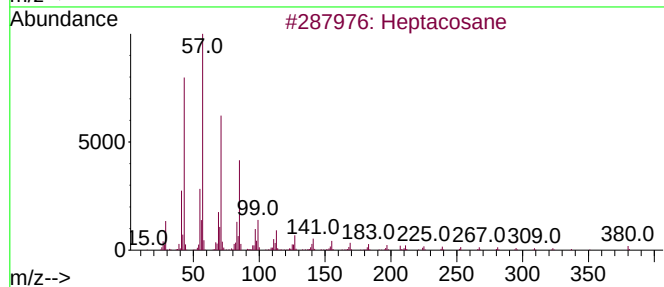
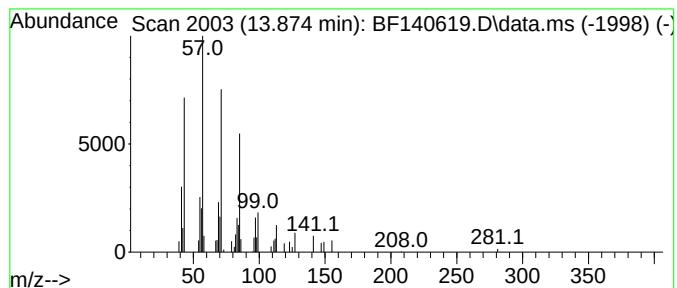
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Peak Number 4 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.06 ng	36381	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



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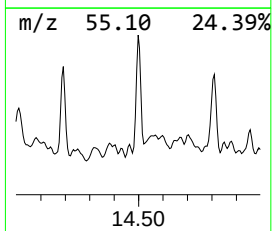
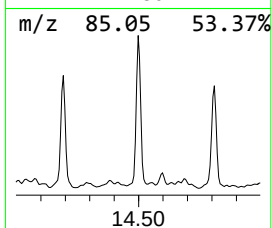
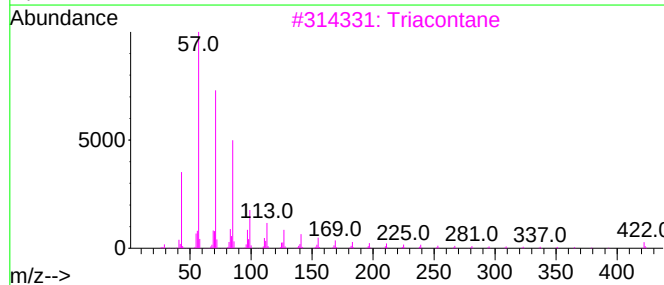
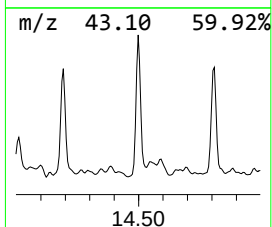
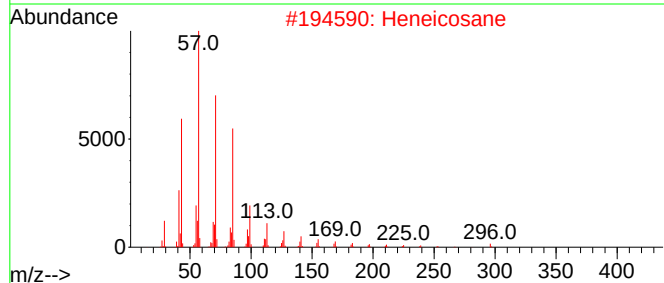
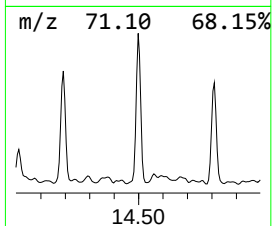
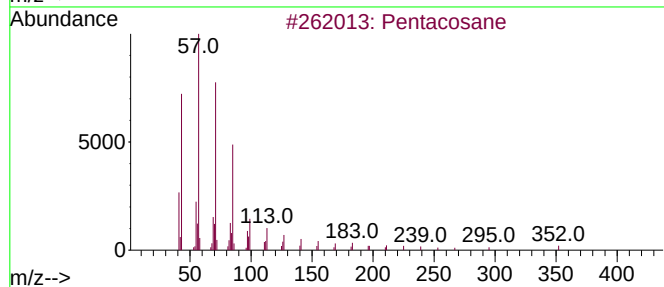
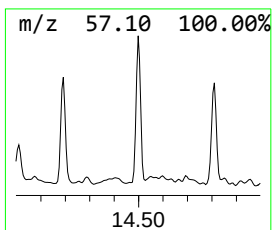
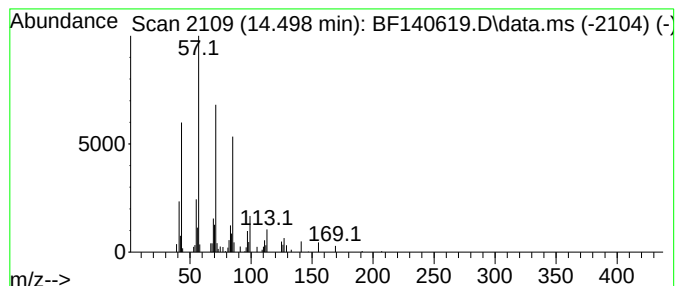
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Peak Number 5 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	2.57 ng	45458	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Hexacosane	366	C26H54	000630-01-3	90



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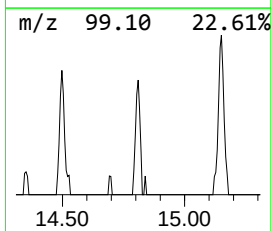
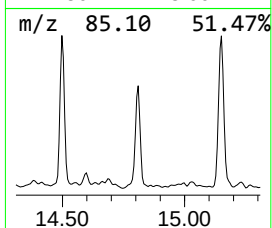
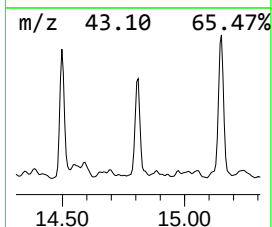
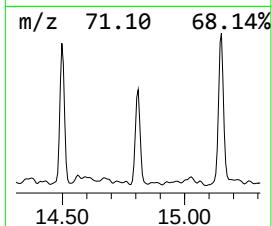
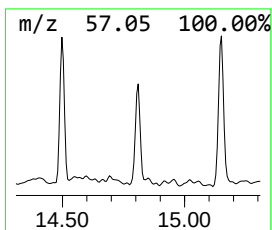
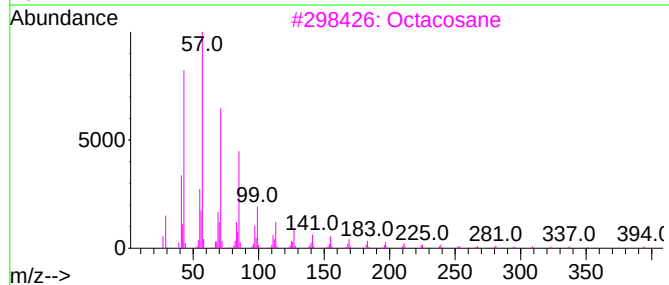
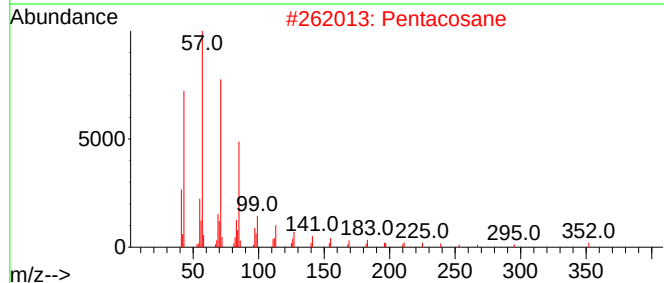
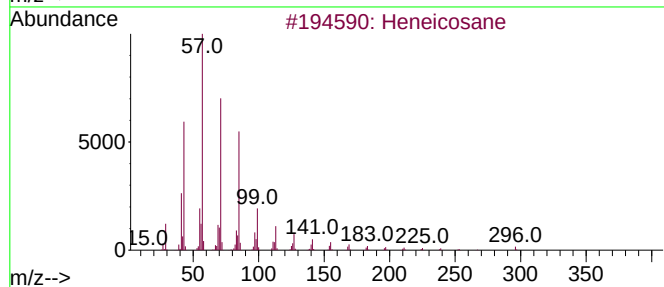
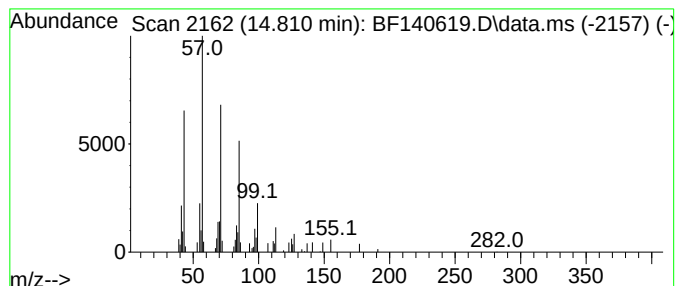
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	2.13 ng	36825	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentacosane	352	C25H52	000629-99-2	87
3	Octacosane	394	C28H58	000630-02-4	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	86
5	triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140619.D
Acq On : 25 Nov 2024 22:29
Operator : RC/JU
Sample : P4860-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-005

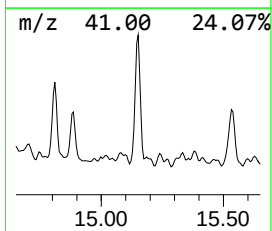
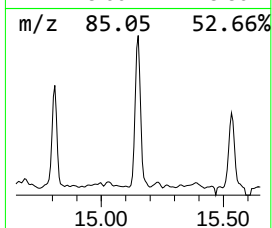
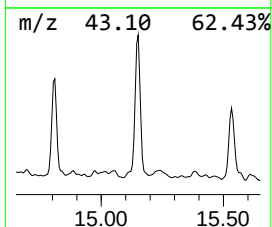
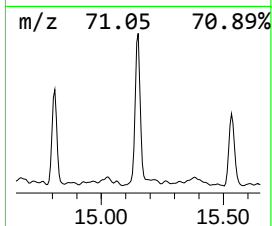
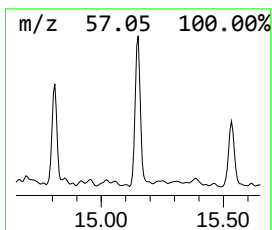
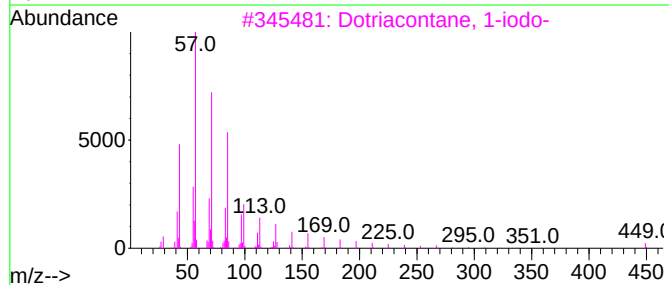
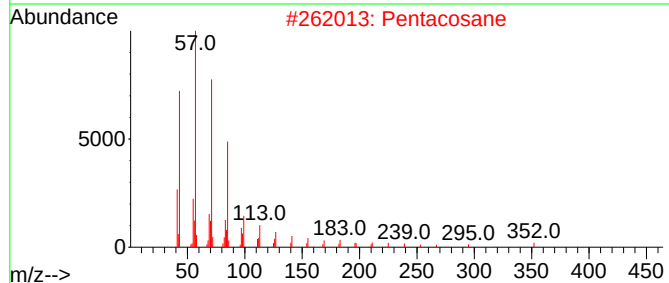
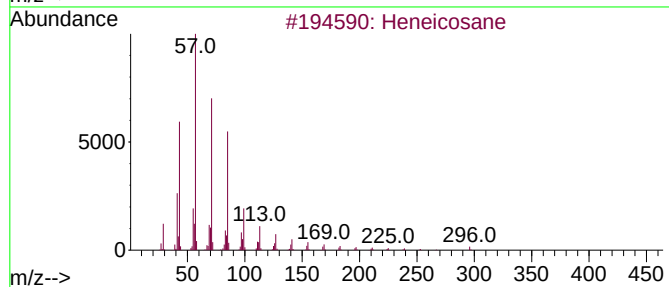
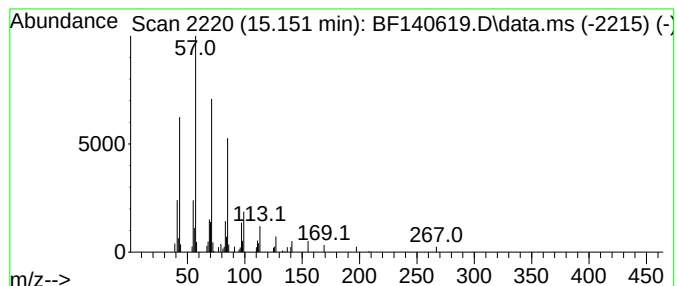
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	3.09 ng	53415	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140619.D
Acq On : 25 Nov 2024 22:29
Operator : RC/JU
Sample : P4860-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-005

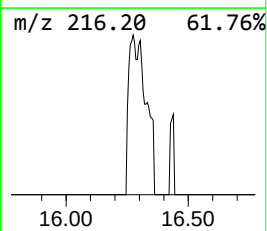
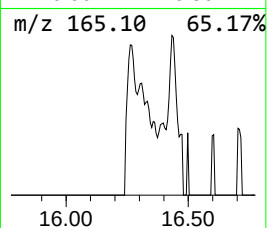
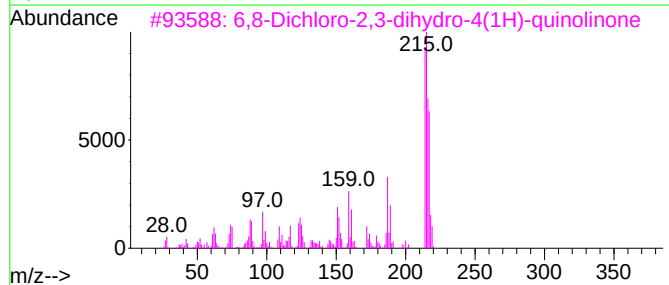
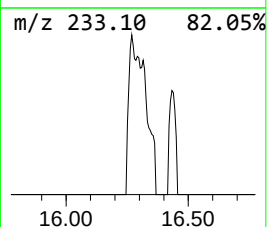
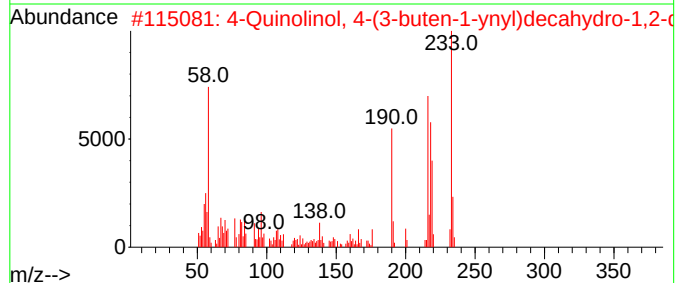
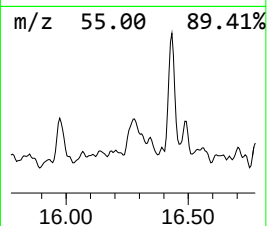
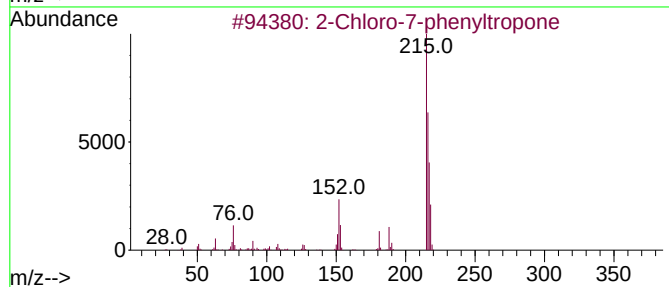
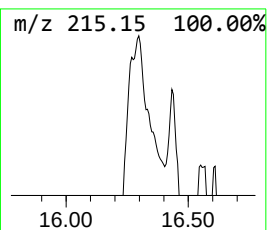
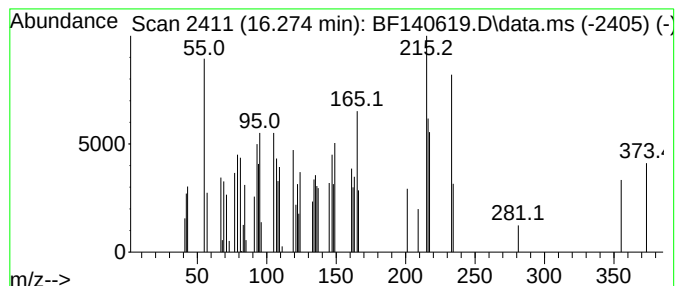
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.274 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.274	3.38 ng	58265	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-7-phenyltropone	216	C13H9ClO	090128-01-1	12
2			4-Quinolinol, 4-(3-buten-1-ynyl)...	233	C15H23NO	037982-01-7	12
3			6,8-Dichloro-2,3-dihydro-4(1H)-q...	215	C9H7Cl2NO	036054-22-5	12
4			Pregnane-3,20-diol, (3.alpha.,5....	320	C21H36O2	000080-92-2	11
5			Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140619.D
Acq On : 25 Nov 2024 22:29
Operator : RC/JU
Sample : P4860-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-005

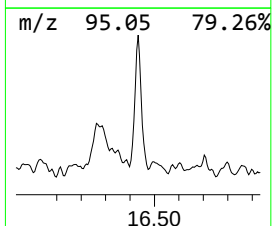
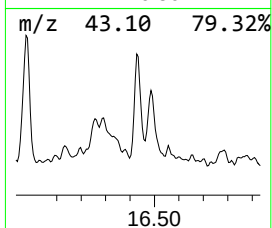
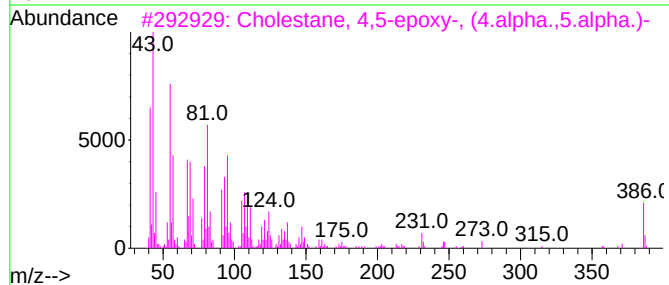
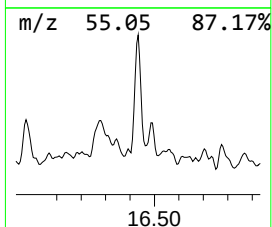
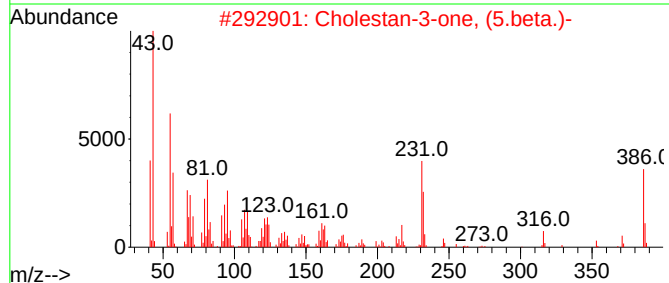
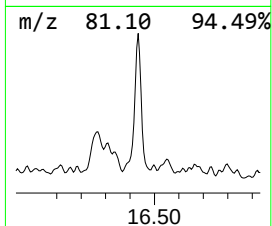
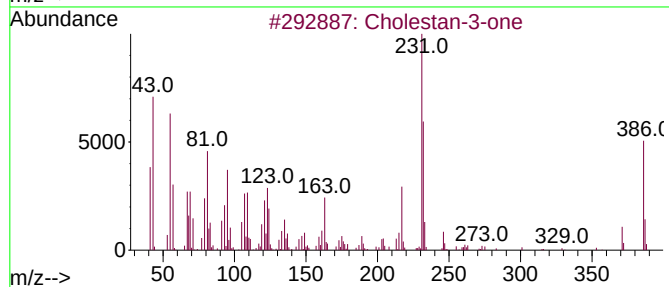
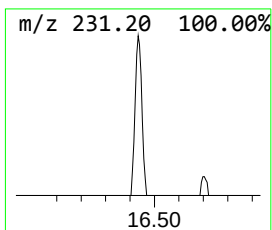
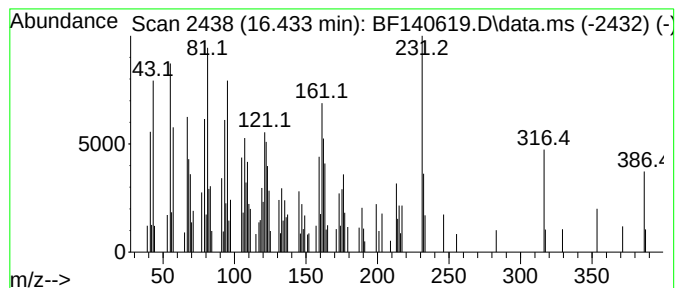
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cholestan-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.433	5.25 ng	90580	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-one	386	C27H46O	015600-08-5	86
2			Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	70
3			Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	46
4			Cholestan-2-one	386	C27H46O	1010210-43-4	46
5			Pregn-5-en-20-one, 3-hydroxy-	316	C21H32O2	038372-24-6	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140619.D
Acq On : 25 Nov 2024 22:29
Operator : RC/JU
Sample : P4860-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-005

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzophenone	10.616	9.7	ng	212183	3	9.904	439751	20.0
n-Hexadecanoic ...	11.916	3.3	ng	78683	4	11.392	475821	20.0
10,18-Bisnorabi...	12.645	2.1	ng	50540	4	11.392	475821	20.0
Heptacosane	13.874	2.1	ng	36381	5	14.039	353128	20.0
Pentacosane	14.498	2.6	ng	45458	5	14.039	353128	20.0
Heneicosane	14.810	2.1	ng	36825	6	15.527	345241	20.0
Dotriacontane, ...	15.151	3.1	ng	53415	6	15.527	345241	20.0
unknown16.274	16.274	3.4	ng	58265	6	15.527	345241	20.0
Cholestan-3-one	16.433	5.3	ng	90580	6	15.527	345241	20.0