

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020922\
 Data File : BF126832.D
 Acq On : 09 Feb 2022 18:33
 Operator : CG\JU
 Sample : PB142553BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB142553BL

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-BF020922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.204	355	360	369	rBV	101821	151434	2.86%	0.459%
2	5.569	416	422	425	rBV	4304623	4620818	87.35%	13.995%
3	6.563	584	591	594	rBV	3797854	4775090	90.27%	14.462%
4	6.940	651	655	658	rBV	1047856	808176	15.28%	2.448%
5	7.504	745	751	754	rBV	2785433	3308257	62.54%	10.020%
6	8.222	868	873	876	rBV	1311383	1112032	21.02%	3.368%
7	9.298	1050	1056	1059	rBV	5087667	5268525	99.59%	15.956%
8	9.981	1167	1172	1175	rBV	1477549	1217005	23.01%	3.686%
9	10.775	1301	1307	1310	rBV	3609234	3420291	64.66%	10.359%
10	11.469	1421	1425	1429	rBV	1483263	1222629	23.11%	3.703%
11	13.063	1691	1696	1699	rBV	5407501	5289967	100.00%	16.021%
12	14.116	1871	1875	1878	rBV	818548	780819	14.76%	2.365%
13	15.621	2125	2131	2144	rBV	468481	653564	12.35%	1.979%
14	16.098	2207	2212	2219	rVB2	37827	58025	1.10%	0.176%
15	16.633	2297	2303	2311	rBV2	32423	60352	1.14%	0.183%
16	17.262	2402	2410	2422	rBV3	28497	69025	1.30%	0.209%
17	17.598	2452	2467	2479	rBV6	46420	202162	3.82%	0.612%

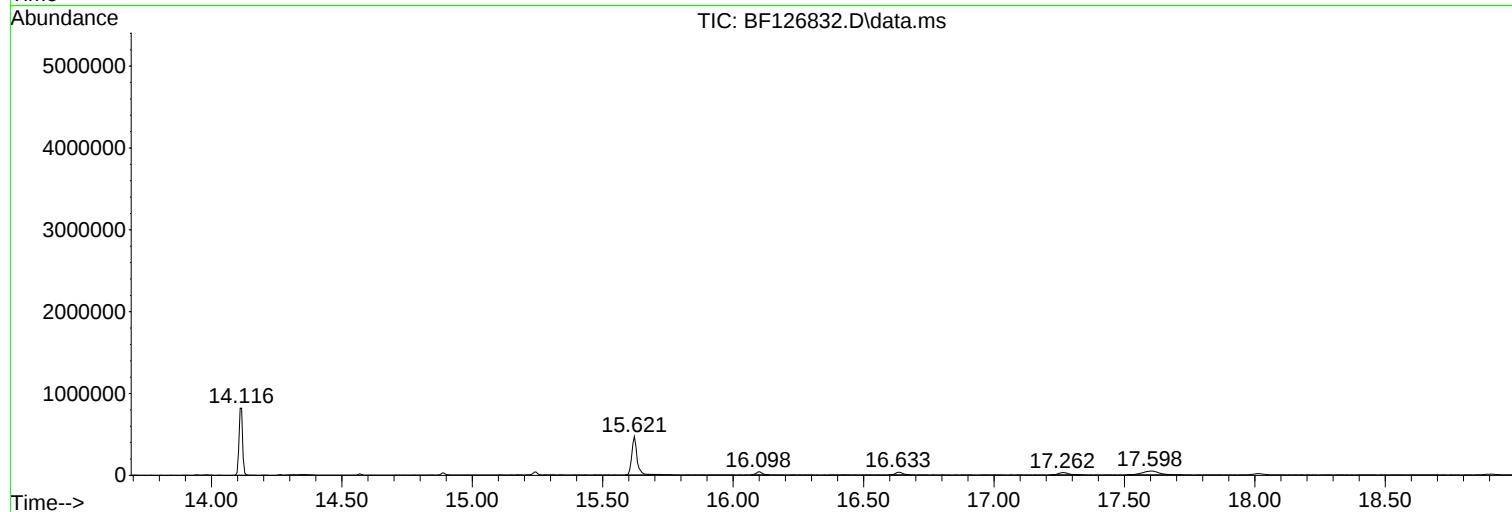
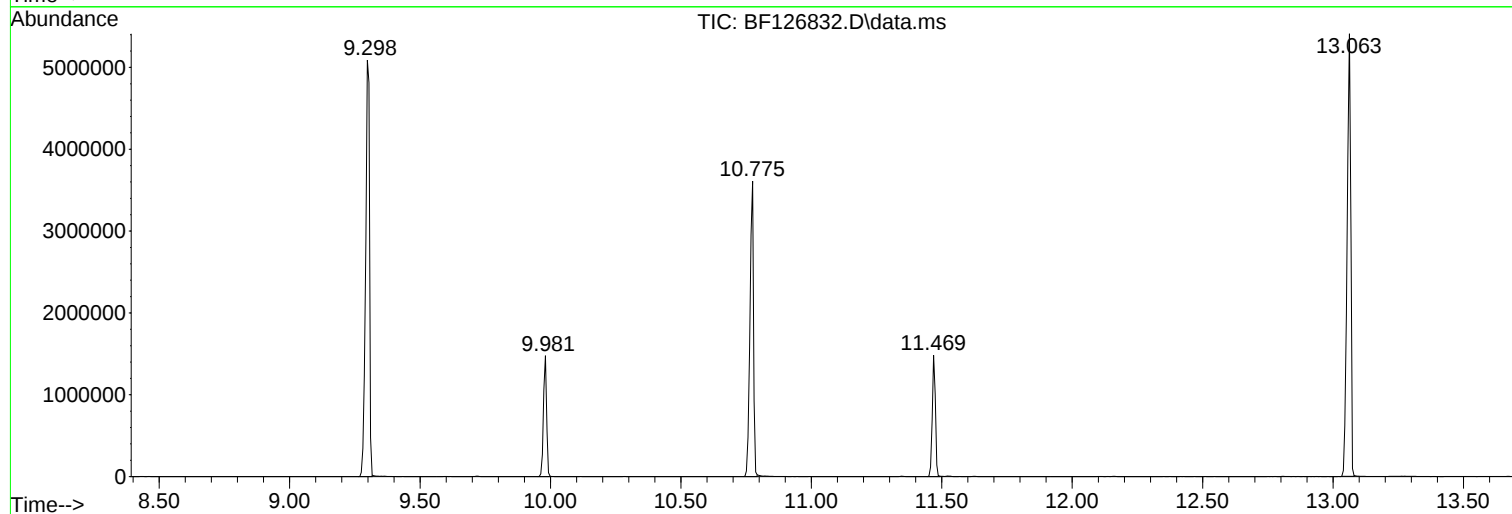
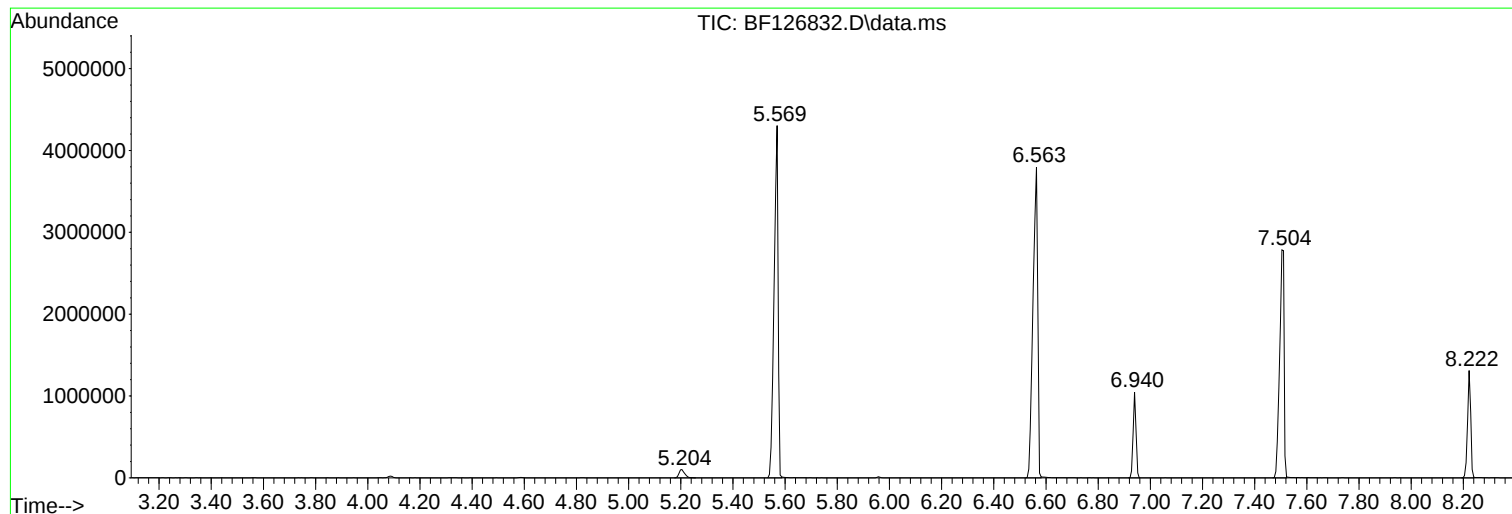
Sum of corrected areas: 33018171

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020922\
Data File : BF126832.D
Acq On : 09 Feb 2022 18:33
Operator : CG\JU
Sample : PB142553BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142553BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.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\BF020922\
Data File : BF126832.D
Acq On : 09 Feb 2022 18:33
Operator : CG\JU
Sample : PB142553BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142553BL

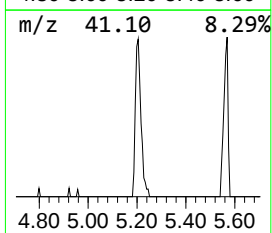
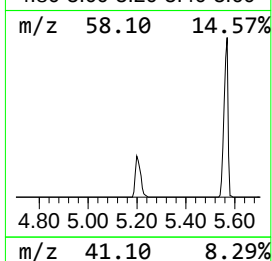
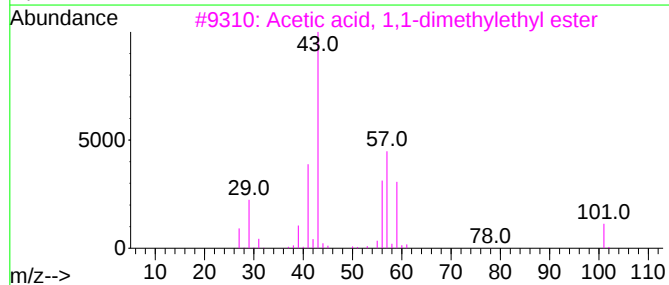
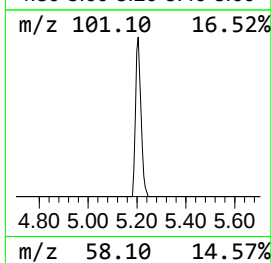
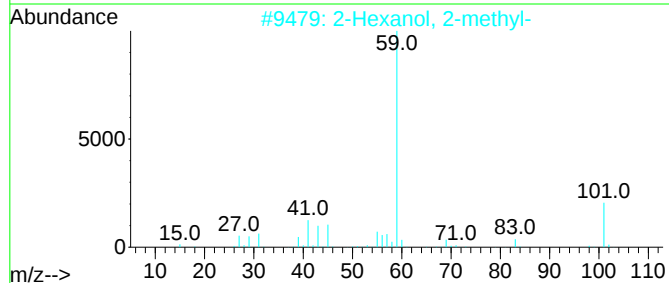
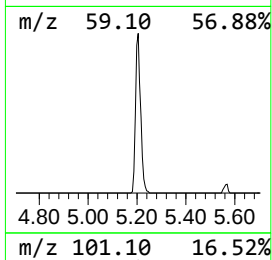
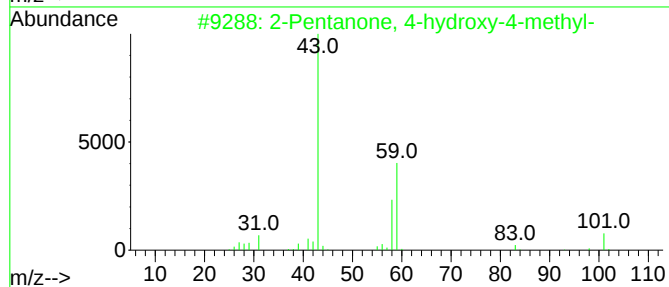
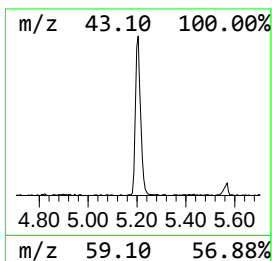
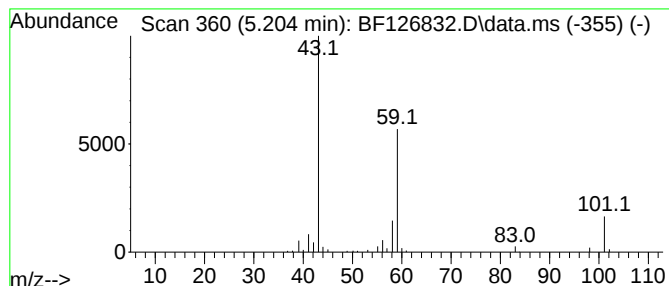
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	3.75 ng	151434	1,4-Dichlorobenzene-d4	6.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020922\
Data File : BF126832.D
Acq On : 09 Feb 2022 18:33
Operator : CG\JU
Sample : PB142553BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142553BL

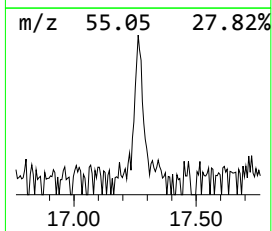
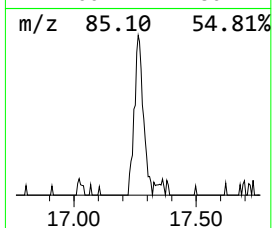
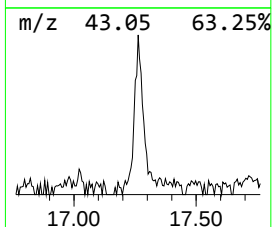
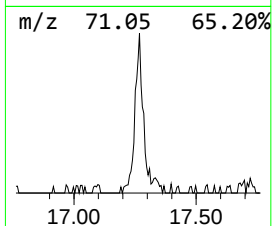
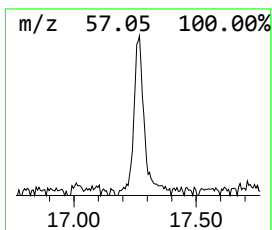
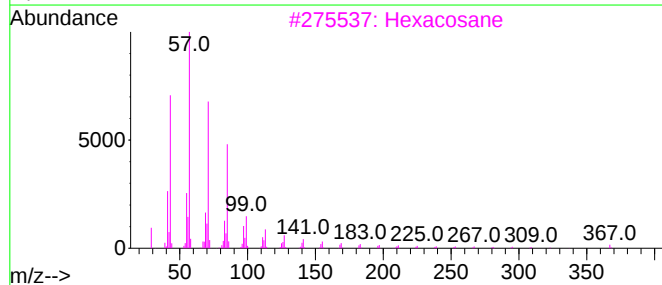
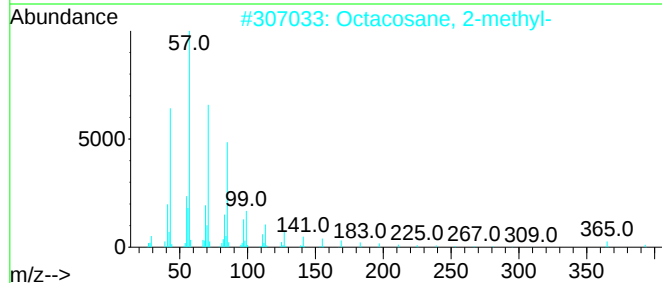
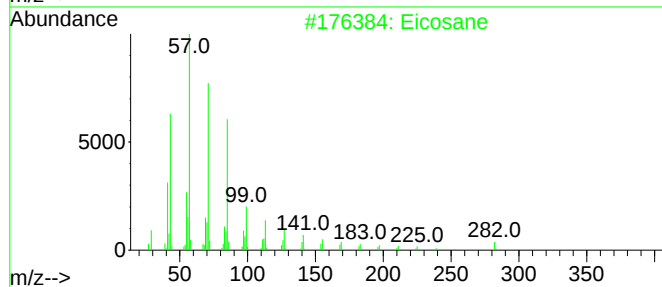
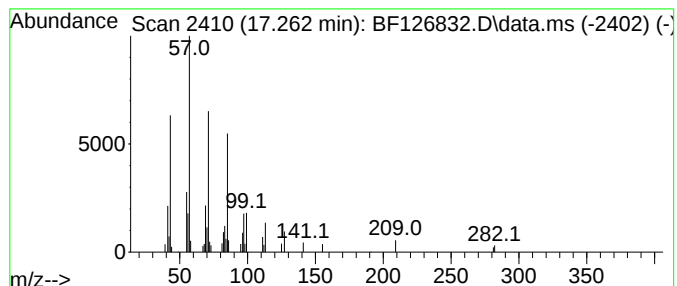
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	2.11 ng	69025	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Pentacosane	352	C25H52	000629-99-2	86
5			Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020922\
Data File : BF126832.D
Acq On : 09 Feb 2022 18:33
Operator : CG\JU
Sample : PB142553BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

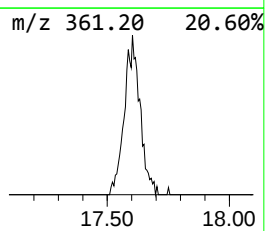
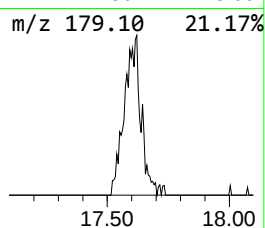
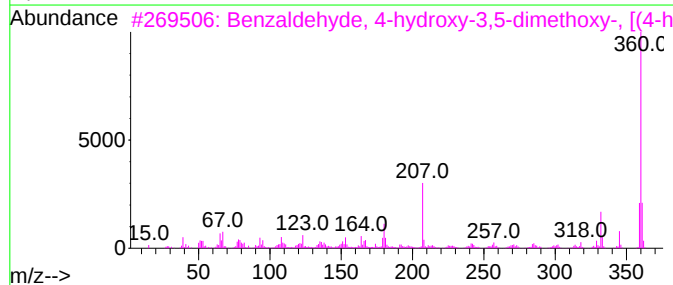
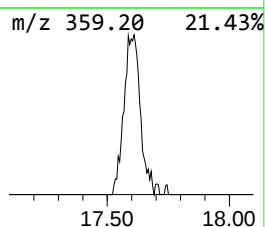
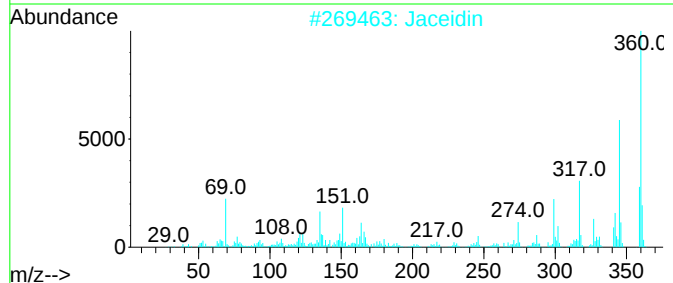
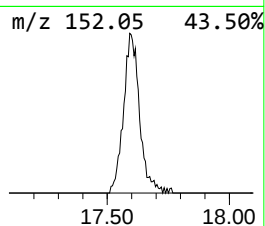
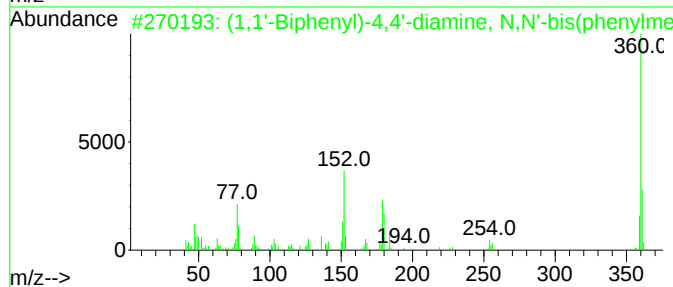
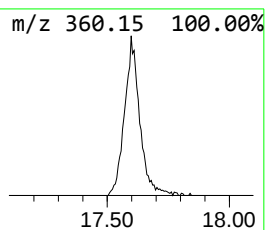
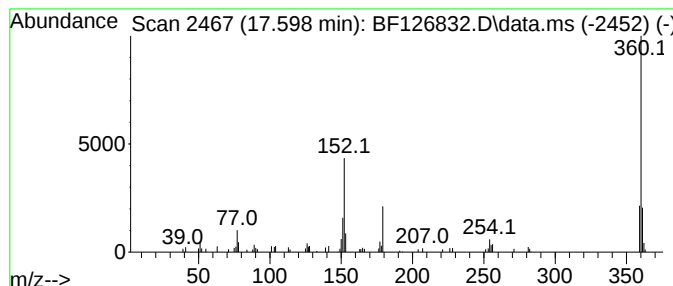
Instrument :
BNA_F
ClientSampleId :
PB142553BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.598	6.19 ng	202162	Perylene-d12	15.621	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,N'-bis(2,2,2-trifluoroethyl)carbamate	360	C26H20N2	006311-48-4	87
2	Jaceidin	360	C18H16O8	010173-01-0	47
3	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	360	C18H20N2O6	014414-32-5	47
4	1,3,2-Dioxaborolane, bis(spiro[4.5]undec-2-en-2-ylidene)-	360	C20H13B06	1000150-23-7	47
5	1,10-Phenanthroline, 2,9-dimethyl-	360	C26H20N2	004733-39-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020922\
Data File : BF126832.D
Acq On : 09 Feb 2022 18:33
Operator : CG\JU
Sample : PB142553BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142553BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.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-...	5.204	3.8	ng	151434	1	6.940	808176	20.0
Eicosane	17.262	2.1	ng	69025	6	15.621	653564	20.0
(1,1'-Biphenyl)...	17.598	6.2	ng	202162	6	15.621	653564	20.0