

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100722\
 Data File : BF130580.D
 Acq On : 07 Oct 2022 17:59
 Operator : CG\JU
 Sample : N5046-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R-7

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.781	453	458	469	rBV	445543	558959	25.38%	3.891%
2	5.210	528	531	551	rBV	1786982	1841120	83.61%	12.817%
3	5.616	597	600	608	rVB	39610	36433	1.65%	0.254%
4	6.257	705	709	727	rBV	1919568	1691409	76.81%	11.775%
5	6.610	766	769	773	rBV	621224	486457	22.09%	3.387%
6	7.181	862	866	869	rBV	1291178	1097307	49.83%	7.639%
7	7.839	970	978	984	rBV6	11509	35189	1.60%	0.245%
8	7.892	984	987	991	rVV	816036	635444	28.86%	4.424%
9	8.969	1166	1170	1173	rBV	2735767	2202125	100.00%	15.331%
10	9.639	1281	1284	1288	rBV	965119	831893	37.78%	5.791%
11	10.427	1415	1418	1433	rBV	1182171	1008752	45.81%	7.023%
12	11.122	1532	1536	1539	rBV	860171	675020	30.65%	4.699%
13	12.704	1801	1805	1809	rBV	1692466	1386023	62.94%	9.649%
14	13.751	1974	1983	1986	rBV	699545	623357	28.31%	4.340%
15	13.927	2009	2013	2022	rVB	34789	40727	1.85%	0.284%
16	14.233	2058	2065	2069	rBV	38744	45747	2.08%	0.318%
17	14.527	2111	2115	2121	rVB	35009	35910	1.63%	0.250%
18	14.827	2162	2166	2169	rBV	35698	36730	1.67%	0.256%
19	15.133	2214	2218	2222	rBV	632098	665843	30.24%	4.635%
20	15.545	2285	2288	2295	rVB3	28033	37706	1.71%	0.263%
21	15.992	2359	2364	2374	rVB5	23548	46202	2.10%	0.322%
22	16.509	2446	2452	2458	rVB4	22250	40871	1.86%	0.285%
23	17.115	2551	2555	2562	rVB7	33699	67381	3.06%	0.469%
24	17.445	2604	2611	2619	rVB2	109624	237567	10.79%	1.654%

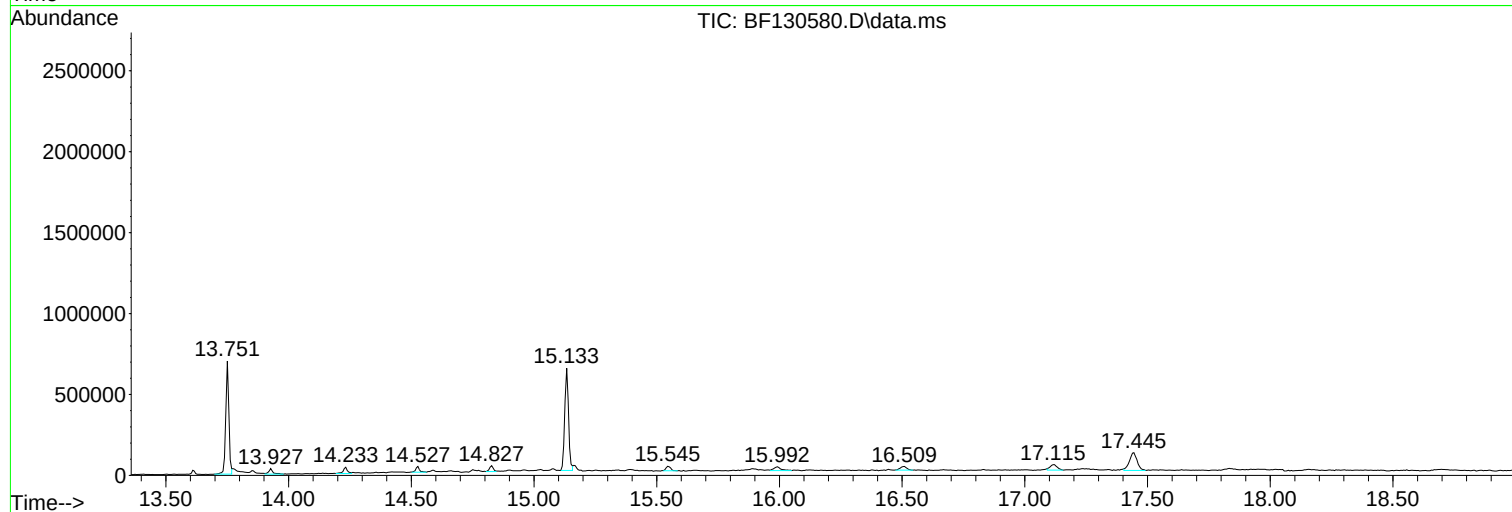
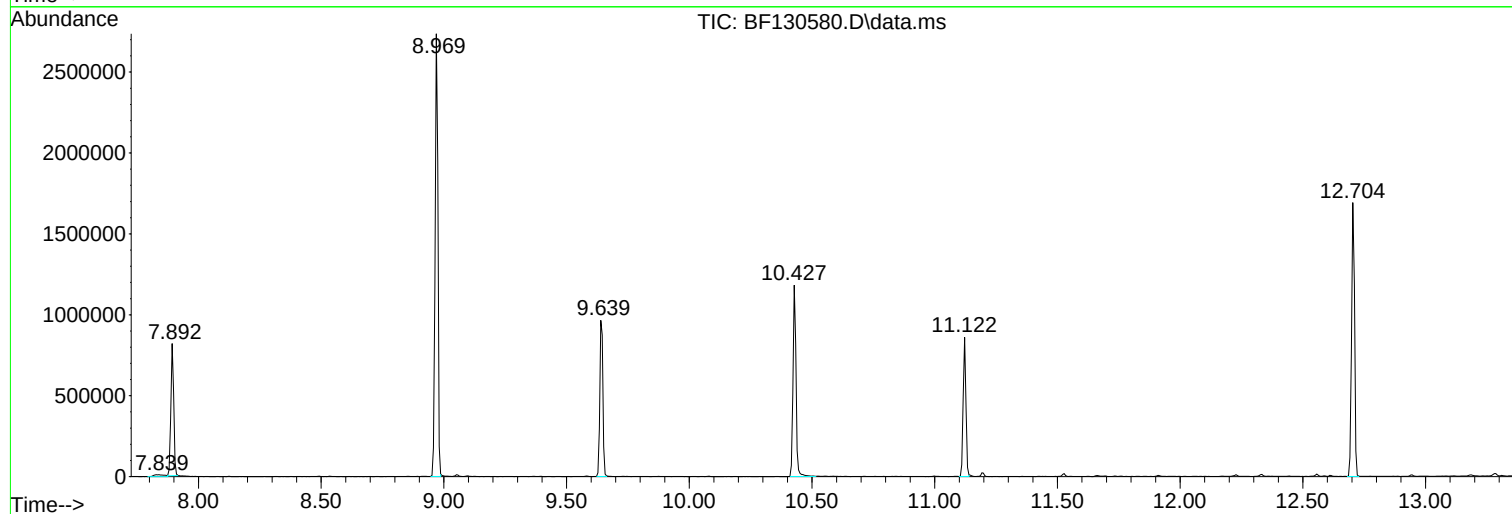
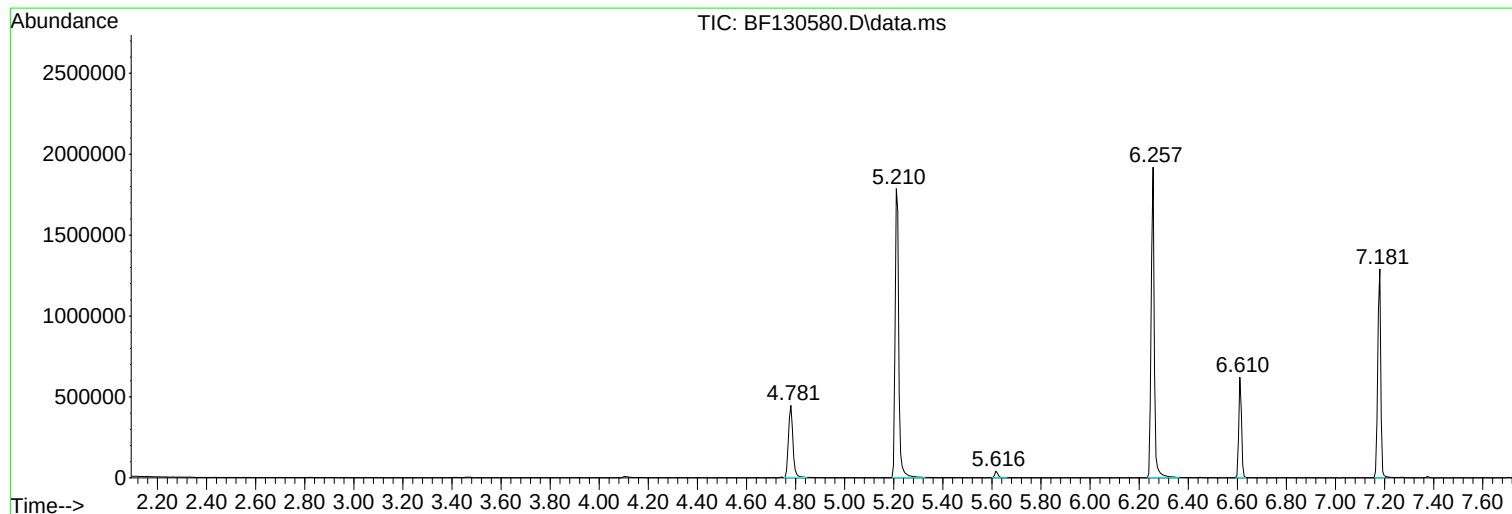
Sum of corrected areas: 14364172

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100722\
Data File : BF130580.D
Acq On : 07 Oct 2022 17:59
Operator : CG\JU
Sample : N5046-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100722\
Data File : BF130580.D
Acq On : 07 Oct 2022 17:59
Operator : CG\JU
Sample : N5046-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

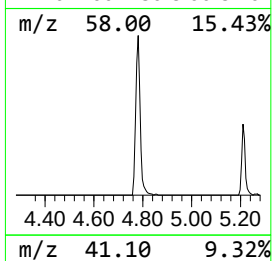
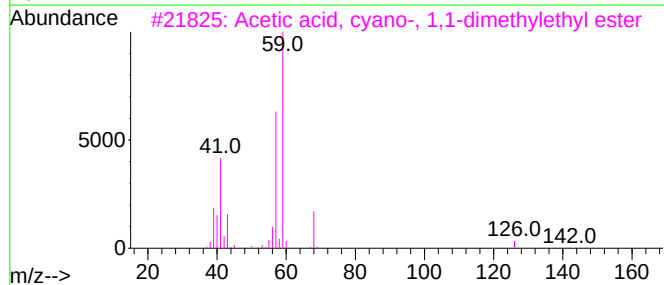
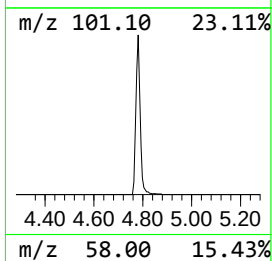
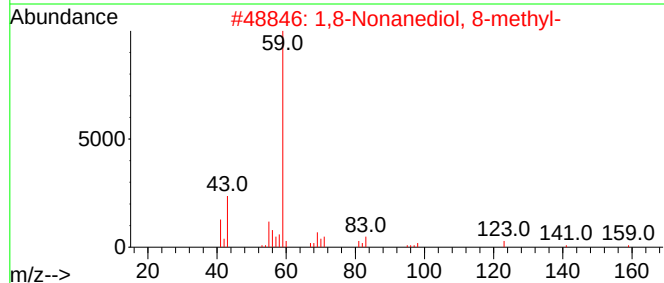
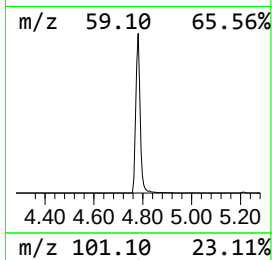
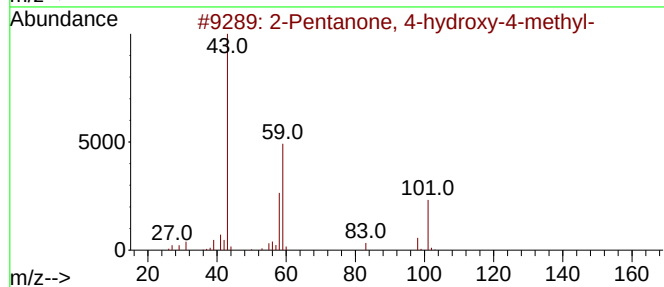
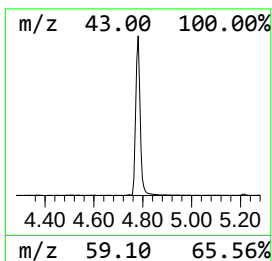
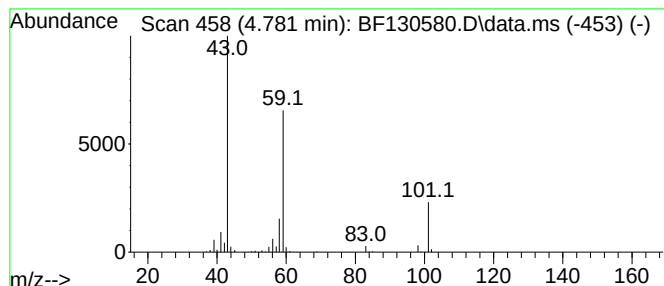
Instrument :
BNA_F
ClientSampleId :
R-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.781	22.98 ng	558959	1,4-Dichlorobenzene-d4	6.610	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100722\
Data File : BF130580.D
Acq On : 07 Oct 2022 17:59
Operator : CG\JU
Sample : N5046-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-7

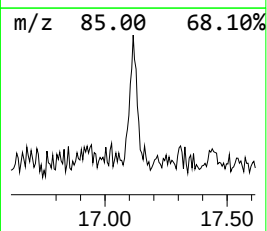
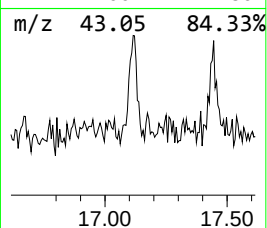
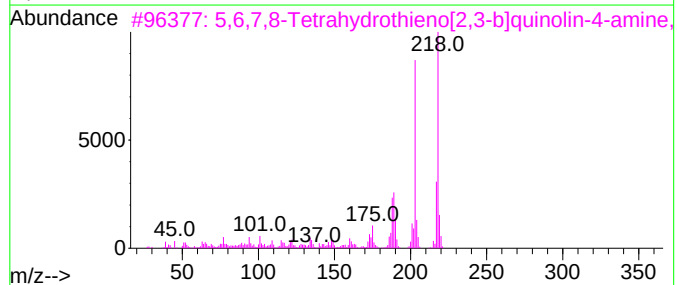
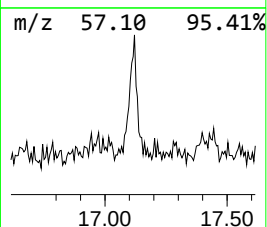
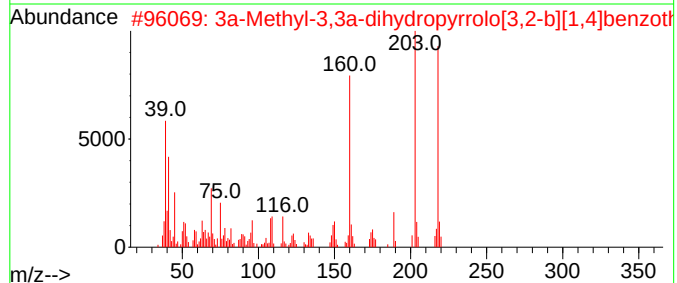
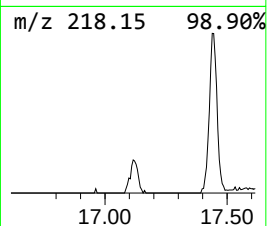
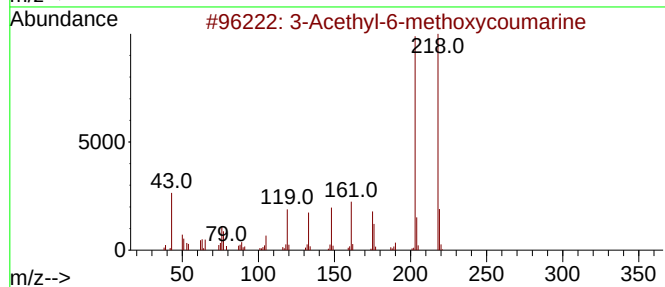
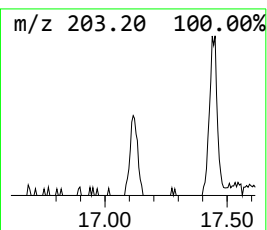
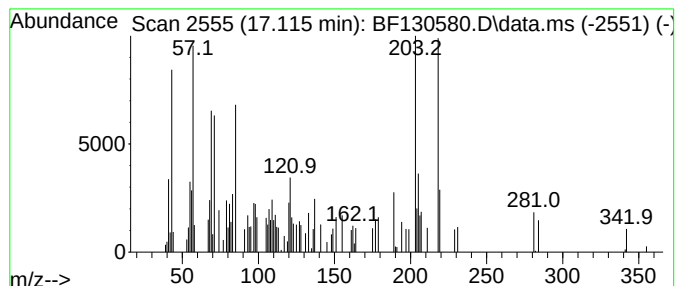
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Acethyl-6-methoxycoumarine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.115	2.02 ng	67381	Perylene-d12	15.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Acethyl-6-methoxycoumarine	218	C12H10O4	013252-80-7	50
2			3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	49
3			5,6,7,8-Tetrahydrothieno[2,3-b]q...	218	C12H14N2S	134315-44-9	47
4			2,4a-Epidioxy-4a,5,6,7,8,8a-hexa...	372	C22H28O5	1000212-01-8	47
5			Quinolin-8-amine, 5,6-dimethoxy-...	218	C12H14N2O2	064992-95-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100722\
Data File : BF130580.D
Acq On : 07 Oct 2022 17:59
Operator : CG\JU
Sample : N5046-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-7

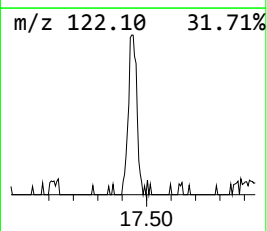
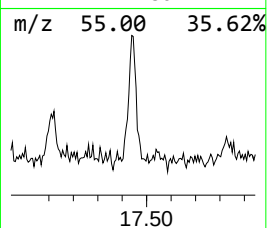
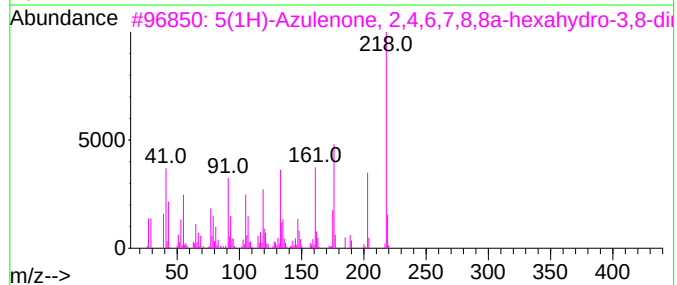
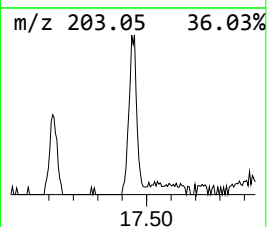
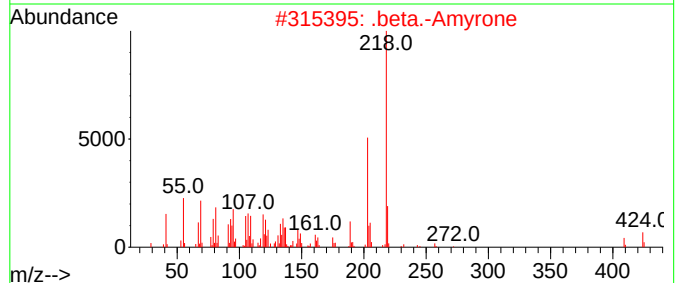
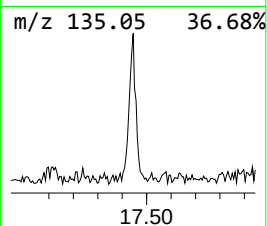
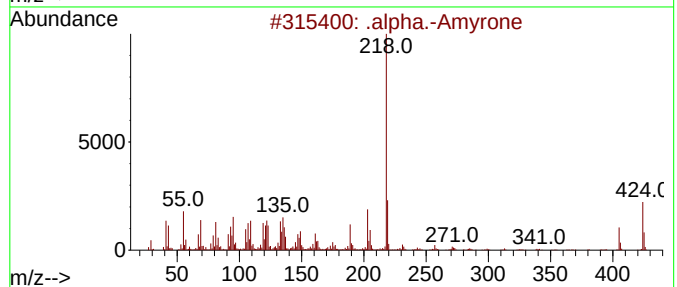
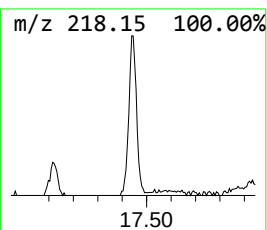
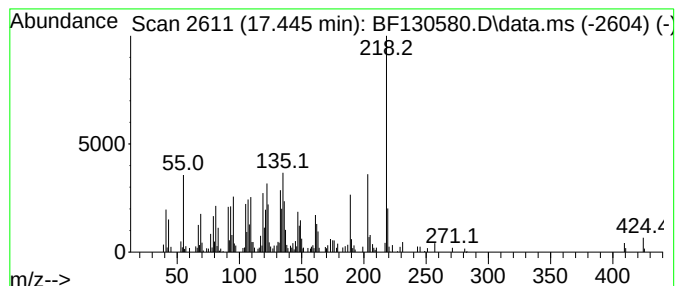
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 .alpha.-Amyrone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.445	7.14 ng	237567	Perylene-d12	15.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Amyrone	424	C30H48O	000638-96-0	93
2			.beta.-Amyrone	424	C30H48O	000638-97-1	90
3			5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	64
4			(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	58
5			2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100722\
Data File : BF130580.D
Acq On : 07 Oct 2022 17:59
Operator : CG\JU
Sample : N5046-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
2-Pentanone, 4-...	4.781	23.0	ng	558959	1	6.610	486457	20.0
3-Acethyl-6-met...	17.115	2.0	ng	67381	6	15.133	665843	20.0
.alpha.-Amyrone	17.445	7.1	ng	237567	6	15.133	665843	20.0