

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
 Data File : BF131843.D
 Acq On : 27 Dec 2022 18:29
 Operator : CG\JU
 Sample : N6190-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LOCATION-3

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-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	496	501	513	rVB	536368	699120	35.95%	4.712%
2	5.446	566	571	574	rBV	1713060	1666764	85.72%	11.235%
3	6.463	739	744	747	rBV	1796416	1697044	87.27%	11.439%
4	6.834	803	807	810	rBV	521852	472399	24.29%	3.184%
5	7.398	898	903	906	rBV	1194975	1115175	57.35%	7.517%
6	8.122	1022	1026	1029	rBV	736159	599250	30.82%	4.039%
7	9.204	1205	1210	1213	rBV	2274414	1944534	100.00%	13.107%
8	9.886	1321	1326	1329	rBV	813361	714295	36.73%	4.815%
9	10.675	1456	1460	1464	rBV	1407766	1302754	67.00%	8.781%
10	11.375	1576	1579	1583	rBV	845278	746013	38.36%	5.029%
11	11.904	1665	1669	1673	rBV	40934	36805	1.89%	0.248%
12	12.969	1846	1850	1854	rBV	2014903	1786659	91.88%	12.043%
13	13.033	1858	1861	1864	rVV	83515	65999	3.39%	0.445%
14	13.851	1990	2000	2002	rBV	97390	125524	6.46%	0.846%
15	13.874	2002	2004	2024	rVV4	98935	399428	20.54%	2.692%
16	14.027	2027	2030	2034	rVB	529181	444007	22.83%	2.993%
17	14.539	2112	2117	2125	rBV	12021	30620	1.57%	0.206%
18	15.145	2216	2220	2226	rVB	25526	31949	1.64%	0.215%
19	15.321	2239	2250	2251	rBV	51583	121538	6.25%	0.819%
20	15.515	2277	2283	2295	rVB	327505	415506	21.37%	2.801%
21	15.974	2357	2361	2366	rBV	21713	30681	1.58%	0.207%
22	16.868	2494	2513	2530	rBV5	42864	234866	12.08%	1.583%
23	17.662	2642	2648	2658	rVB5	27682	58438	3.01%	0.394%
24	18.156	2725	2732	2743	rVB10	28774	69677	3.58%	0.470%
25	18.627	2805	2812	2813	rBV4	15367	26627	1.37%	0.179%

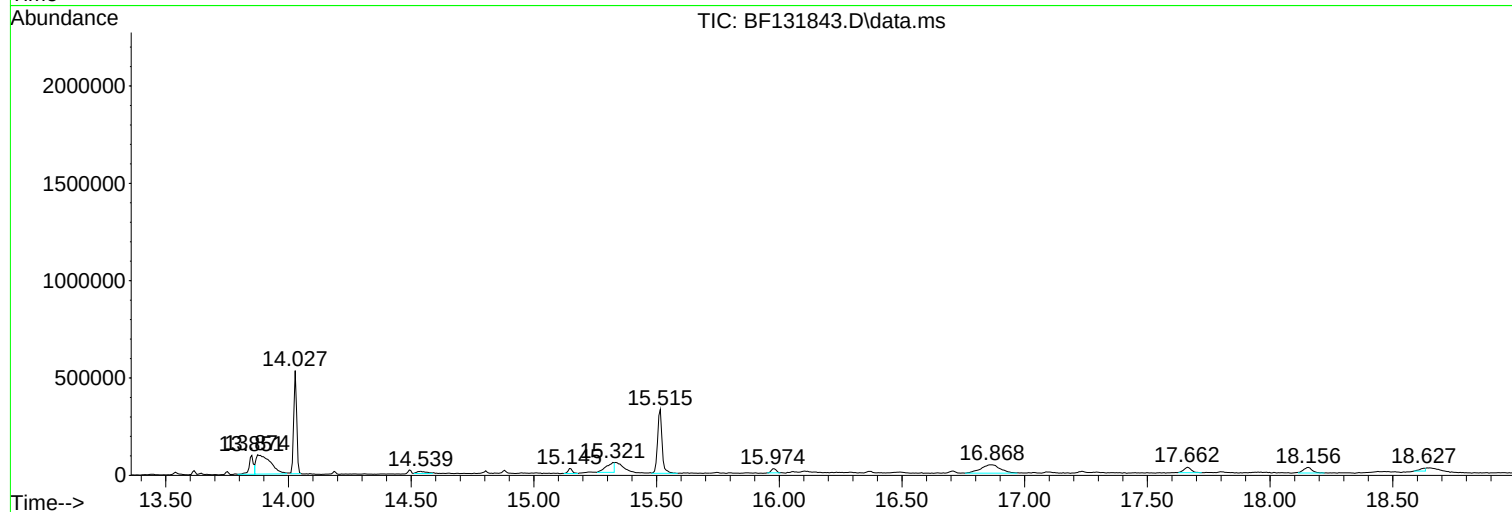
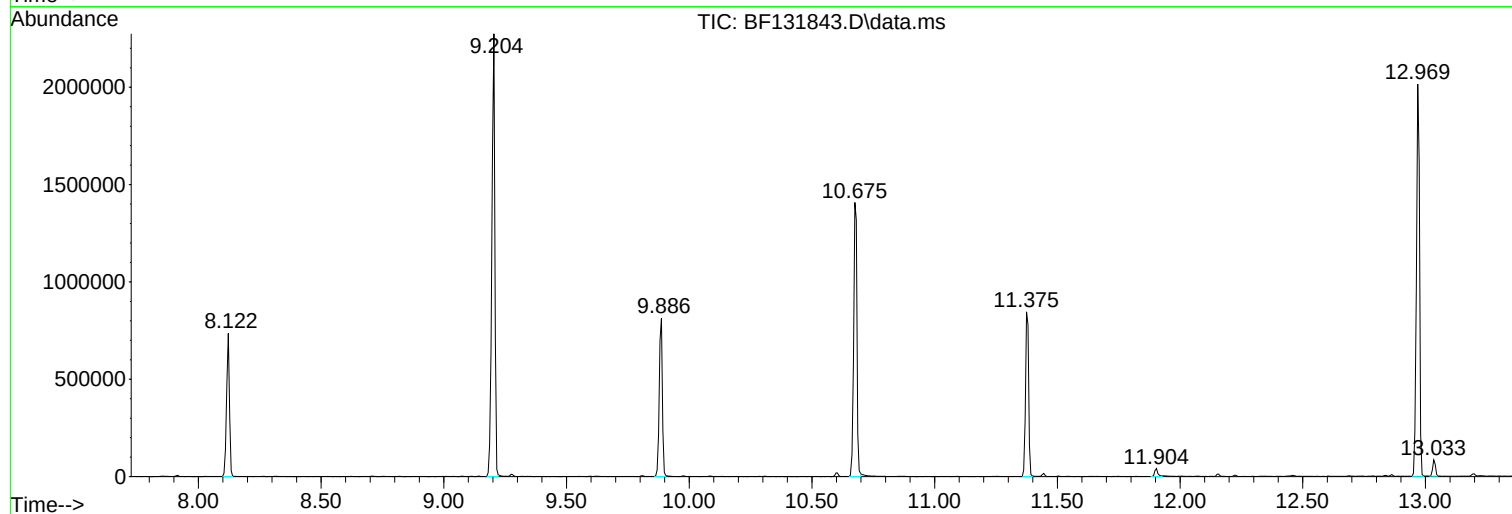
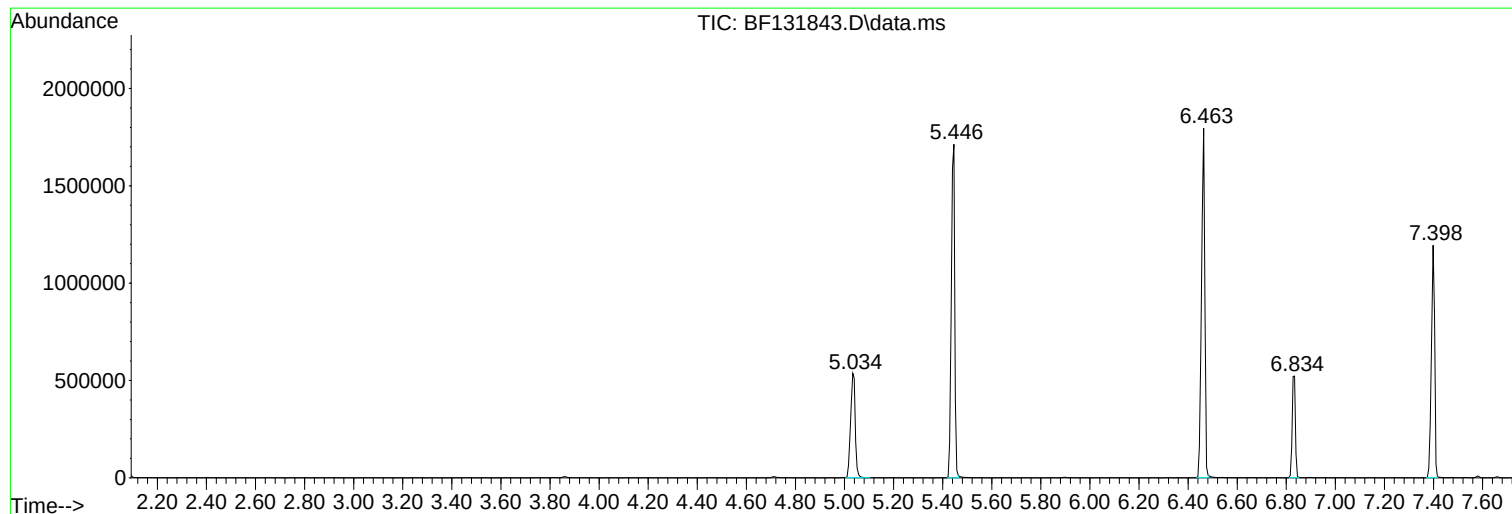
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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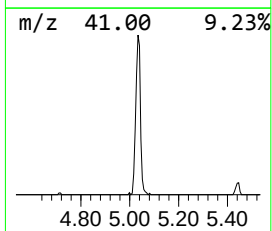
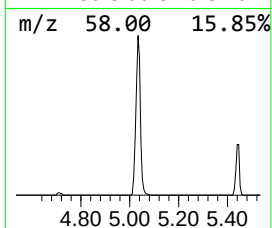
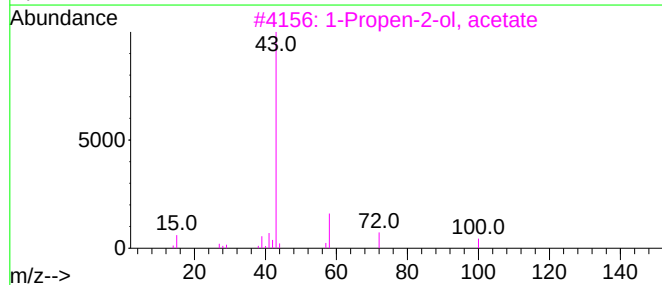
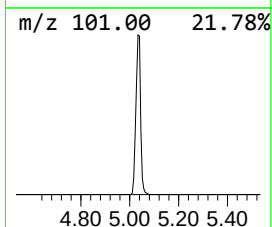
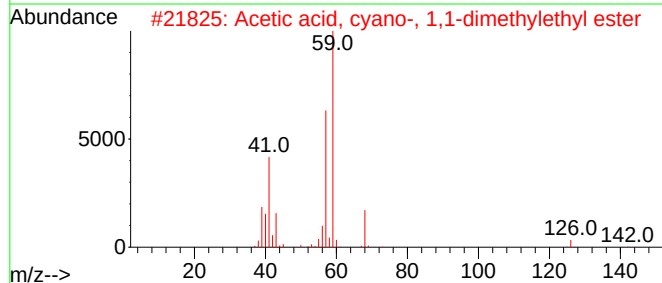
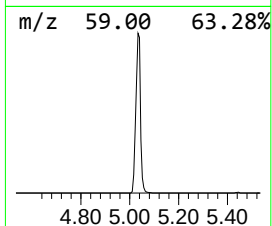
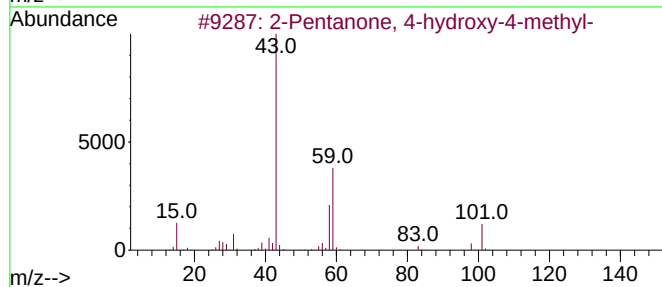
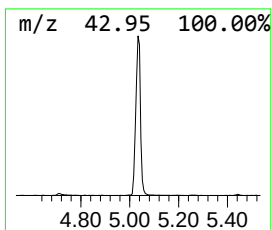
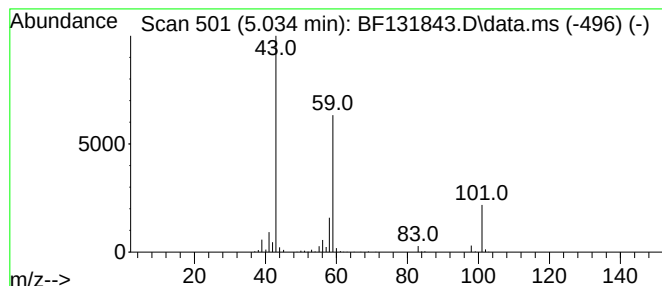
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.034	29.60 ng	699120	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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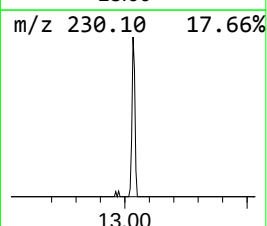
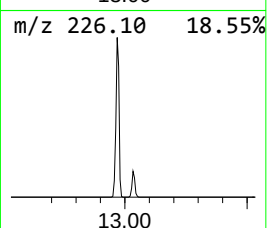
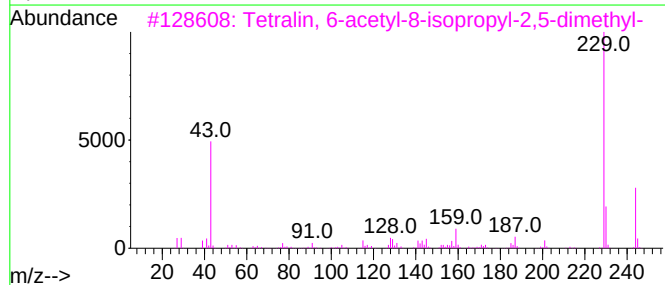
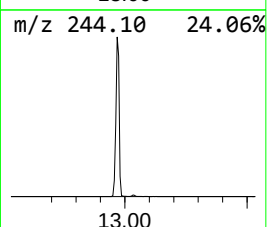
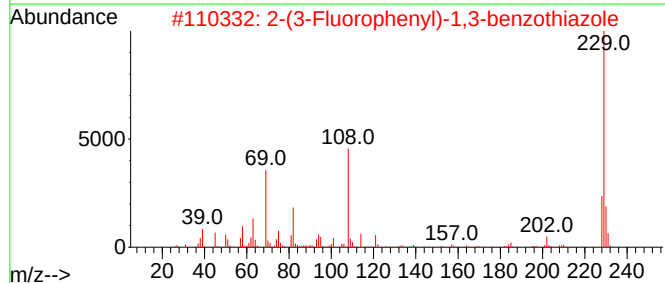
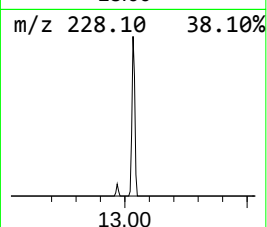
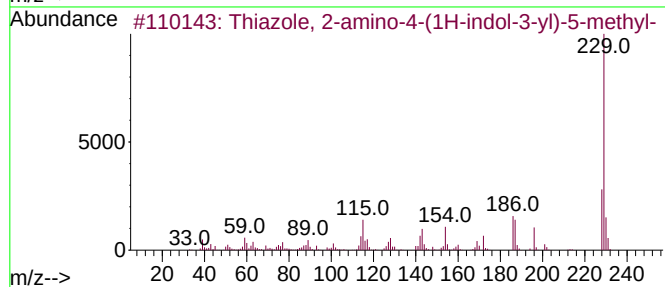
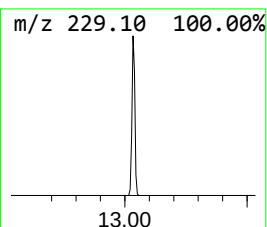
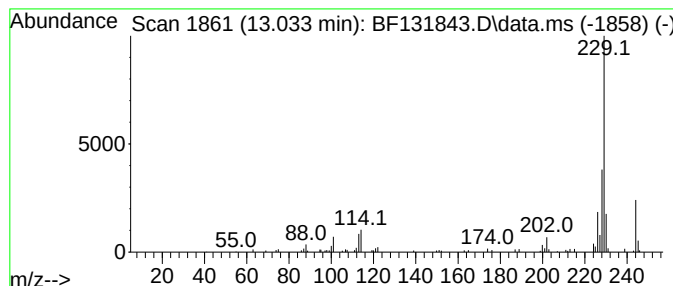
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Thiazole, 2-amino-4-(1H-indol-3-yl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.033	2.97 ng	65999	Chrysene-d12	14.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole, 2-amino-4-(1H-indol-3-...	229	C12H11N3S	1000304-18-3	53
2	2-(3-Fluorophenyl)-1,3-benzothia...	229	C13H8FNS	1000298-18-6	50
3	Tetralin, 6-acetyl-8-isopropyl-2...	244	C17H24O	1000155-43-5	47
4	2-{Bicyclo[2.2.1]heptan-2-yl}-4-...	244	C17H24O	1000411-56-7	47
5	Ethanone, 1-(2,3-dihydro-1,1,2,3...	244	C17H24O	015323-35-0	47



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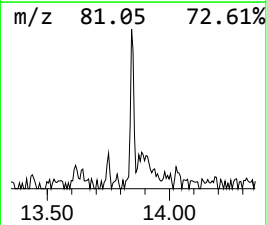
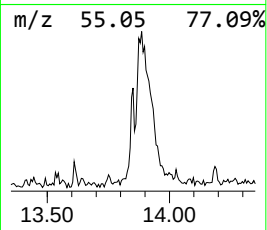
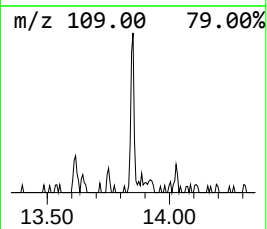
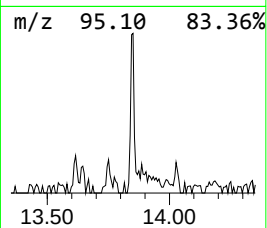
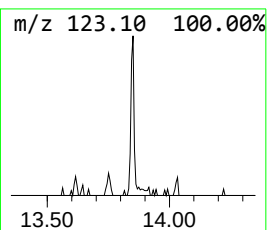
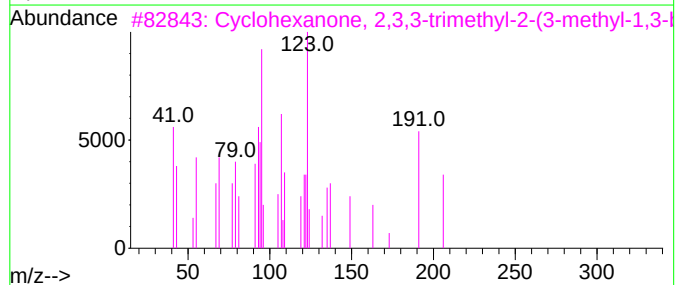
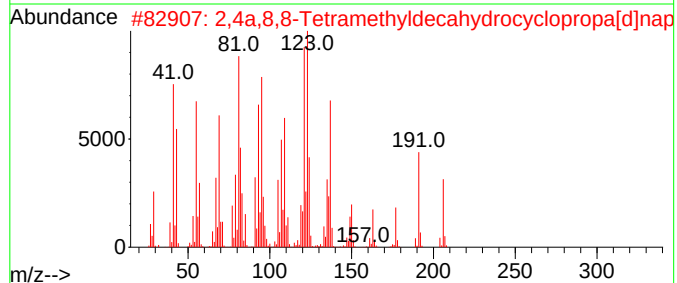
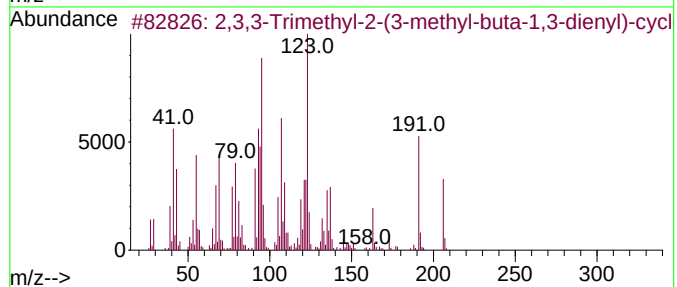
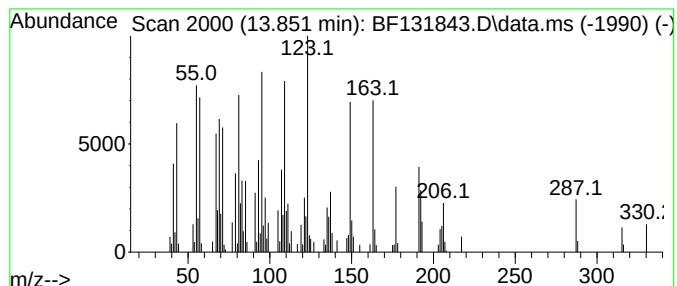
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Peak Number 3 unknown13.851 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	5.65 ng	125524	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	46		
2	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	46		
3	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	46		
4	4-[(Bicyclo[4.1.0]heptane-7-carb...	287	C17H21NO3	1000297-42-7	30		
5	Spiro[2.5]octane, 3,3-dimethyl-2...	206	C14H22O	1000197-07-6	30		



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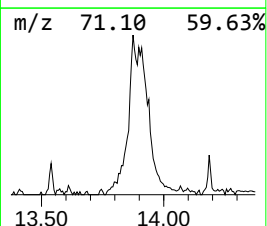
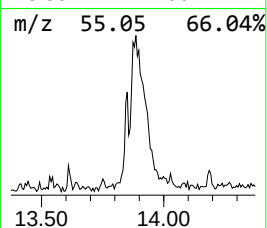
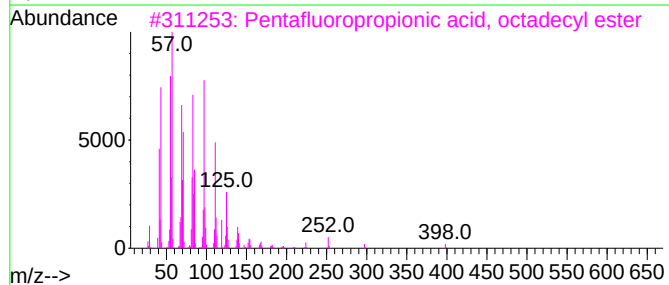
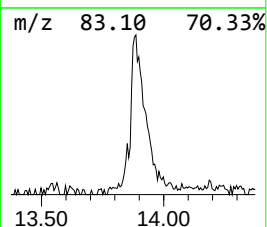
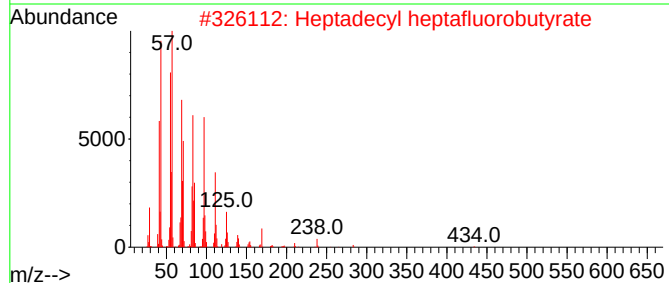
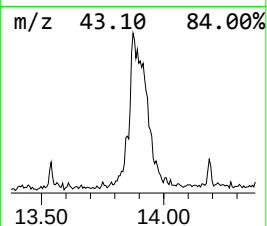
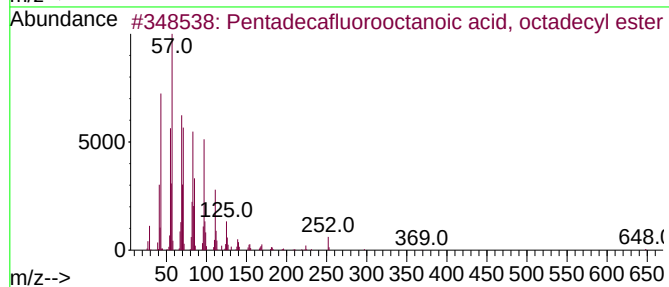
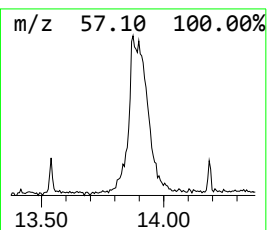
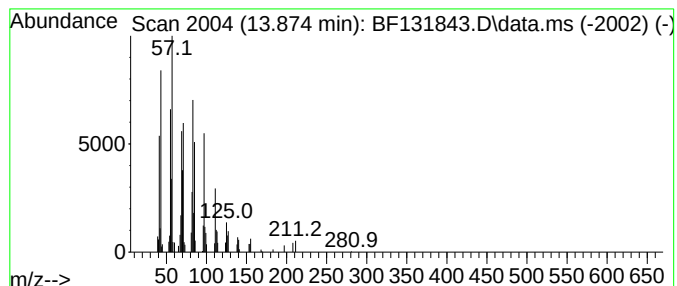
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	17.99 ng	399428	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	76
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	74
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	70



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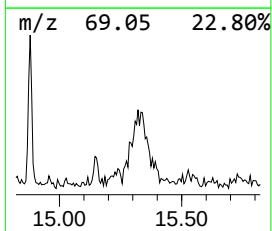
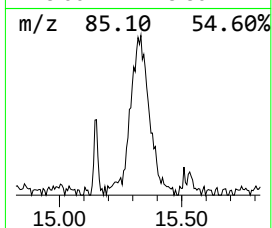
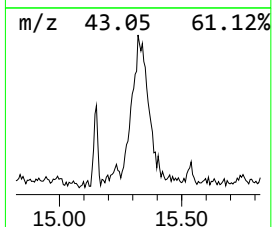
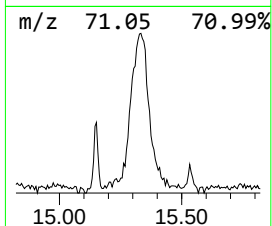
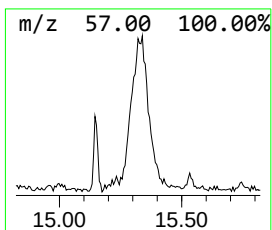
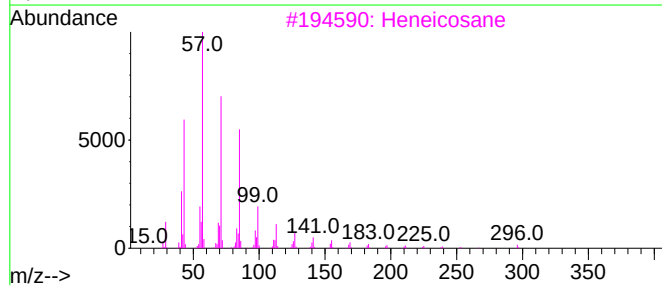
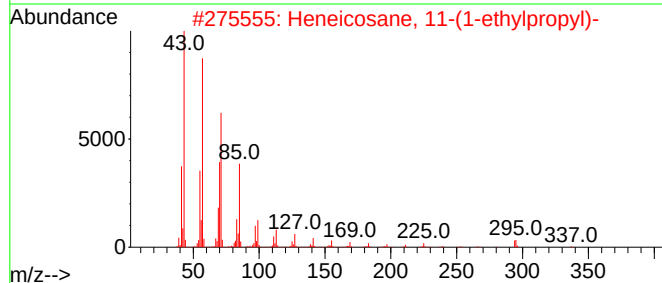
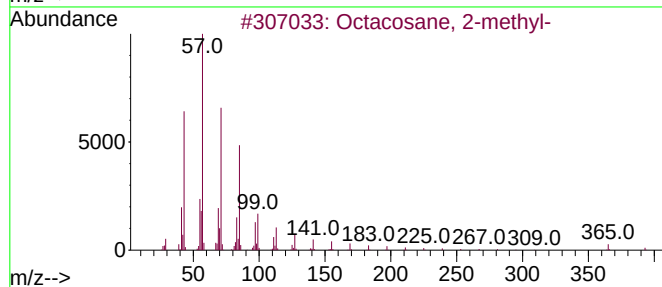
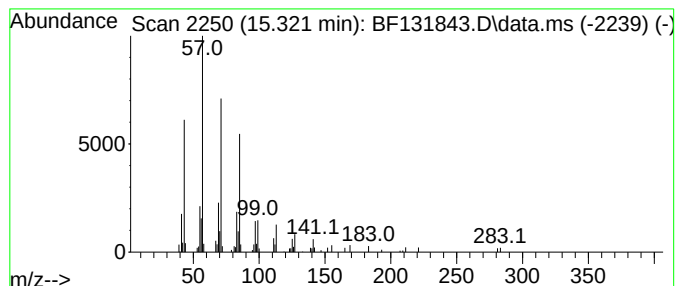
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Peak Number 5 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	5.85 ng	121538	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			2-Methyltetracosane	352	C25H52	001560-78-7	91
5			Tetracosane	338	C24H50	000646-31-1	90



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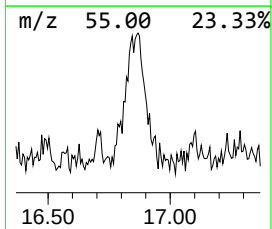
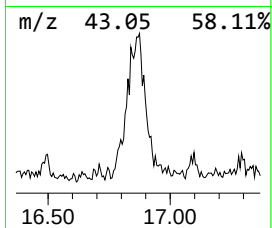
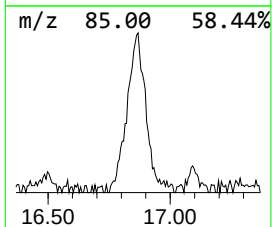
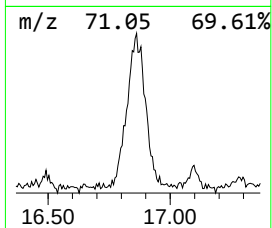
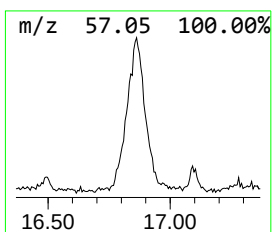
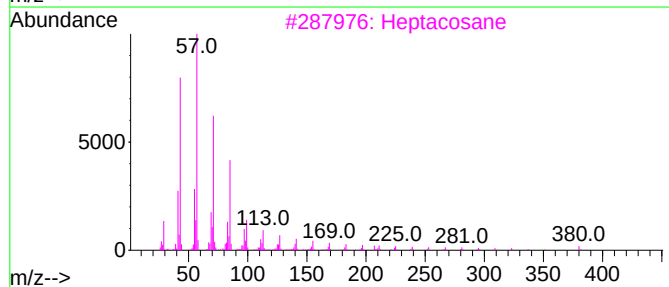
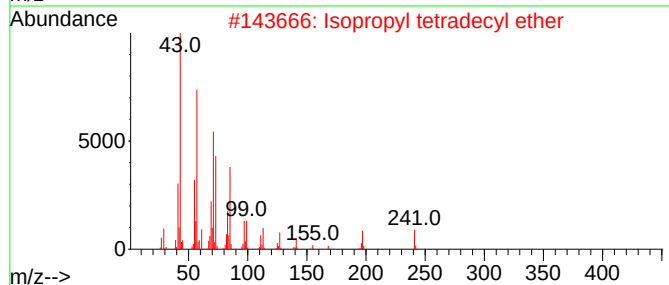
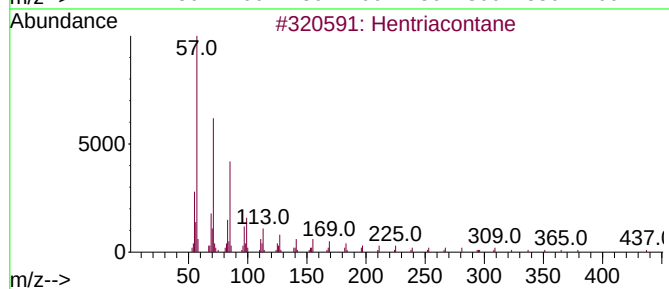
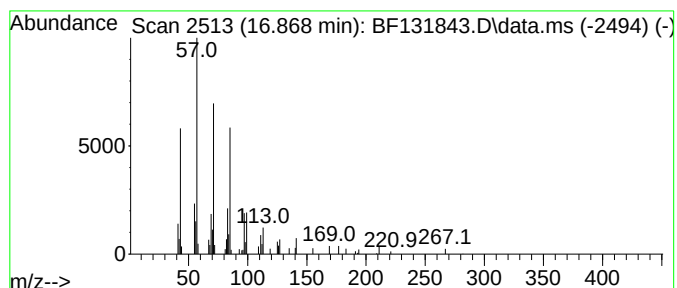
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hentriacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.868	11.31 ng	234866	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Isopropyl tetradecyl ether	256	C17H36O	1000406-34-0	90
3			Heptacosane	380	C27H56	000593-49-7	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131843.D
Acq On : 27 Dec 2022 18:29
Operator : CG\JU
Sample : N6190-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-3

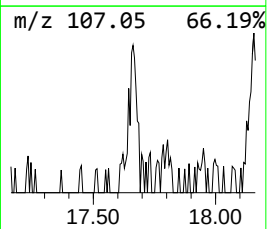
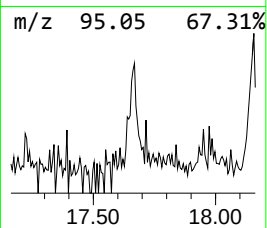
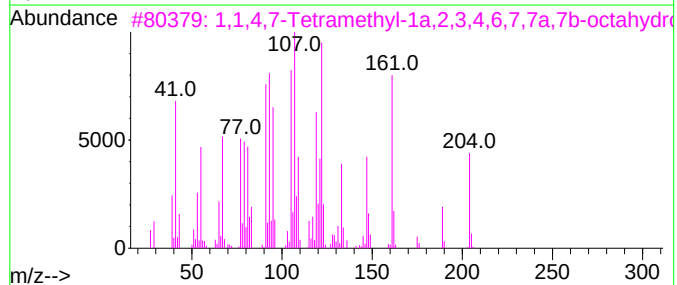
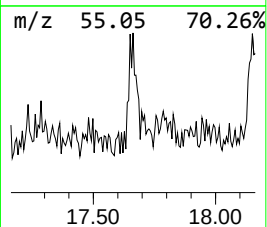
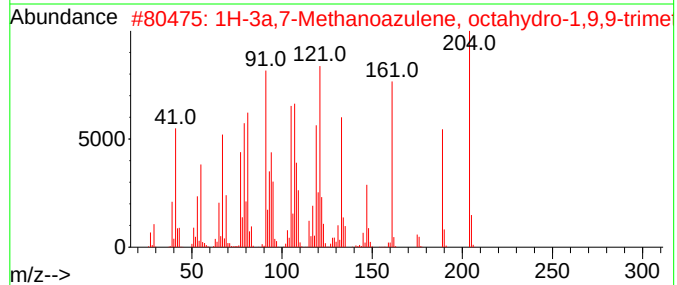
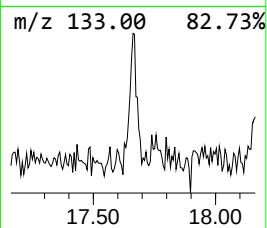
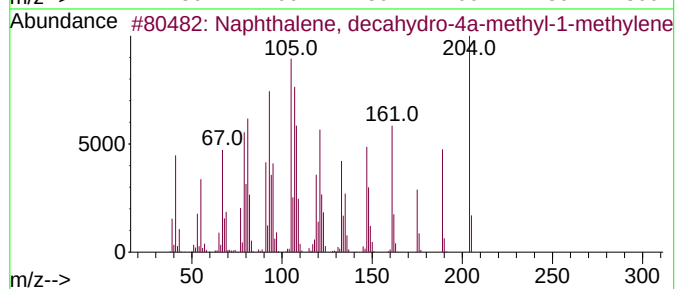
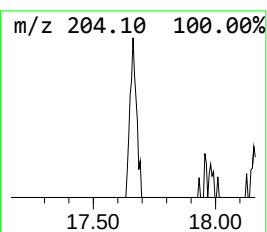
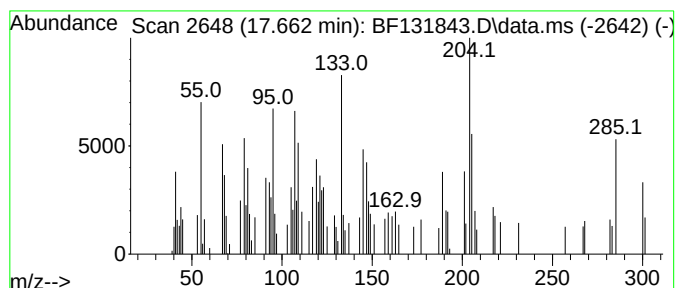
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.662 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.662	2.81 ng	58438	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	38
2			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	30
3			1,1,4,7-Tetramethyl-1a,2,3,4,6,7...	204	C15H24	405112-35-8	30
4			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	30
5			1,3-Dimethyl-5-(propen-1-yl)adam...	204	C15H24	057040-48-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131843.D
Acq On : 27 Dec 2022 18:29
Operator : CG\JU
Sample : N6190-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-3

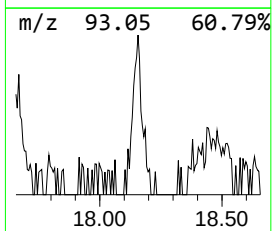
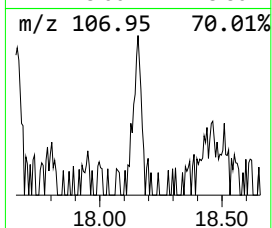
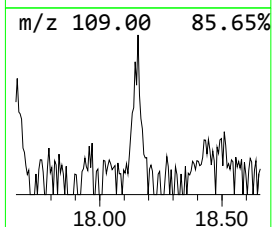
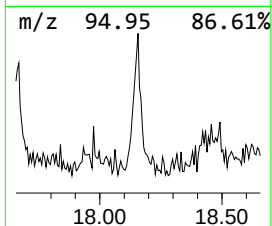
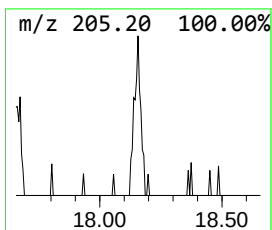
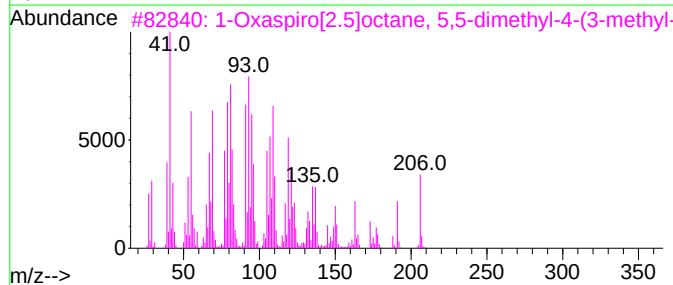
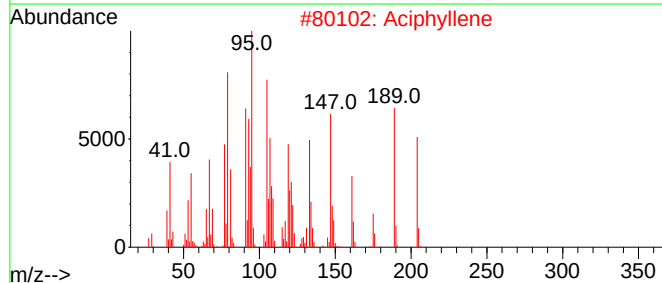
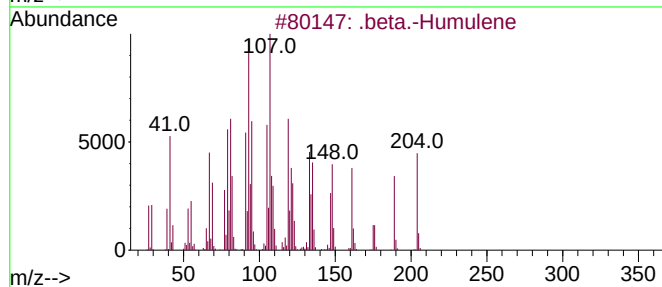
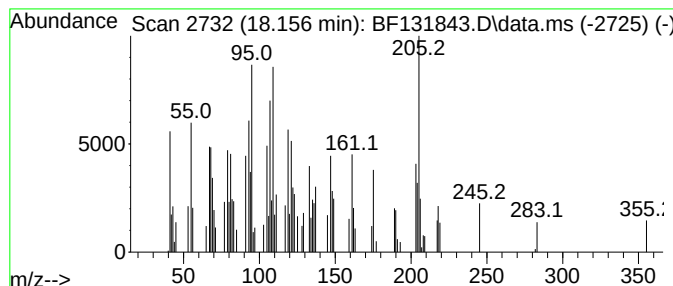
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .beta.-Humulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	3.35 ng	69677	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Humulene	204	C15H24	000116-04-1	90
2			Aciphyllene	204	C15H24	087745-31-1	56
3			1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	38
4			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	25
5			1,1,4,7-Tetramethyl-1a,2,3,4,6,7...	204	C15H24	405112-35-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131843.D
Acq On : 27 Dec 2022 18:29
Operator : CG\JU
Sample : N6190-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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-...	5.034	29.6	ng	699120	1	6.834	472399	20.0
Thiazole, 2-am...	13.033	3.0	ng	65999	5	14.027	444007	20.0
unknown13.851	13.851	5.7	ng	125524	5	14.027	444007	20.0
Pentadecafluoro...	13.874	18.0	ng	399428	5	14.027	444007	20.0
Octacosane, 2-m...	15.321	5.8	ng	121538	6	15.515	415506	20.0
Hentriacontane	16.868	11.3	ng	234866	6	15.515	415506	20.0
unknown17.662	17.662	2.8	ng	58438	6	15.515	415506	20.0
.beta.-Humulene	18.157	3.4	ng	69677	6	15.515	415506	20.0