

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
 Data File : BF135202.D
 Acq On : 13 Sep 2023 02:53
 Operator : CG\JU
 Sample : 04343-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-1-14TH-ST

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135202.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	488	493	505	rVB	648788	728741	18.40%	3.633%
2	5.393	558	562	573	rBV	1315601	1252201	31.61%	6.243%
3	6.398	729	733	746	rBV	933824	848939	21.43%	4.232%
4	6.763	791	795	798	rBV	839956	709416	17.91%	3.537%
5	7.328	885	891	894	rBV	2262064	2373132	59.91%	11.831%
6	8.039	1008	1012	1016	rBV	1168210	948755	23.95%	4.730%
7	9.122	1190	1196	1199	rBV	4102461	3961300	100.00%	19.748%
8	9.239	1212	1216	1220	rVB2	58547	59624	1.51%	0.297%
9	9.798	1307	1311	1314	rBV	1261965	1023790	25.84%	5.104%
10	10.592	1441	1446	1449	rBV	1641473	1674934	42.28%	8.350%
11	10.780	1475	1478	1480	rBV	43286	48164	1.22%	0.240%
12	10.810	1480	1483	1486	rVB2	39822	45121	1.14%	0.225%
13	10.957	1505	1508	1512	rVB3	55935	62503	1.58%	0.312%
14	10.998	1512	1515	1520	rBV	36392	48395	1.22%	0.241%
15	11.286	1560	1564	1568	rBV	1169589	977397	24.67%	4.873%
16	11.827	1652	1656	1668	rBV2	339527	372470	9.40%	1.857%
17	12.616	1787	1790	1795	rBV	86525	98528	2.49%	0.491%
18	12.886	1832	1836	1840	rBV	2774694	2833049	71.52%	14.124%
19	13.827	1993	1996	2004	rBV2	113108	186948	4.72%	0.932%
20	13.945	2011	2016	2019	rBV	563169	580270	14.65%	2.893%
21	14.580	2122	2124	2128	rVB	49032	46644	1.18%	0.233%
22	15.410	2261	2265	2270	rVB	504076	590295	14.90%	2.943%
23	15.545	2285	2288	2294	rVB3	92586	122472	3.09%	0.611%
24	15.915	2348	2351	2356	rVB3	80562	114049	2.88%	0.569%
25	16.104	2380	2383	2390	rVB3	78042	150159	3.79%	0.749%
26	16.539	2453	2457	2467	rVB2	113741	201780	5.09%	1.006%

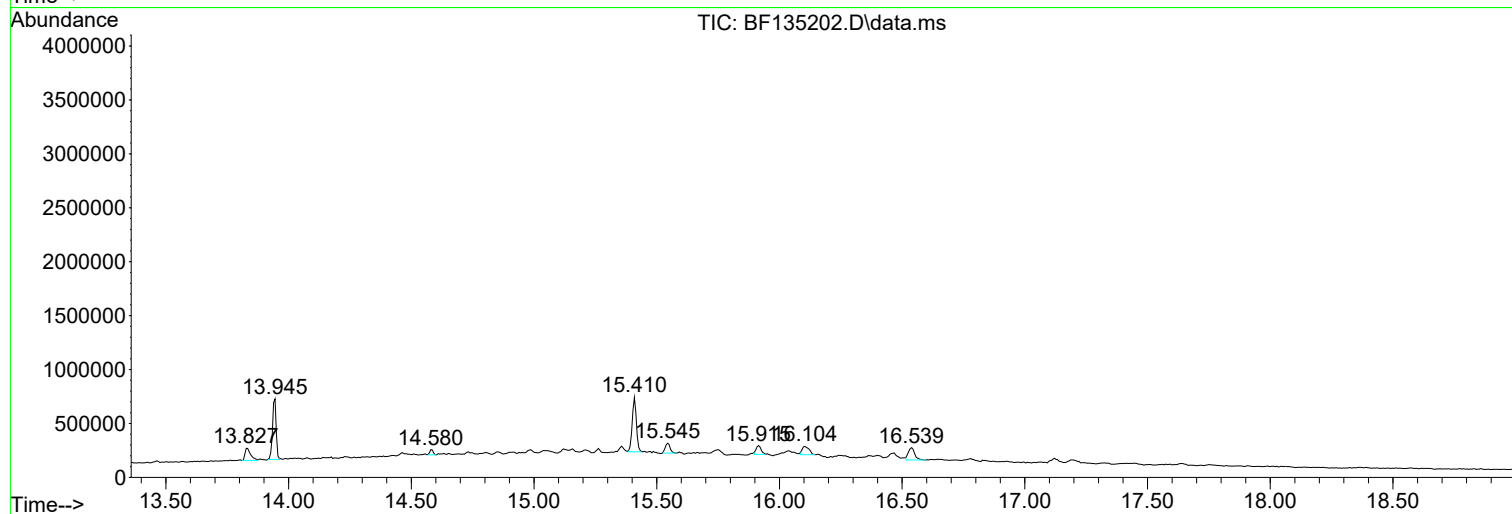
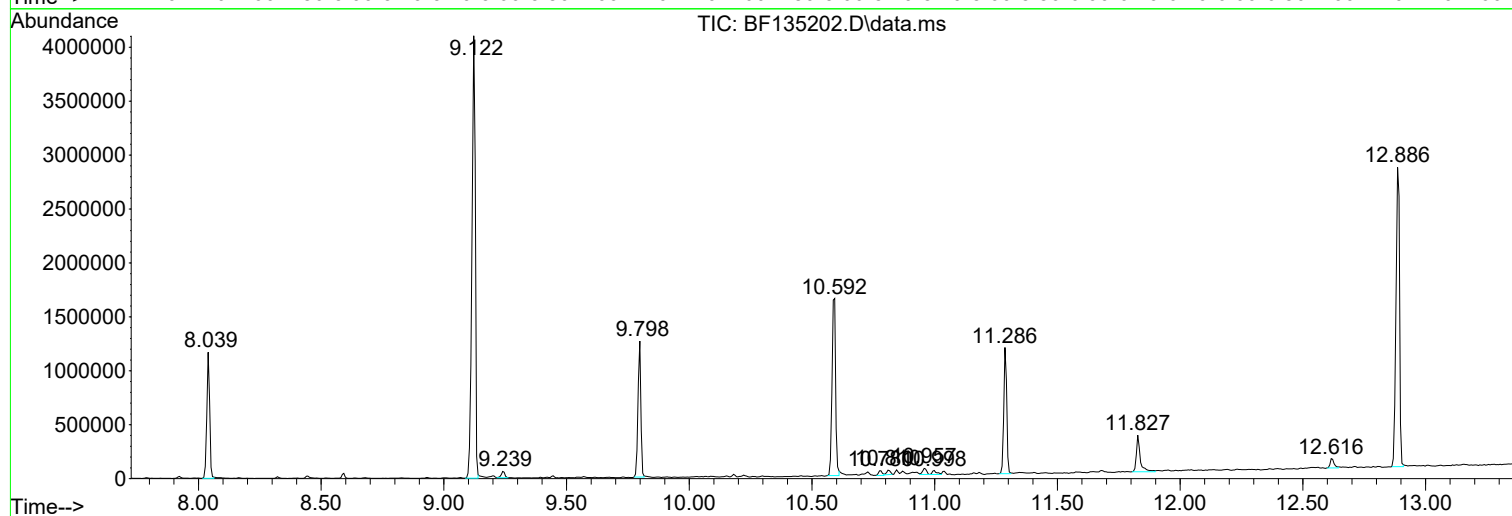
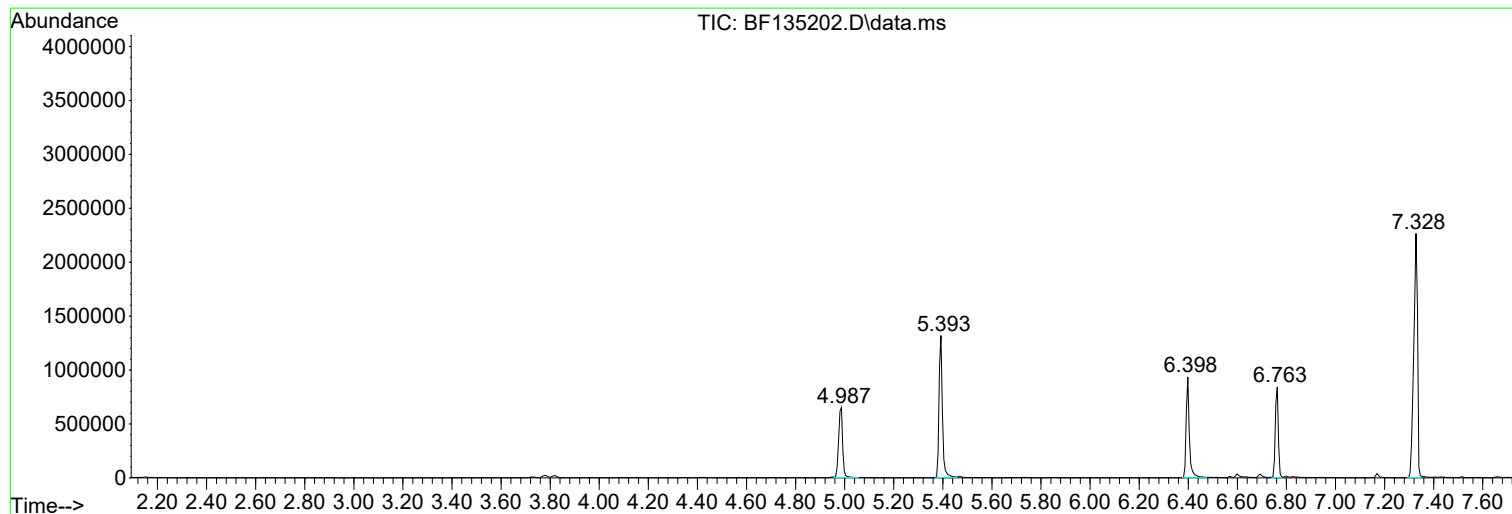
Sum of corrected areas: 20059076

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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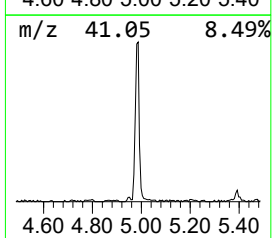
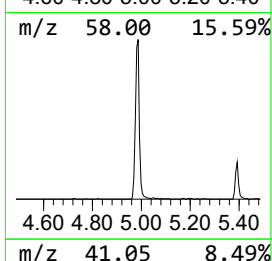
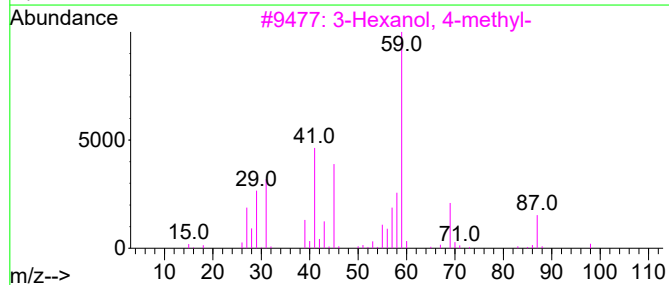
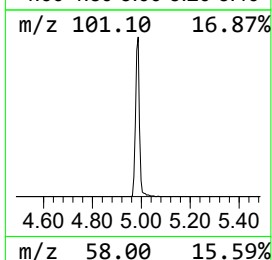
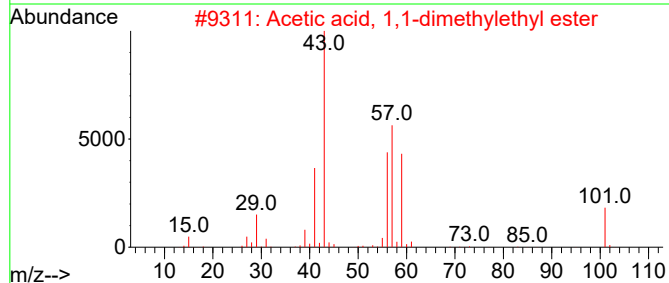
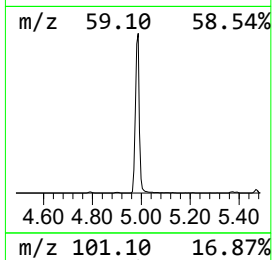
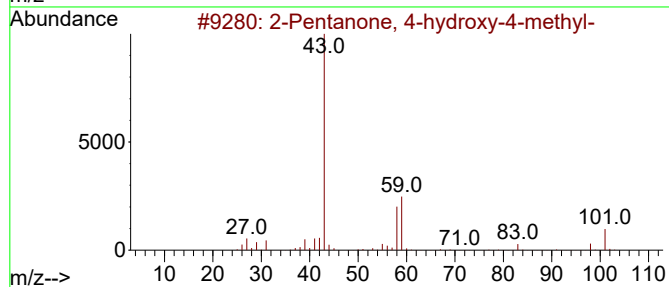
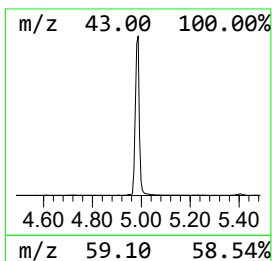
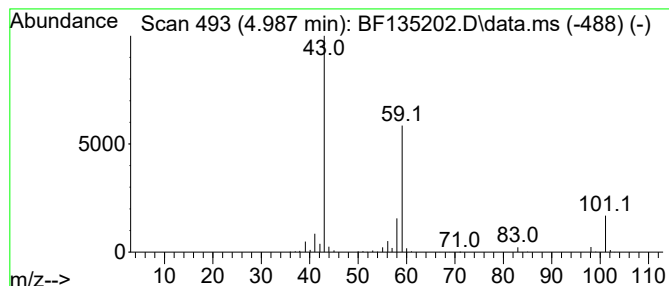
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.987	20.54 ng	728741	1,4-Dichlorobenzene-d4			6.763
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10



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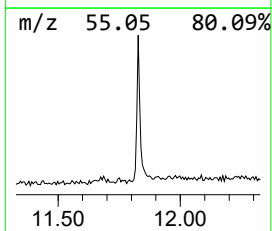
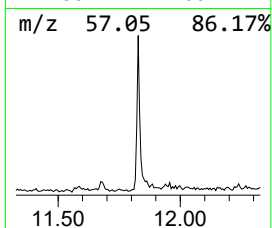
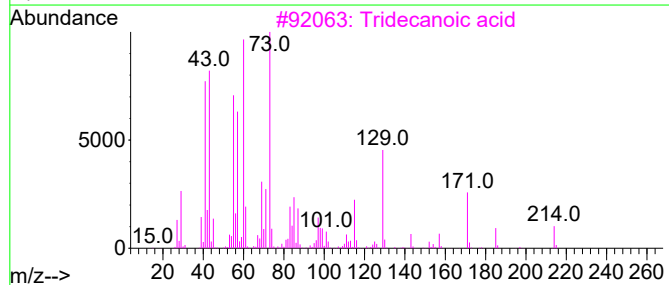
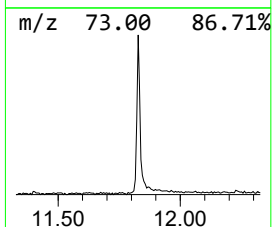
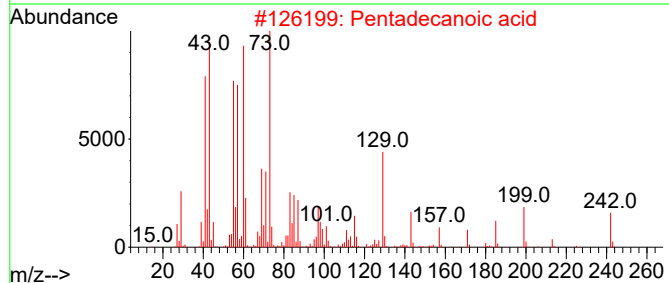
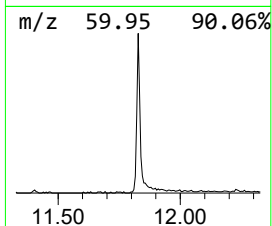
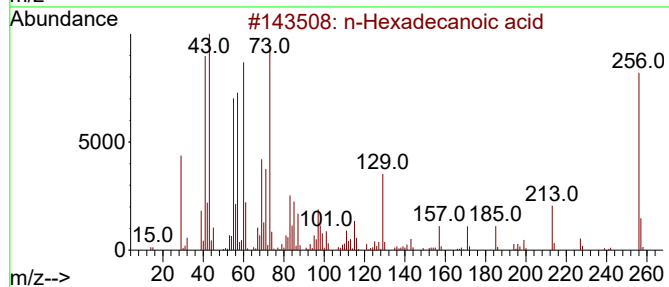
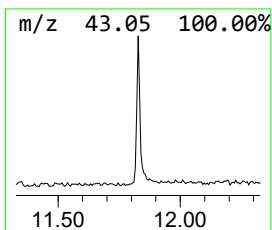
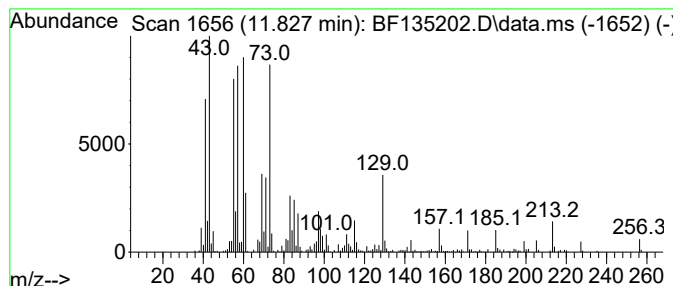
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	7.62 ng	372470	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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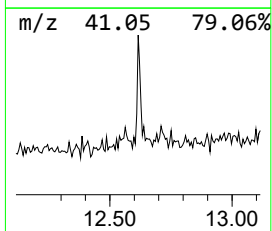
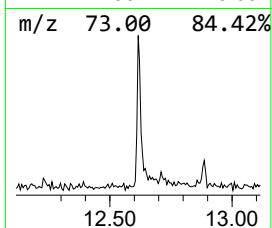
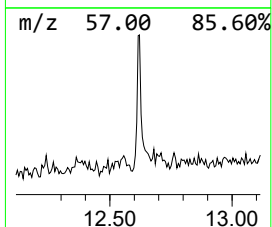
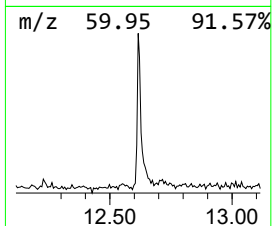
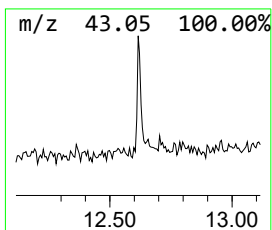
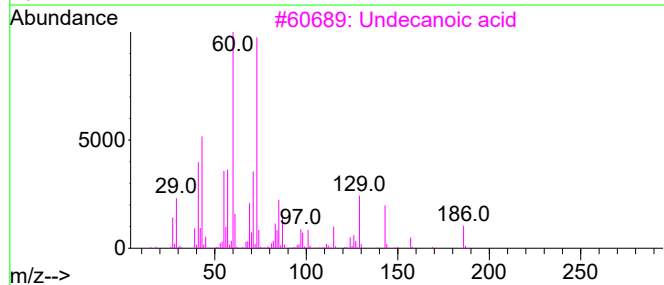
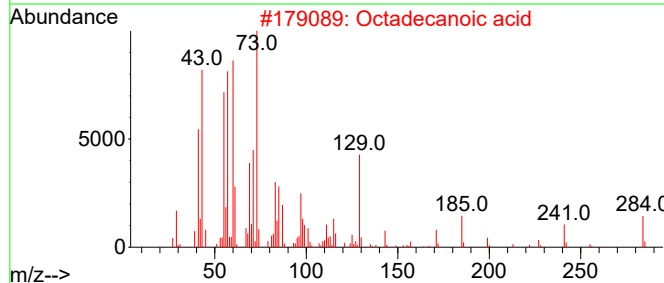
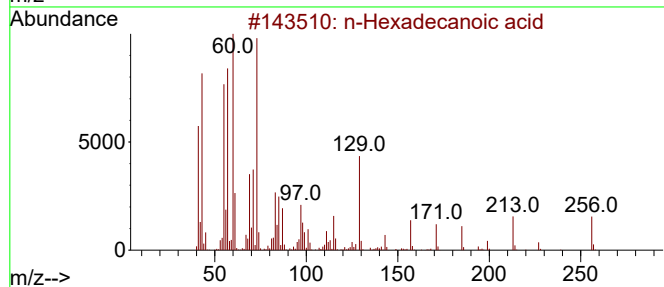
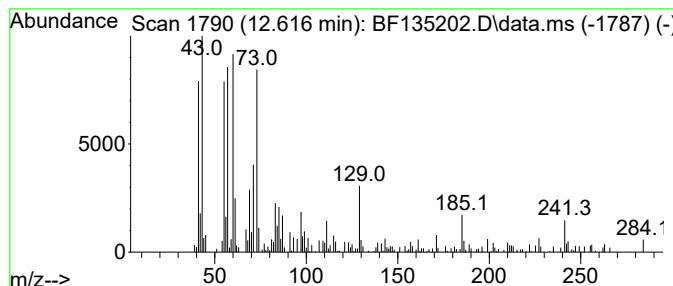
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	3.40 ng	98528	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Undecanoic acid	186	C11H22O2	000112-37-8	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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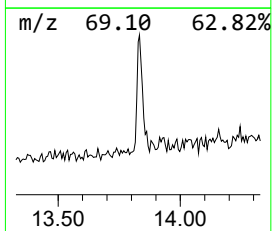
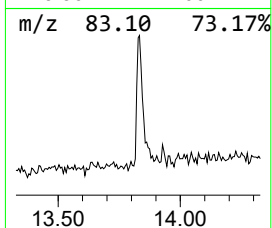
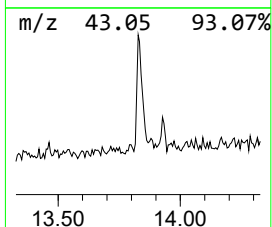
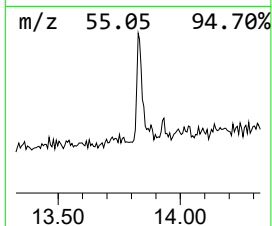
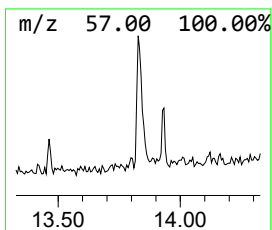
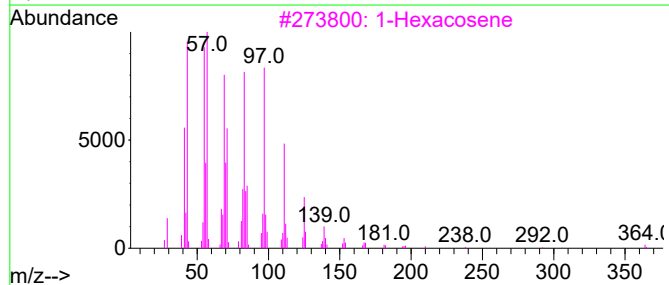
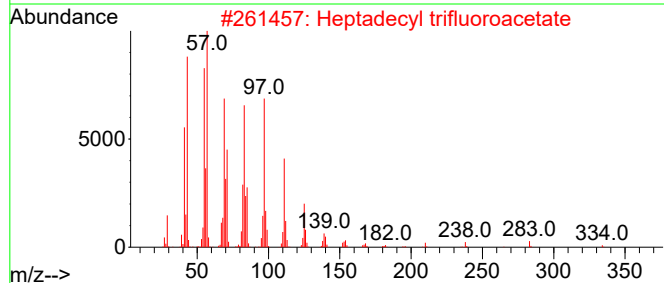
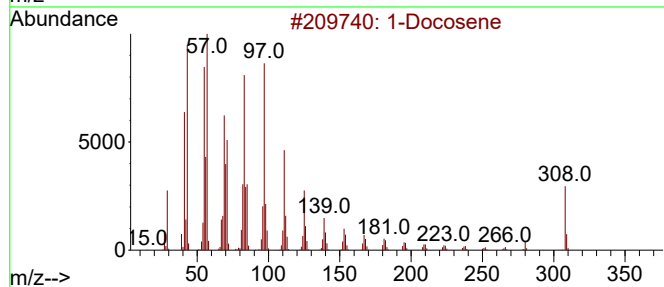
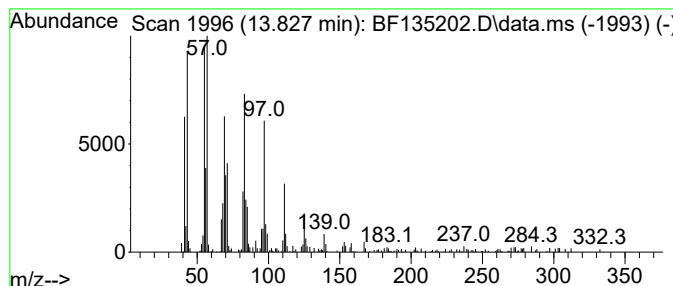
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	6.44 ng	186948	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	98
2	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	94
3	1-Hexacosene			364	C26H52	018835-33-1	93
4	9-Eicosene, (E)-			280	C20H40	074685-29-3	91
5	1-Nonadecene			266	C19H38	018435-45-5	91



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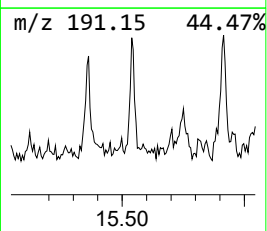
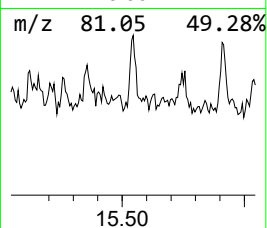
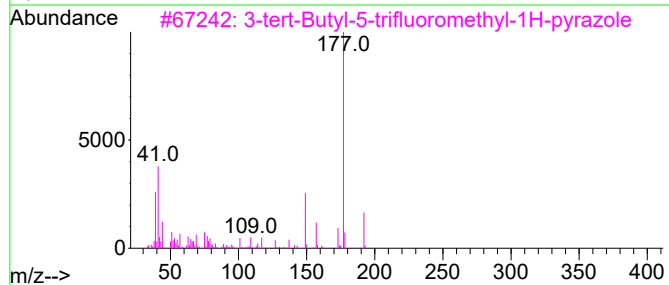
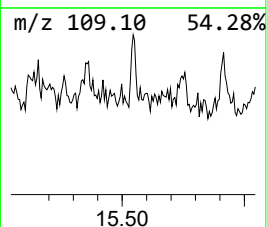
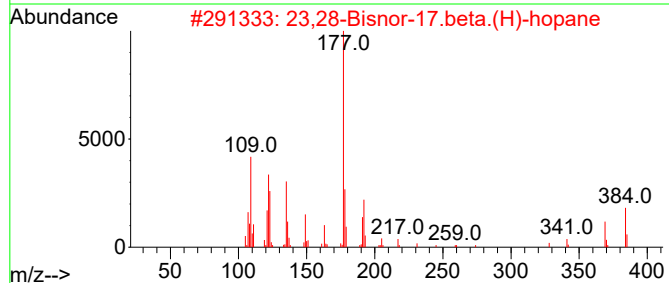
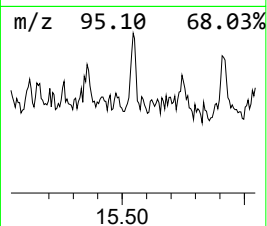
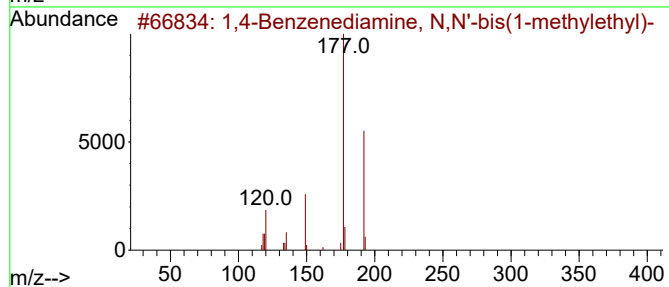
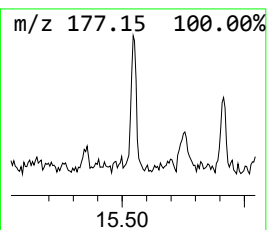
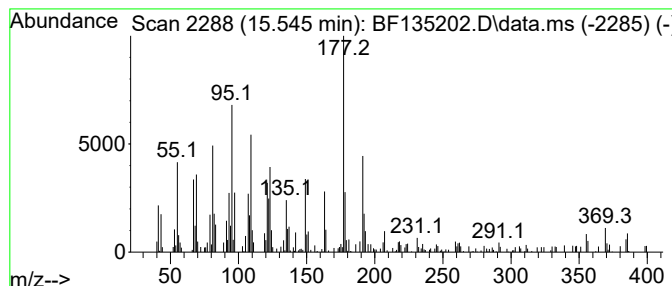
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Peak Number 5 unknown15.545 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	4.15 ng	122472	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	35
2			23,28-Bisnor-17.beta.(H)-hopane	384	C28H48	1000101-35-0	27
3			3-tert-Butyl-5-trifluoromethyl-1...	192	C8H11F3N2	150433-22-0	22
4			8H-[1,2,3]Triazolo[4',5':3,4]ben...	177	C6H3N5S	1000306-38-7	22
5			trans-.beta.-Ionone	192	C13H20O	000079-77-6	22



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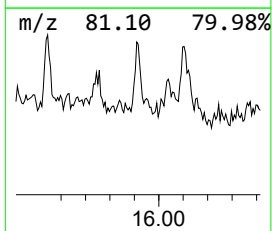
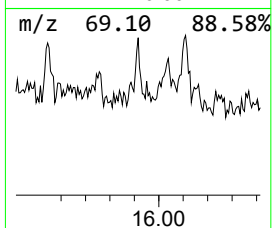
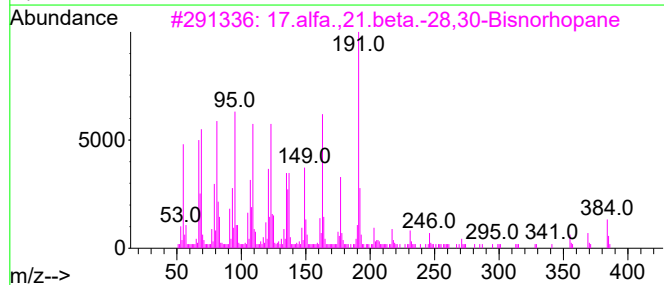
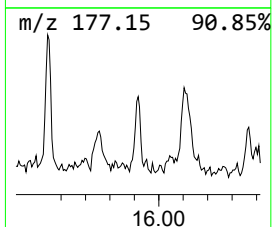
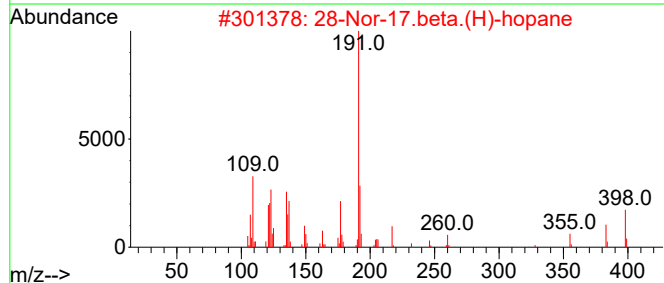
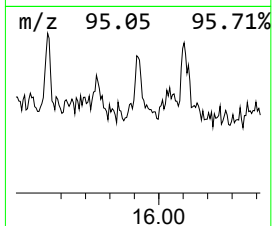
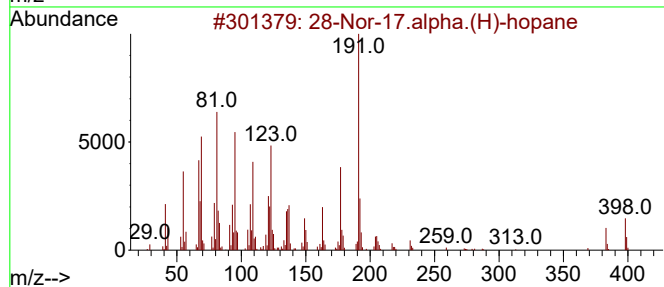
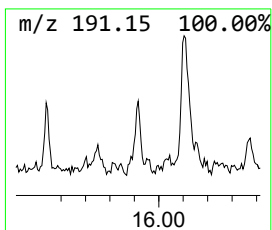
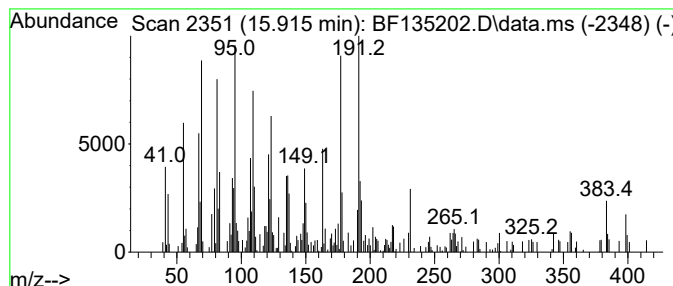
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 28-Nor-17.alpha.(H)-hopane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	3.86 ng	114049	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	95
2			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	86
3			17.alpha.,21.beta.-28,30-Bisnorho...	384	C28H48	1000360-26-1	83
4			(1R,2S,8R,8Ar)-8-acetoxy-1-(2-hy...	296	C18H32O3	1000298-98-4	59
5			(4aS,8aS)-8-Isopentyl-4,4,7,8a-t...	262	C19H34	220766-79-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135202.D
Acq On : 13 Sep 2023 02:53
Operator : CG\JU
Sample : 04343-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

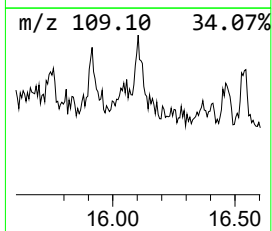
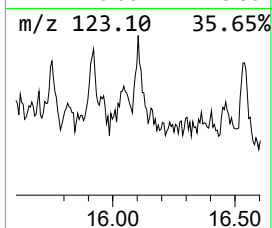
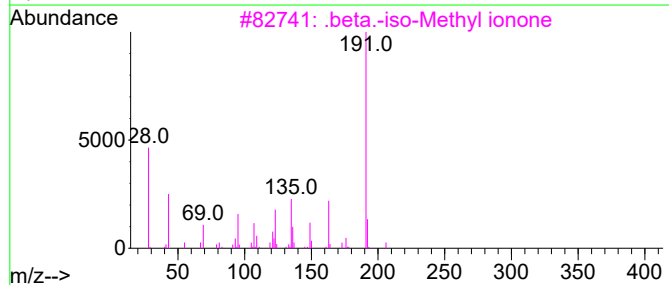
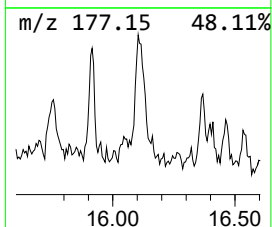
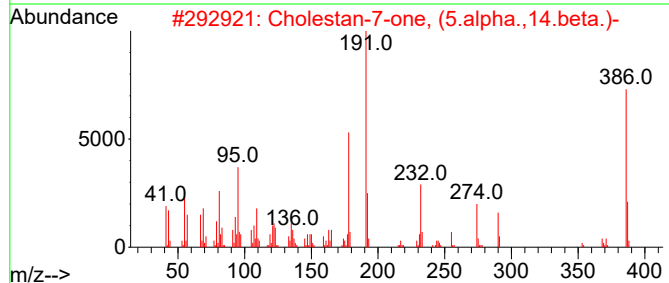
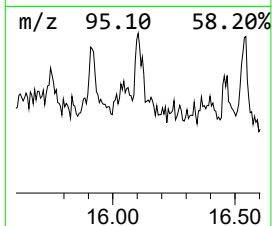
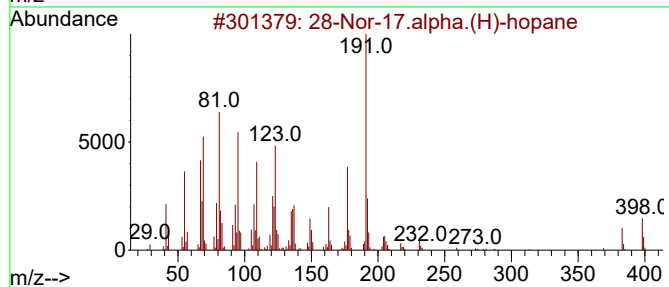
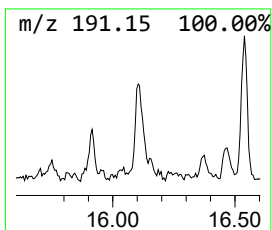
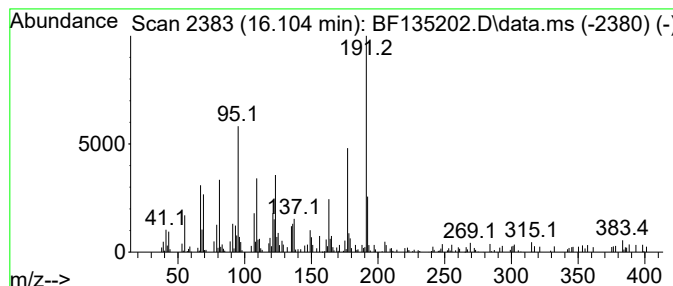
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ClientSampleId :
SAMPLE-1-14TH-ST

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cholestan-7-one, (5.alpha.,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.104	5.09 ng	150159	Perylene-d12	15.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	70
2	Cholestan-7-one, (5.alpha.,14.be...	386	C27H46O	040072-53-5	53
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
4	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	52
5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135202.D
Acq On : 13 Sep 2023 02:53
Operator : CG\JU
Sample : 04343-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

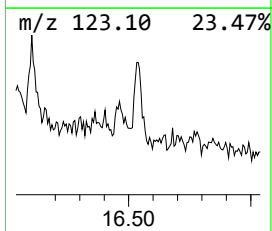
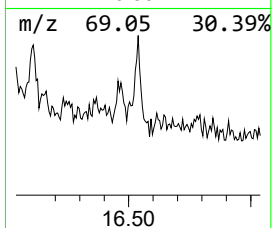
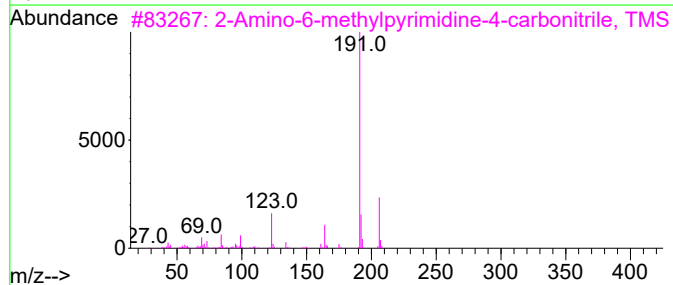
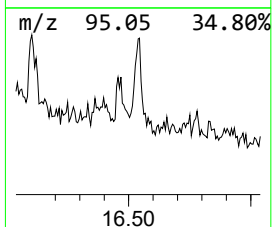
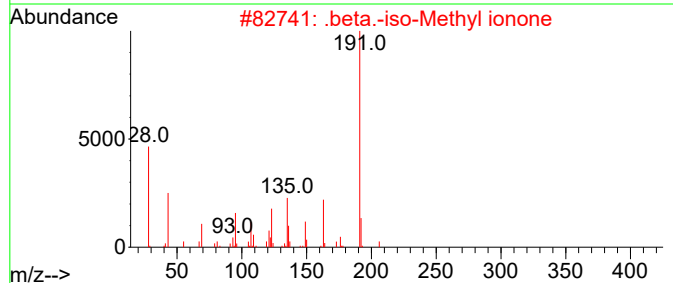
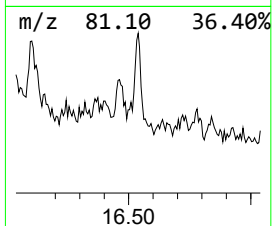
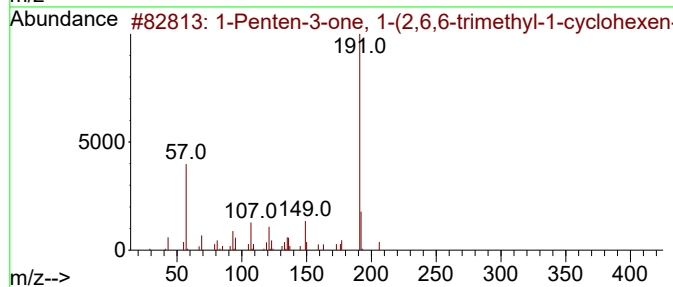
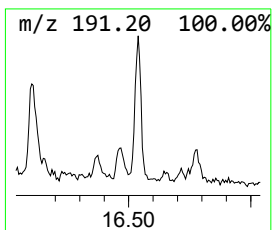
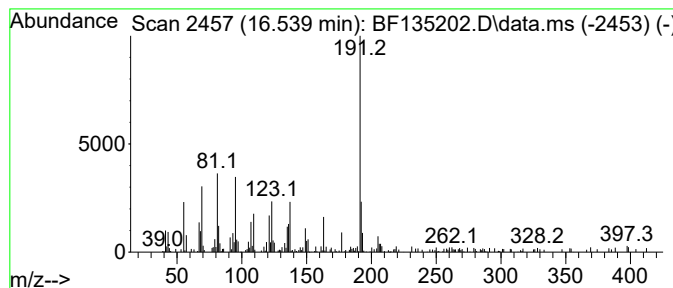
Instrument :
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ClientSampleId :
SAMPLE-1-14TH-ST

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Penten-3-one, 1-(2,6,6-tr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.539	6.84 ng	201780	Perylene-d12	15.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	58
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
3	2-Amino-6-methylpyrimidine-4-car...	206	C9H14N4Si	1000496-37-8	50
4	Isophthalic acid, 2-methyloct-5-...	330	C20H26O4	1000343-92-3	38
5	Succinic acid, di(3-methylphenyl...	298	C18H18O4	1000329-96-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135202.D
Acq On : 13 Sep 2023 02:53
Operator : CG\JU
Sample : 04343-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-14TH-ST

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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-...	4.987	20.5	ng	728741	1	6.763	709416	20.0
n-Hexadecanoic ...	11.827	7.6	ng	372470	4	11.286	977397	20.0
Octadecanoic acid	12.616	3.4	ng	98528	5	13.945	580270	20.0
1-Docosene	13.827	6.4	ng	186948	5	13.945	580270	20.0
unknown15.545	15.545	4.2	ng	122472	6	15.410	590295	20.0
28-Nor-17.alpha...	15.915	3.9	ng	114049	6	15.410	590295	20.0
Cholestan-7-one...	16.104	5.1	ng	150159	6	15.410	590295	20.0
1-Penten-3-one,...	16.539	6.8	ng	201780	6	15.410	590295	20.0