

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
 Data File : BF129817.D
 Acq On : 16 Aug 2022 18:38
 Operator : CG\JU
 Sample : N4208-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-1

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-BF081422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	465	468	484	rVB	291399	337582	13.19%	1.732%
2	5.463	536	540	554	rBV	1695315	1805880	70.54%	9.265%
3	6.475	708	712	726	rBV	1972652	1916307	74.85%	9.832%
4	6.816	767	770	780	rVB	951060	881760	34.44%	4.524%
5	7.386	863	867	870	rBV	1484630	1294444	50.56%	6.641%
6	8.104	984	989	992	rBV	1271051	1178530	46.03%	6.047%
7	9.175	1166	1171	1174	rBV	3097340	2560128	100.00%	13.135%
8	9.439	1213	1216	1219	rVB	66867	53601	2.09%	0.275%
9	9.480	1219	1223	1225	rBV	185674	161987	6.33%	0.831%
10	9.504	1225	1227	1229	rVV	79149	67876	2.65%	0.348%
11	9.557	1233	1236	1240	rVB	65237	62637	2.45%	0.321%
12	9.751	1263	1269	1271	rBV	29806	38023	1.49%	0.195%
13	9.786	1271	1275	1283	rVB2	34099	39420	1.54%	0.202%
14	9.857	1283	1287	1291	rBV	1669424	1348431	52.67%	6.918%
15	10.245	1347	1353	1356	rBV2	69592	59249	2.31%	0.304%
16	10.527	1398	1401	1408	rVB	31418	30384	1.19%	0.156%
17	10.651	1418	1422	1427	rBV	1513245	1268370	49.54%	6.507%
18	10.698	1427	1430	1432	rVV	47488	40543	1.58%	0.208%
19	11.351	1537	1541	1544	rBV	1404364	1293857	50.54%	6.638%
20	12.433	1715	1725	1728	rBV5	18057	31011	1.21%	0.159%
21	12.933	1805	1810	1813	rBV	2412693	2205926	86.16%	11.318%
22	13.251	1860	1864	1873	rVB3	62168	95123	3.72%	0.488%
23	13.357	1879	1882	1885	rBV	324159	321882	12.57%	1.651%
24	13.392	1885	1888	1895	rVB	176522	234262	9.15%	1.202%
25	13.868	1963	1969	1982	rBV	23660	81311	3.18%	0.417%
26	13.998	1987	1991	1995	rBV	830558	767109	29.96%	3.936%
27	14.421	2060	2063	2069	rVB3	38218	54648	2.13%	0.280%
28	14.886	2139	2142	2146	rBV2	71306	64498	2.52%	0.331%
29	15.068	2170	2173	2177	rVB2	37019	41379	1.62%	0.212%
30	15.462	2235	2240	2249	rVB2	571886	750660	29.32%	3.851%
31	15.645	2267	2271	2276	rBV3	60213	80987	3.16%	0.416%
32	15.868	2304	2309	2314	rVB	57186	84160	3.29%	0.432%
33	16.656	2438	2443	2450	rVB2	56407	97060	3.79%	0.498%
34	16.945	2488	2492	2499	rVB3	22714	41332	1.61%	0.212%
35	18.068	2678	2683	2692	rVB4	40760	100719	3.93%	0.517%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

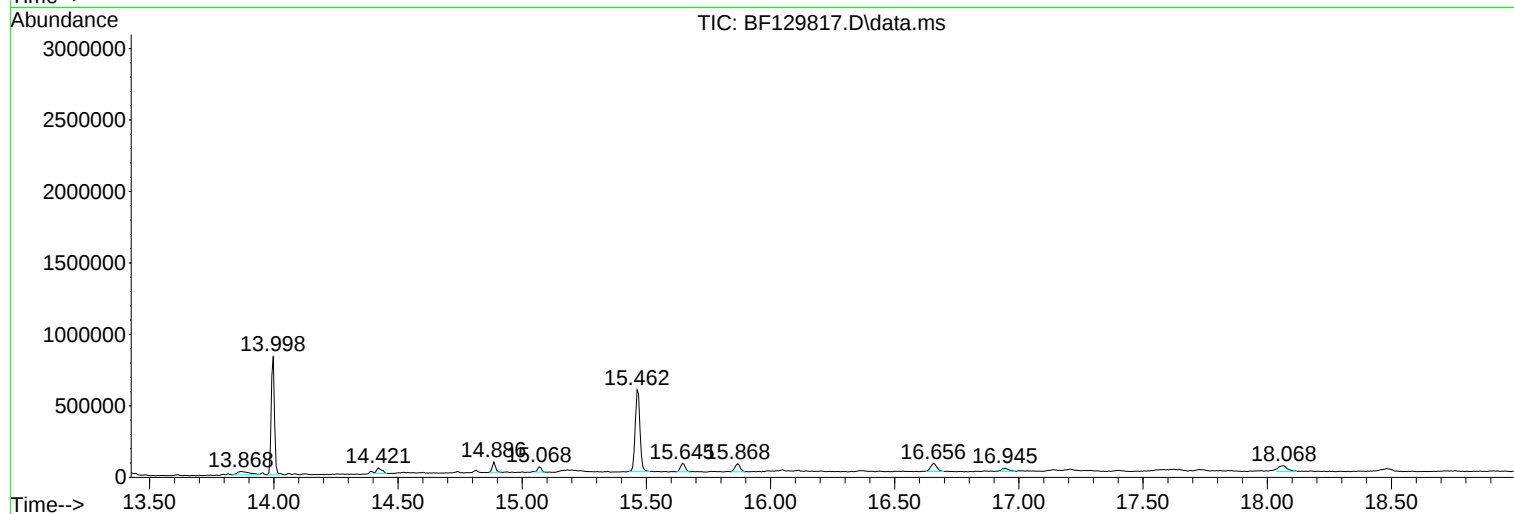
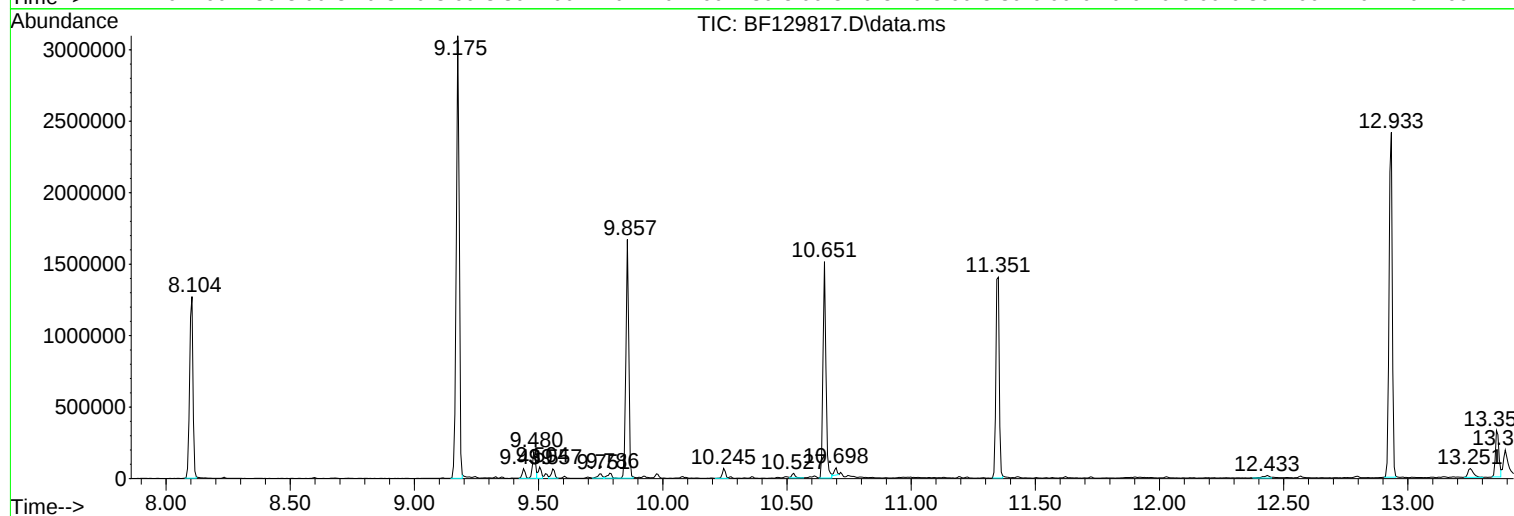
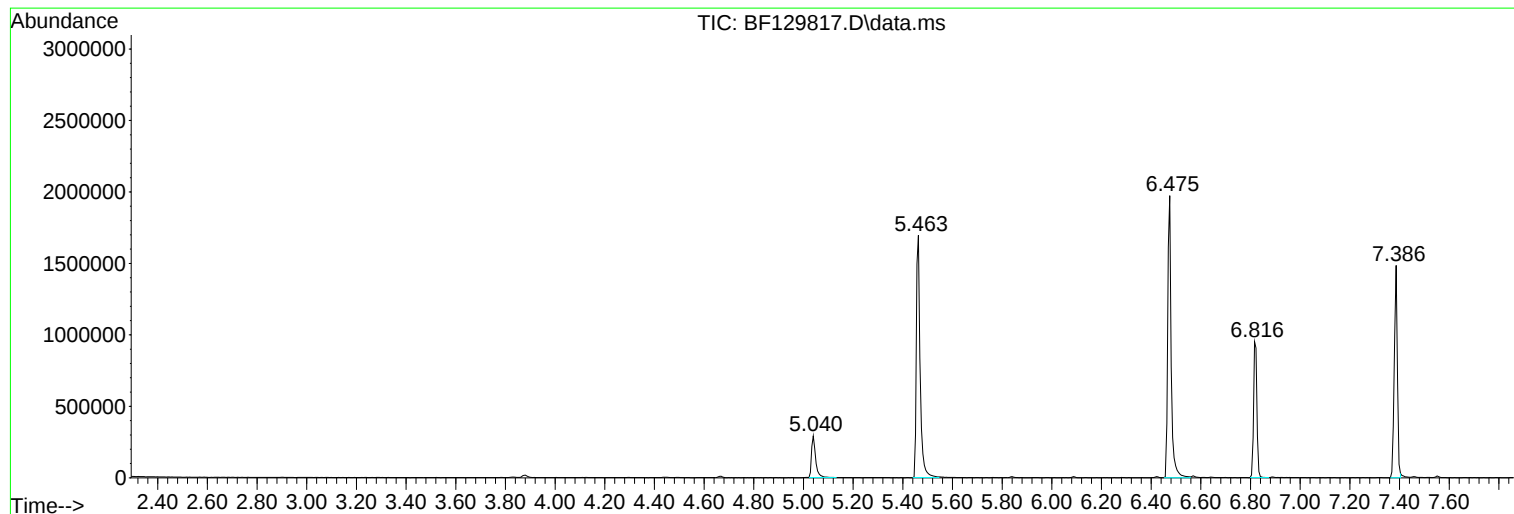
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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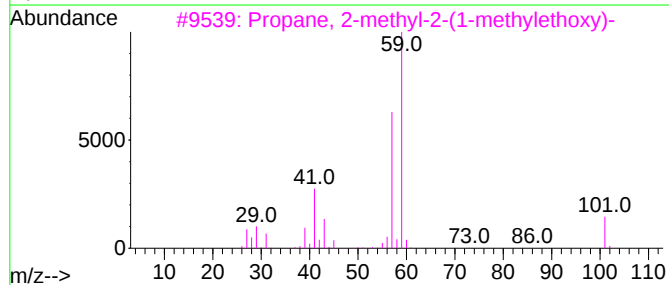
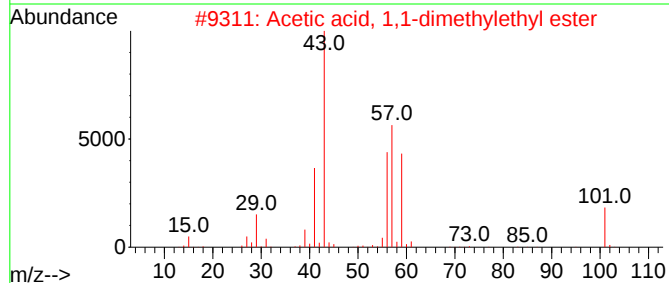
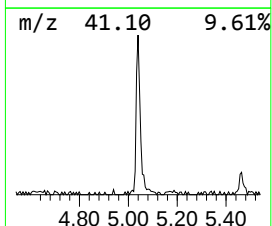
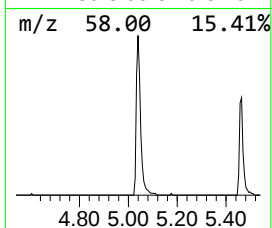
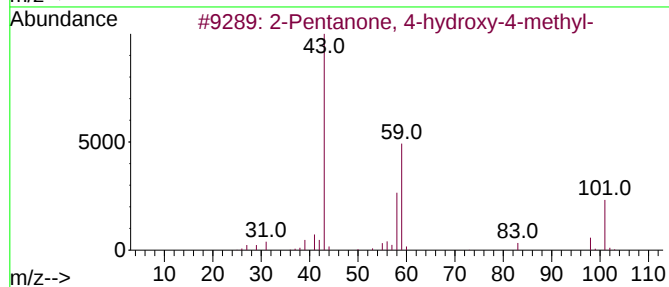
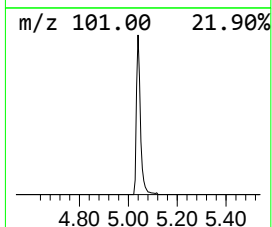
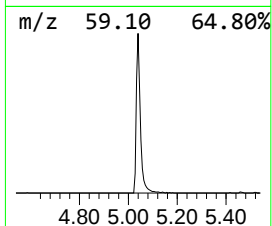
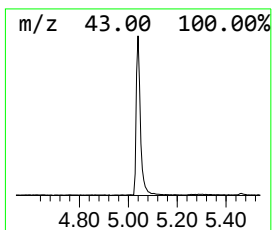
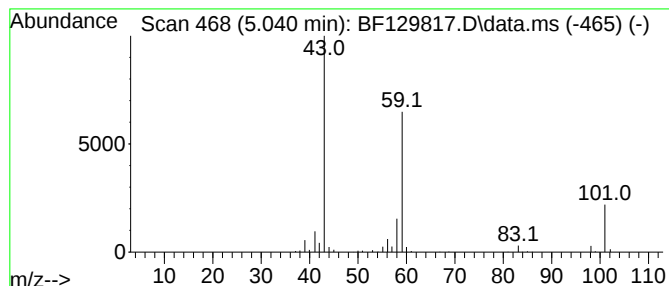
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	7.66 ng	337582	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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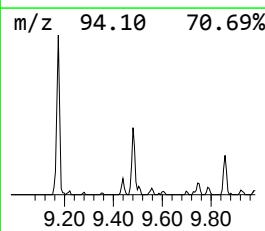
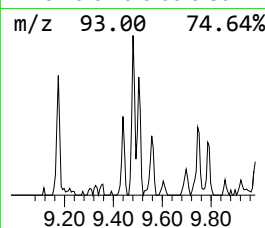
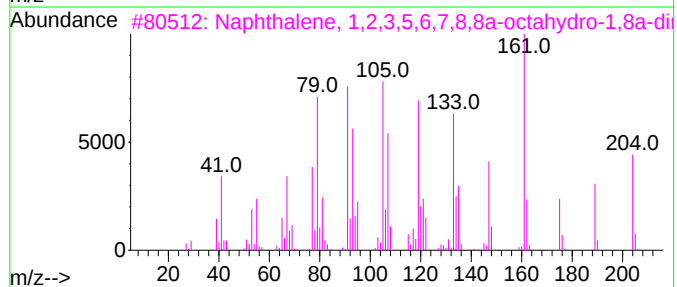
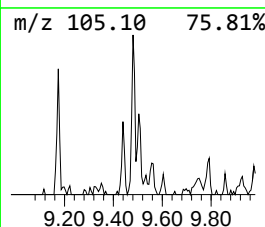
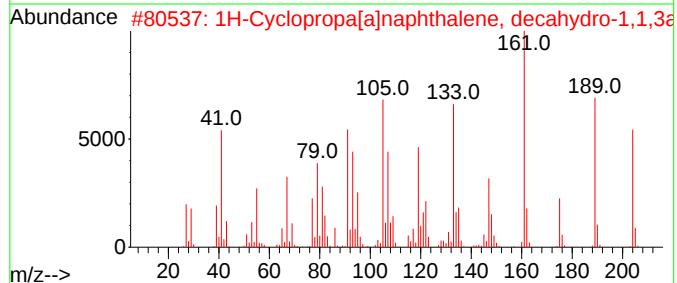
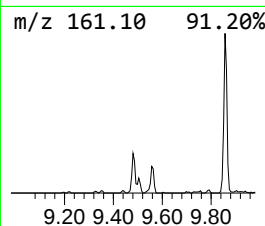
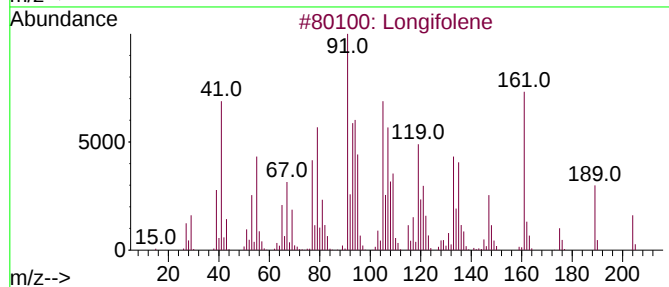
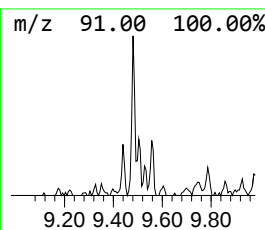
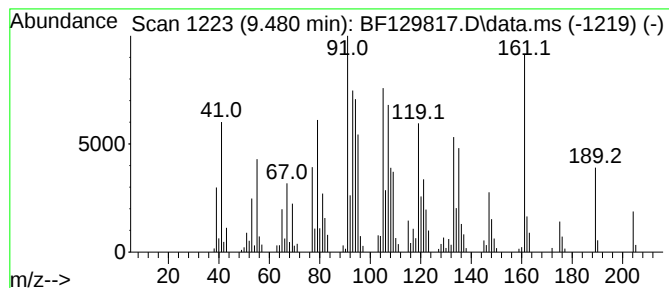
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Peak Number 2 Longifolene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.480	2.40 ng	161987	Acenaphthene-d10	9.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			1H-Cyclopropa[a]naphthalene, dec...	204	C15H24	020071-49-2	91
3			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	87
4			Aromandendrene	204	C15H24	000489-39-4	87
5			1,2,4-Methenoazulene, decahydro-...	204	C15H24	001137-12-8	86



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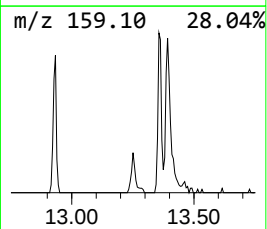
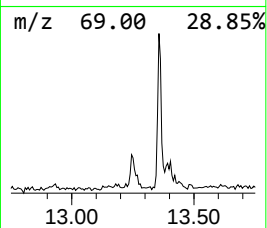
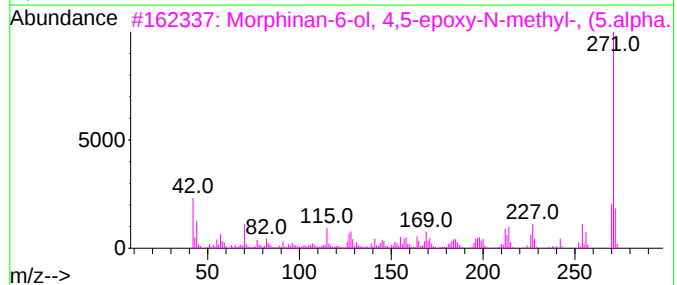
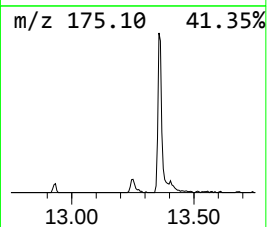
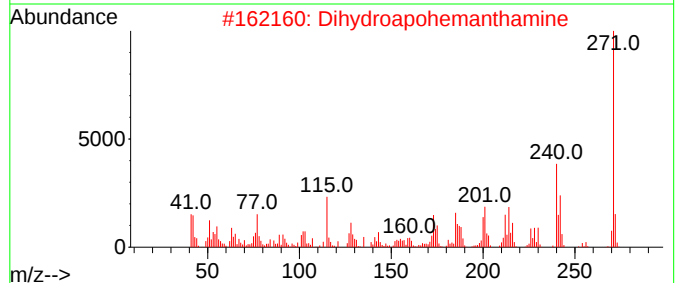
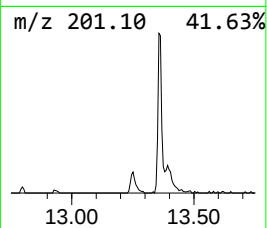
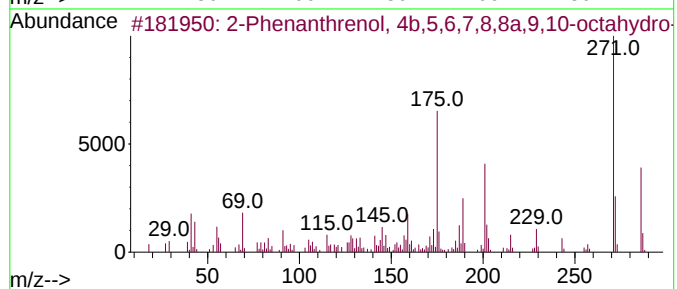
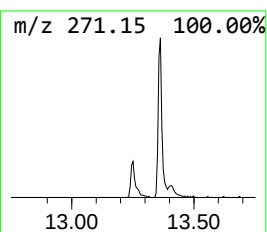
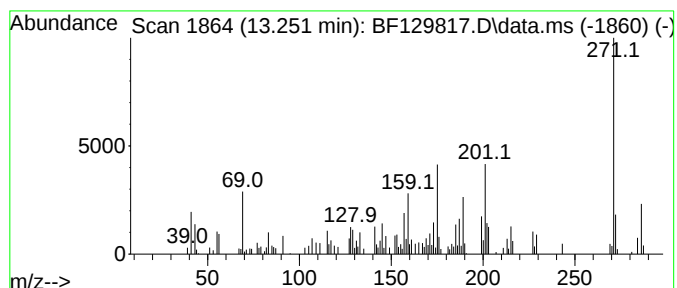
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.251 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	2.48 ng	95123	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	49		
2	Dihydroapohemanthamine	271	C16H17NO3	001153-01-1	27		
3	Morphinan-6-ol, 4,5-epoxy-N-meth...	271	C17H21NO2	083475-40-5	27		
4	phenol, 4-[2-(4-methoxyphenyl)et...	271	C15H13NO4	1000396-99-6	25		
5	[1,2,4]Triazolo[1,5-a]pyrimidin...	271	C13H13N5O2	1000351-09-3	25		



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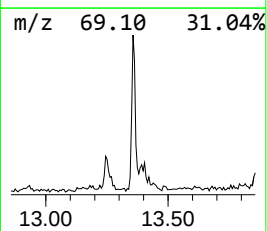
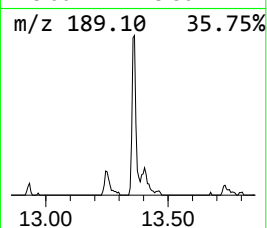
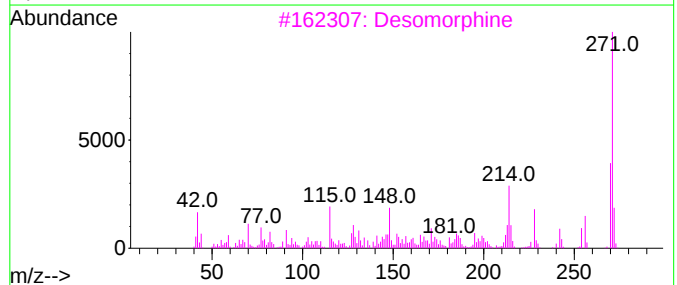
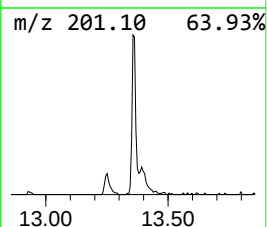
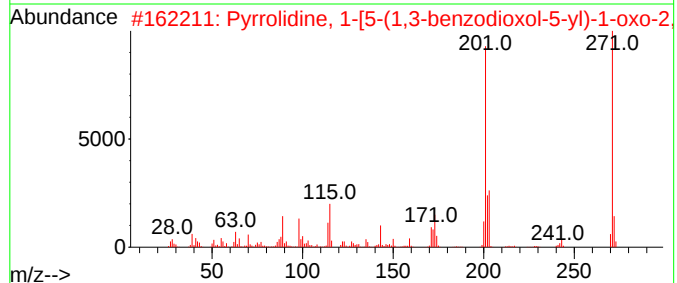
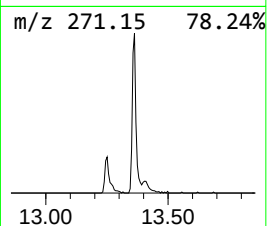
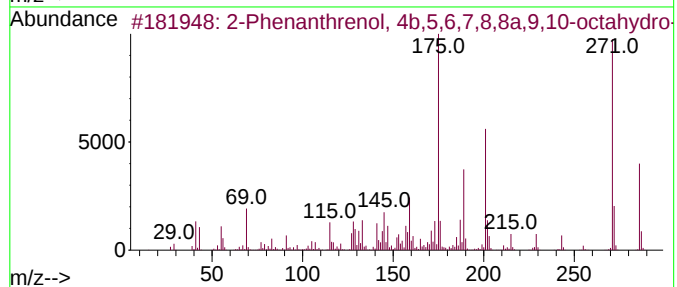
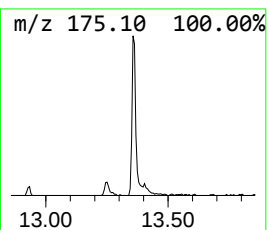
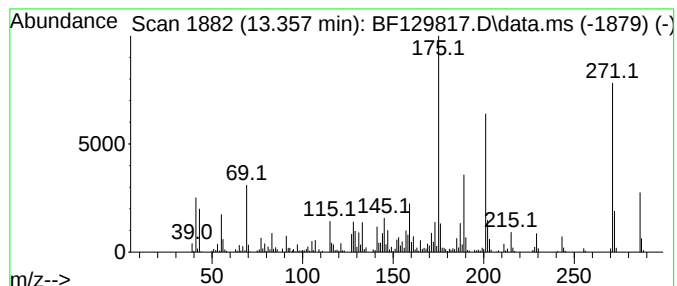
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Peak Number 4 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	8.39 ng	321882	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2			Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	35
3			Desomorphine	271	C17H21NO2	000427-00-9	20
4			2H-Naphtho[2,3-d]-1,2,3-triazole...	271	C18H13N3	1000327-40-5	18
5			3-Acridinol, 9-phenyl-	271	C19H13NO	109553-65-3	18



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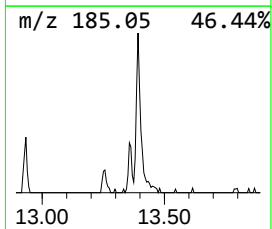
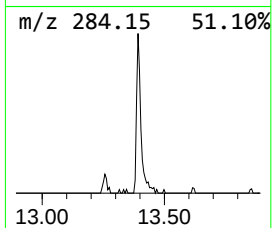
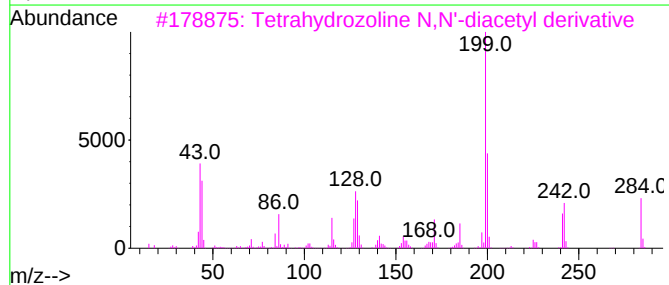
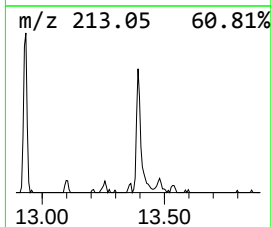
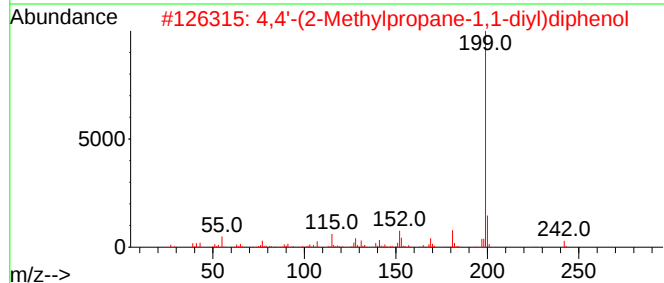
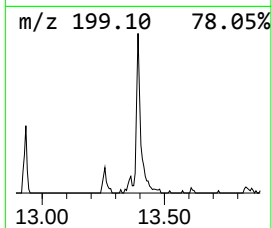
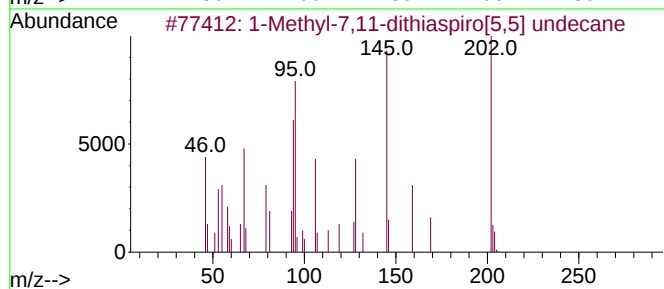
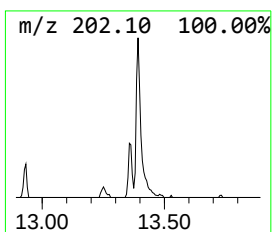
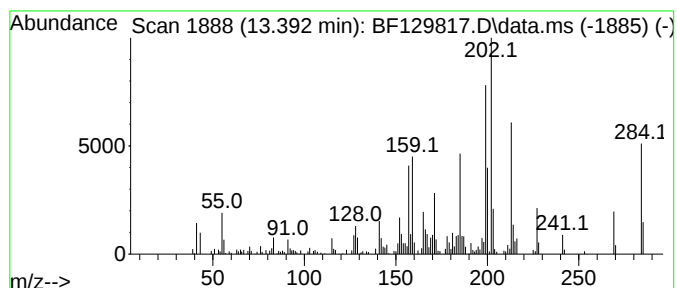
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Methyl-7,11-dithiaspiro[5... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.392	6.11 ng	234262	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	53
2			4,4'-(2-Methylpropane-1,1-diyl)d...	242	C16H18O2	001844-00-4	45
3			Tetrahydrozoline N,N'-diacetyl d...	284	C17H20N2O2	1010442-80-7	22
4			9-Methyl-2,9-dihydropyridazino(3...	199	C11H9N3O	022294-02-6	15
5			4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129817.D
Acq On : 16 Aug 2022 18:38
Operator : CG\JU
Sample : N4208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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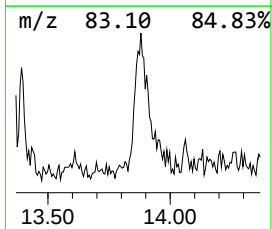
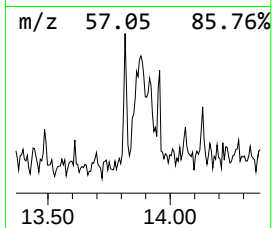
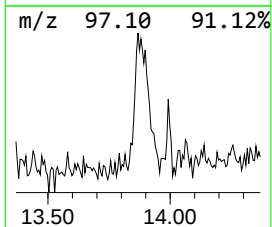
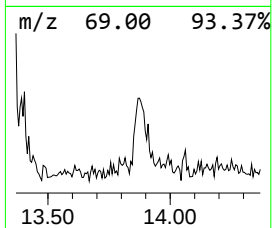
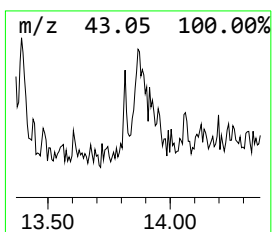
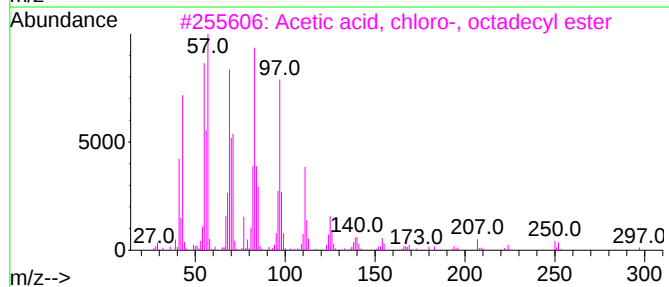
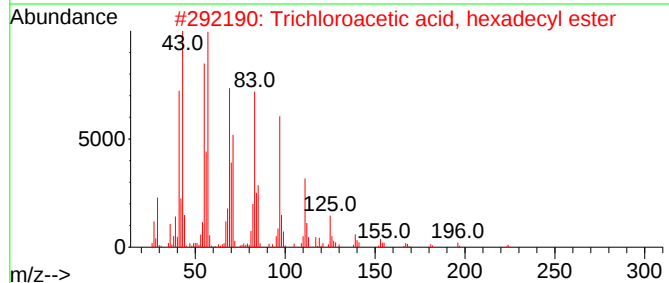
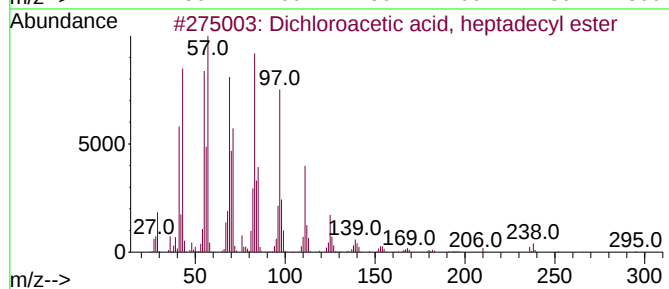
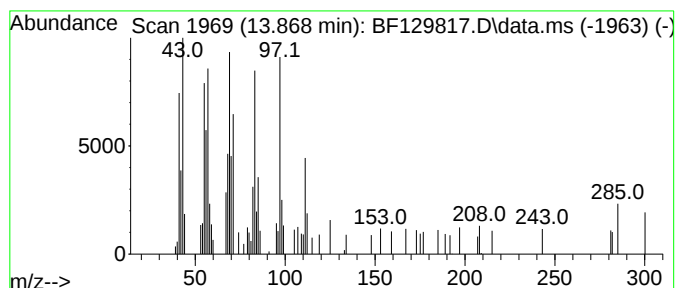
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	2.12 ng	81311	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74
3			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	72
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	72
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	72



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Sample : N4208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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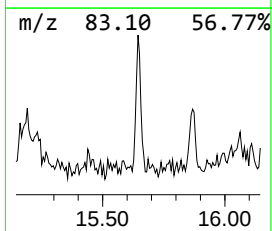
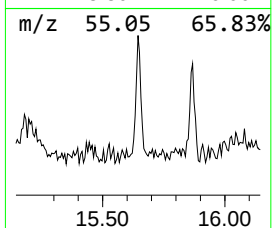
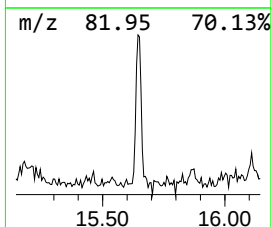
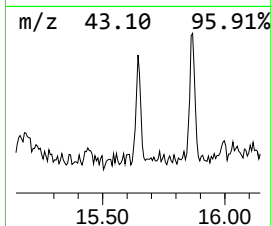
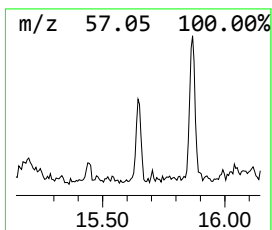
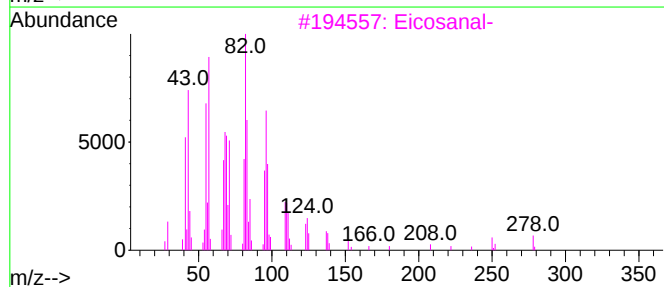
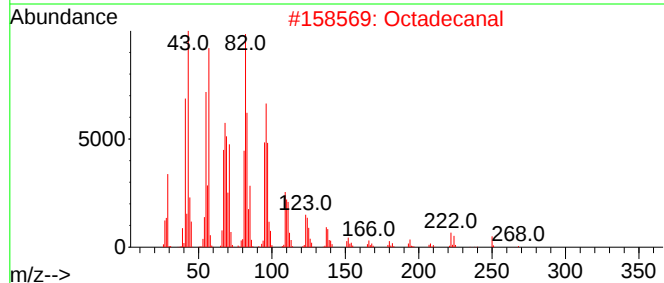
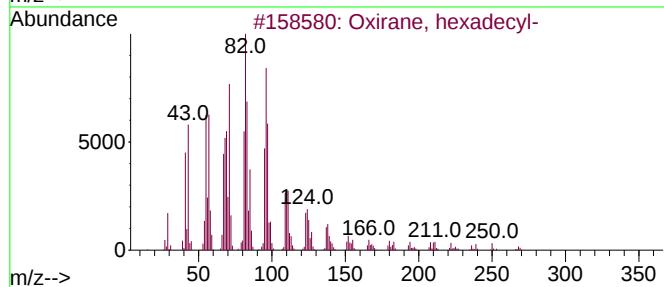
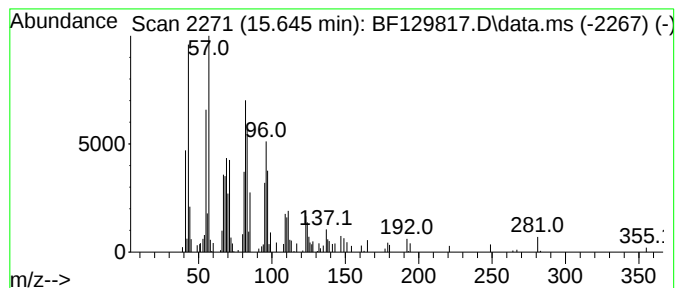
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	2.16 ng	80987	Perylene-d12	15.462

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Octadecanal	268	C18H36O	000638-66-4	90
3		Eicosanal-	296	C20H40O	002400-66-0	87
4		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
5		Tetracosanal	352	C24H48O	057866-08-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129817.D
Acq On : 16 Aug 2022 18:38
Operator : CG\JU
Sample : N4208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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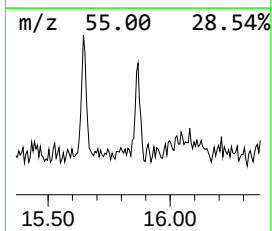
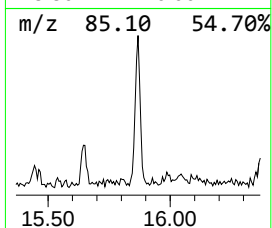
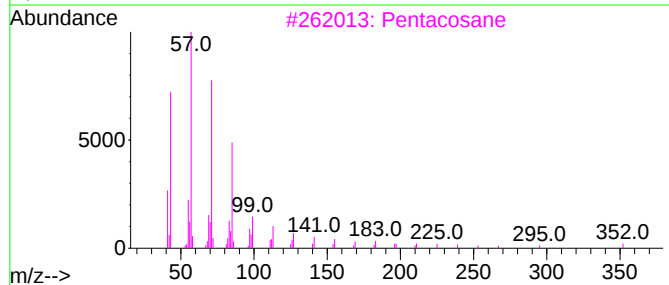
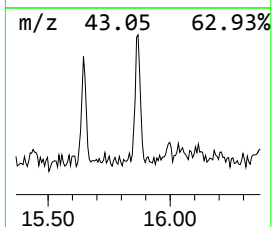
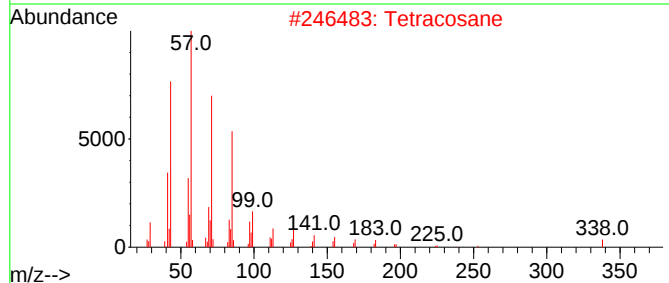
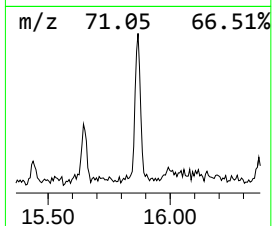
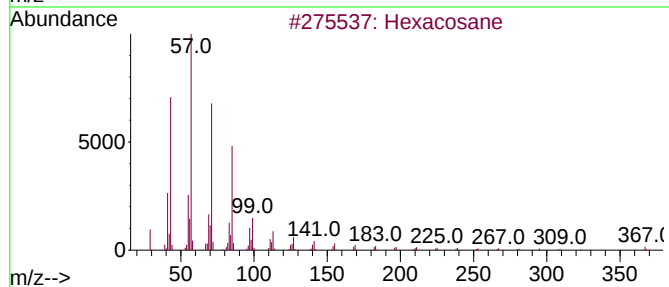
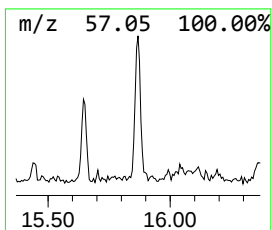
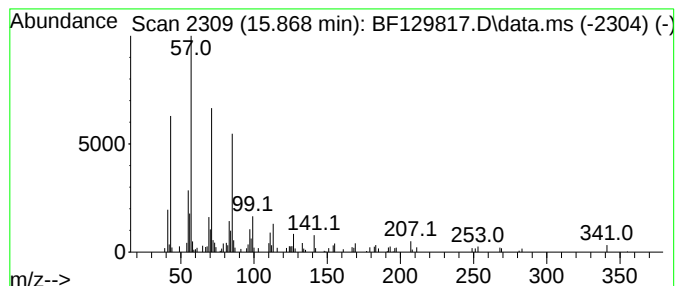
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.868	2.24 ng	84160	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Docosane	310	C22H46	000629-97-0	91
5			triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
Data File : BF129817.D
Acq On : 16 Aug 2022 18:38
Operator : CG\JU
Sample : N4208-01
Misc :
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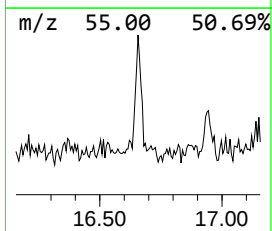
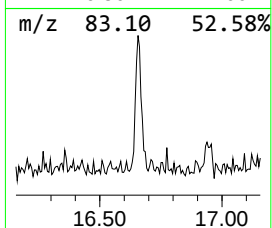
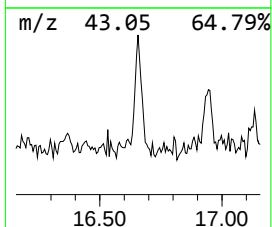
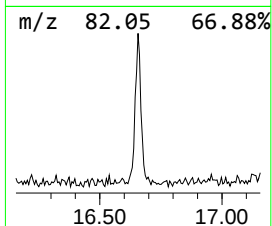
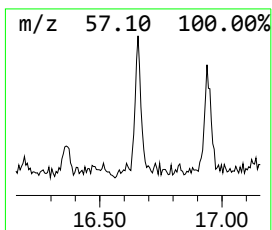
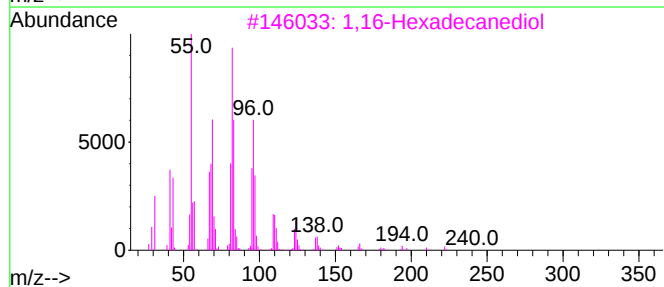
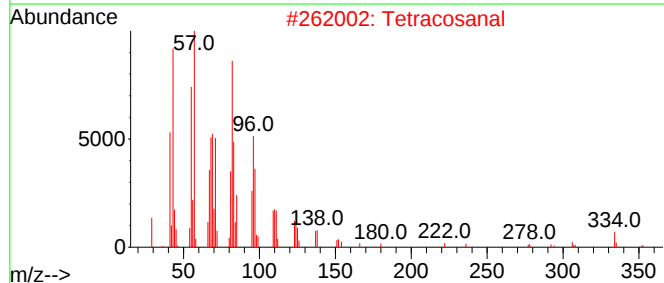
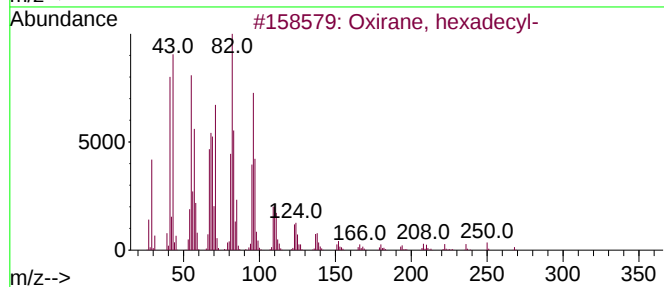
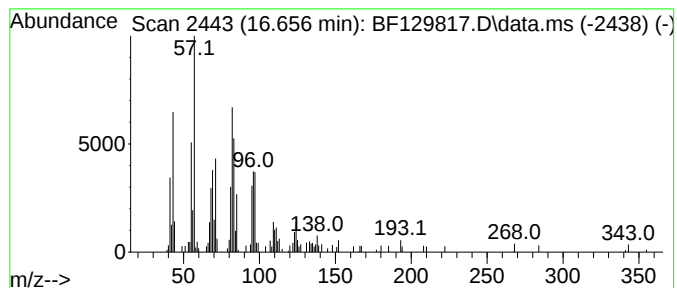
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.657	2.59 ng	97060	Perylene-d12	15.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
2	Tetracosanal	352	C24H48O	057866-08-7	64
3	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
4	1,19-Eicosadiene	278	C20H38	014811-95-1	52
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
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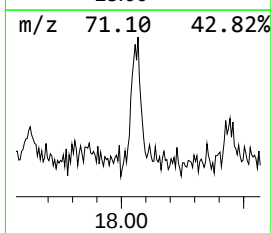
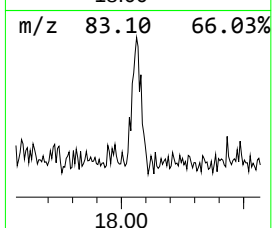
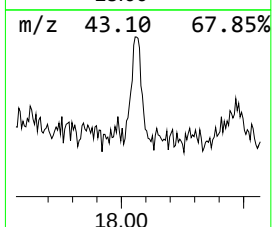
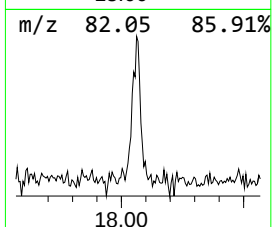
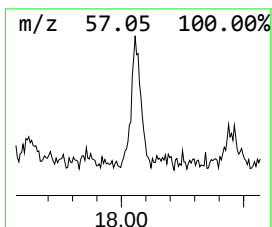
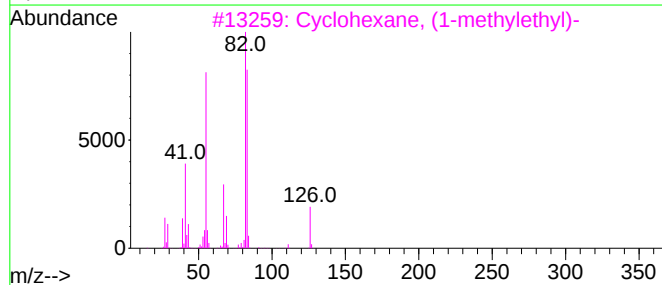
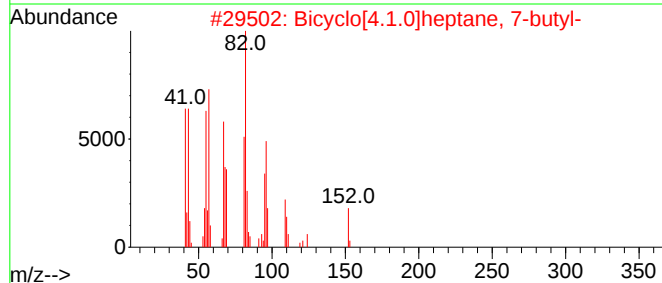
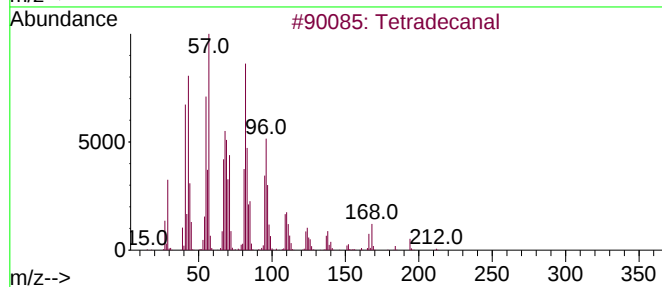
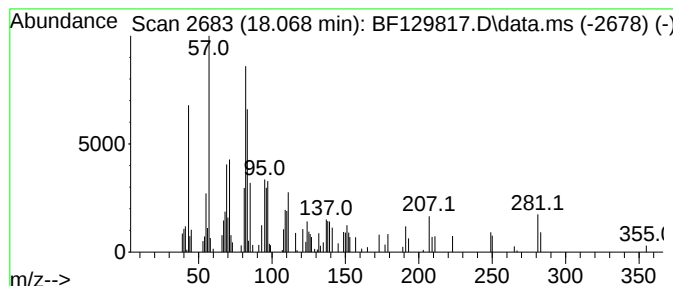
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.068	2.68 ng	100719	Perylene-d12		15.462	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanal		212	C14H28O	000124-25-4	72
2	Bicyclo[4.1.0]heptane, 7-butyl-		152	C11H20	018645-10-8	38
3	Cyclohexane, (1-methylethyl)-		126	C9H18	000696-29-7	35
4	Cyclohexane, 1,1'-(1-methyl-1,3-...		222	C16H30	041851-35-8	35
5	3,3'-Bi-p-menthane		278	C20H38	003294-50-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081622\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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

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

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					#	RT	Resp	Conc
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Longifolene	9.480	2.4	ng	161987	3	9.857	1348430	20.0
unknown13.251	13.251	2.5	ng	95123	5	13.998	767109	20.0
2-Phenanthrenol...	13.357	8.4	ng	321882	5	13.998	767109	20.0
1-Methyl-7,11-d...	13.392	6.1	ng	234262	5	13.998	767109	20.0
Dichloroacetic ...	13.868	2.1	ng	81311	5	13.998	767109	20.0
Oxirane, hexade...	15.645	2.2	ng	80987	6	15.462	750660	20.0
Hexacosane	15.868	2.2	ng	84160	6	15.462	750660	20.0
Tetracosanal	16.657	2.6	ng	97060	6	15.462	750660	20.0
Tetradecanal	18.068	2.7	ng	100719	6	15.462	750660	20.0