LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137064.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	9	14	19	rBV	11268	15841	1.51%	0.189%
2	5.022	495	499	511	rVB	69198	86083	8.19%	1.028%
3	5.434	565	569	588	rBV	966799	885172	84.17%	10.570%
4	6.434	735	739	758	rBV	917656	814824	77.48%	9.730%
5	6.781	795	798	802	rBV	288918	250921	23.86%	2.996%
6	7.345	890	894	897	rBV	659581	531960	50.59%	6.352%
7	8.057	1012	1015	1021	rBV	333462	291864	27.75%	3.485%
8	9.133	1195	1198	1202	rBV	1095715	962388	91.52%	11.492%
9	9.816	1311	1314	1324	rBV	403397	310803	29.55%	3.711%
10	10.610	1446	1449	1461	rBV	559303	512341	48.72%	6.118%
11	11.263	1557	1560	1564	rBV4	10652	11547	1.10%	0.138%
12	11.310	1564	1568	1571	rVV	401896	330187	31.40%	3.943%
13	11.333	1571	1572	1576	rVB	19572	13788	1.31%	0.165%
14	11.774	1644	1647	1651	rBV5	10755	16868	1.60%	0.201%
15	11.845	1656	1659	1671	rVB	138273	162320	15.44%	1.938%
16	12.404	1752	1754	1758	rVB5	14924	12898	1.23%	0.154%
17	12.533	1773	1776	1778	rBV	67225	62564	5.95%	0.747%
18	12.633	1790	1793	1801	rVB3	26507	30263	2.88%	0.361%
19	12.763	1810	1815	1820	rVB	51381	54023	5.14%	0.645%
20	12.904	1835	1839	1843	rBV	1153237	1051613	100.00%	12.558%
21	13.198	1885	1889	1892	rBV4	16207	21075	2.00%	0.252%
22	13.292	1903	1905	1908	rBV3	17703	21286	2.02%	0.254%
23	13.339	1909	1913	1916	rVV	182074	209271	19.90%	2.499%
24	13.380	1916	1920	1924	rVV3	43719	88345	8.40%	1.055%
25	13.421	1926	1927	1933	rVB5	13330	16766	1.59%	0.200%
26	13.610	1955	1959	1962	rVB5	9699	12744	1.21%	0.152%
27	13.674	1965	1970	1973	rBV7	12010	17539	1.67%	0.209%
28	13.763	1982	1985	1991	rBV6	20024	29673	2.82%	0.354%
29	13.827	1991	1996	2011	rVB6	42120	109646	10.43%	1.309%
30	13.968	2016	2020	2023	rVV	423156	421810	40.11%	5.037%
31	13.992	2023	2024	2028	rVB	33381	27764	2.64%	0.332%
32	14.063	2033	2036	2040	rVB2	17872	18538	1.76%	0.221%
33	14.127	2044	2047	2054	rVB2	17678	25258	2.40%	0.302%
34	14.433	2096	2099	2102	rVB	30703	27689	2.63%	0.331%
35	14.486	2104	2108	2111	rVV6	14032	20586	1.96%	0.246%
36	14.745	2149	2152	2155	rVB	23987	24182	2.30%	0.289%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.815	2161	2164	2169	rVB2	26361	30399	2.89%	0.363%
38	15.021	2195	2199	2206	rBV	32663	64512	6.13%	0.770%
39	15.086	2206	2210	2216	rVB	52249	65327	6.21%	0.780%
40	15.327	2248	2251	2256	rBV	18798	24594	2.34%	0.294%
41	15.398	2259	2263	2268	rVB2	23512	33658	3.20%	0.402%
42	15.462	2268	2274	2285	rBV	307648	428032	40.70%	5.111%
43	15.692	2308	2313	2315	rBV6	12337	21099	2.01%	0.252%
44	15.921	2348	2352	2358	rVB	37951	53844	5.12%	0.643%
45	16.015	2363	2368	2369	rBV5	12523	20504	1.95%	0.245%
46	17.621	2635	2641	2646	rVB9	14626	36302	3.45%	0.434%
47	18.627	2804	2812	2823	rVB9	27015	95396	9.07%	1.139%

Sum of corrected areas: 8374107

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
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Instrument :
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ClientSampleId :
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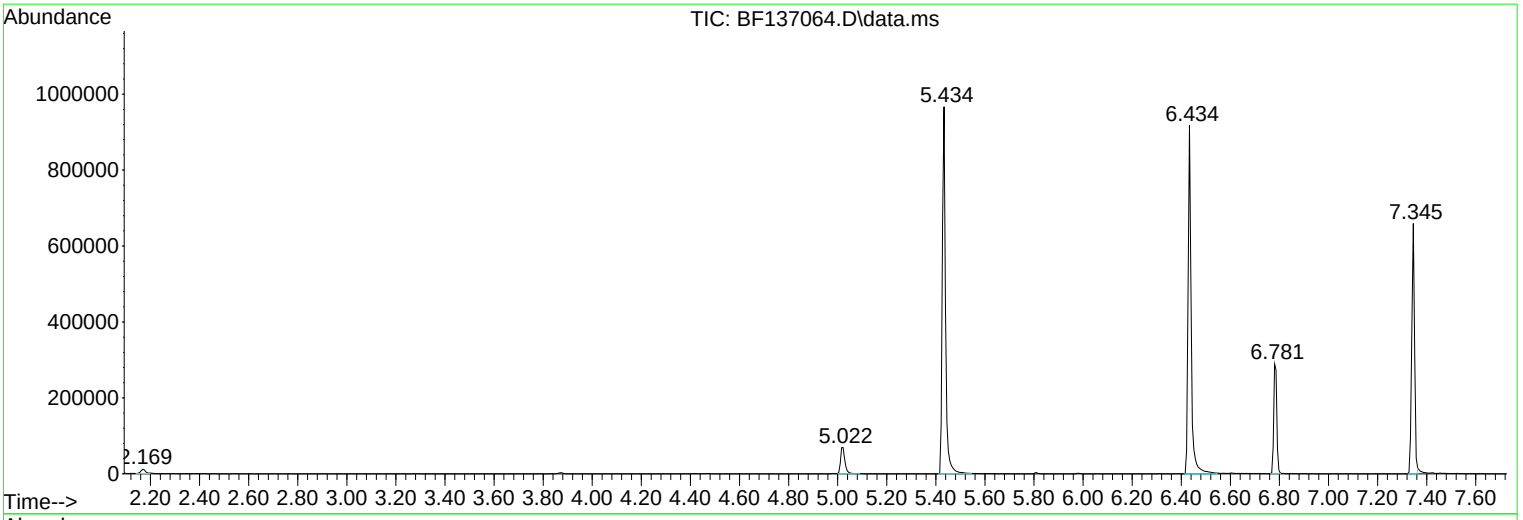
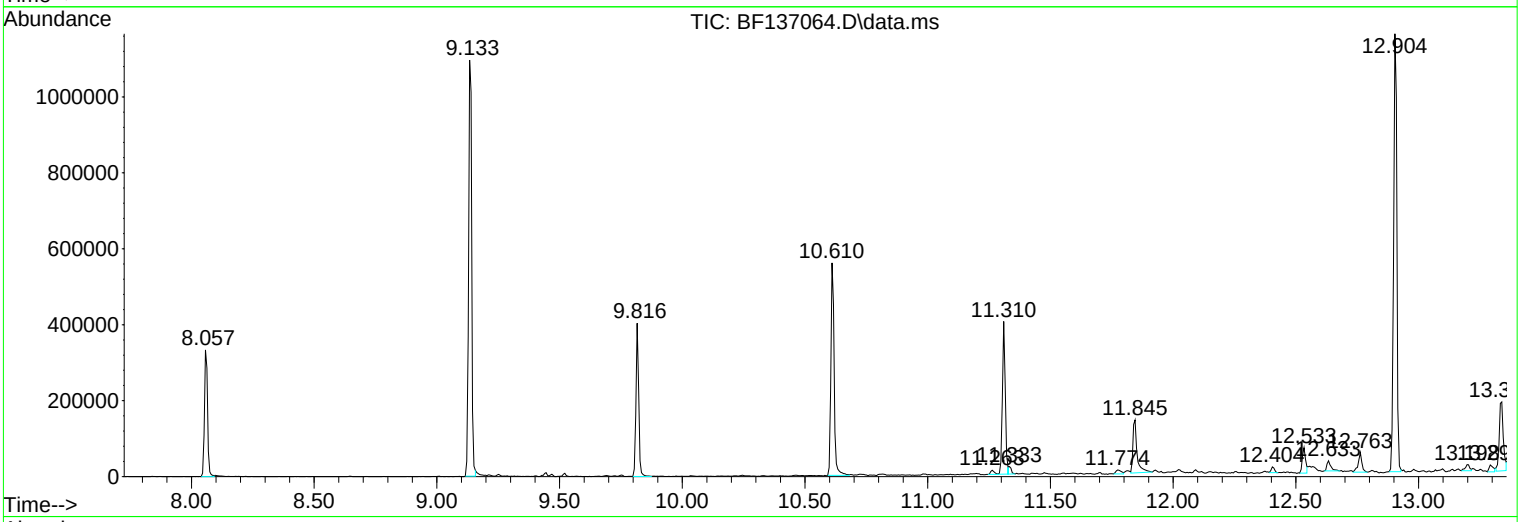
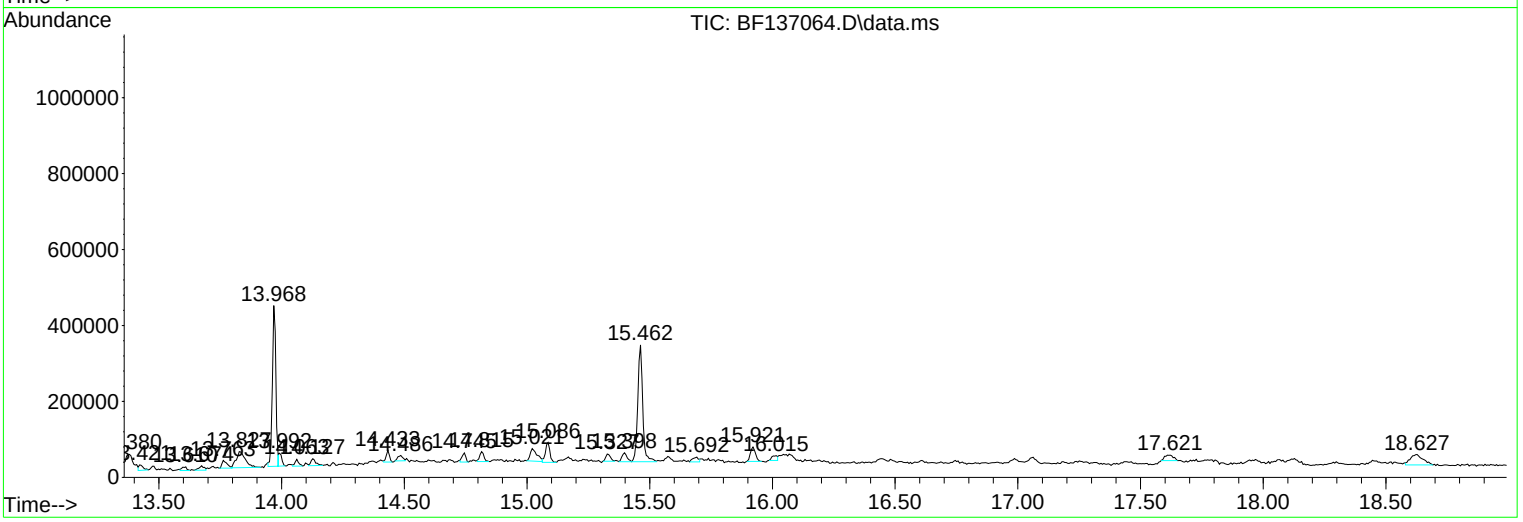
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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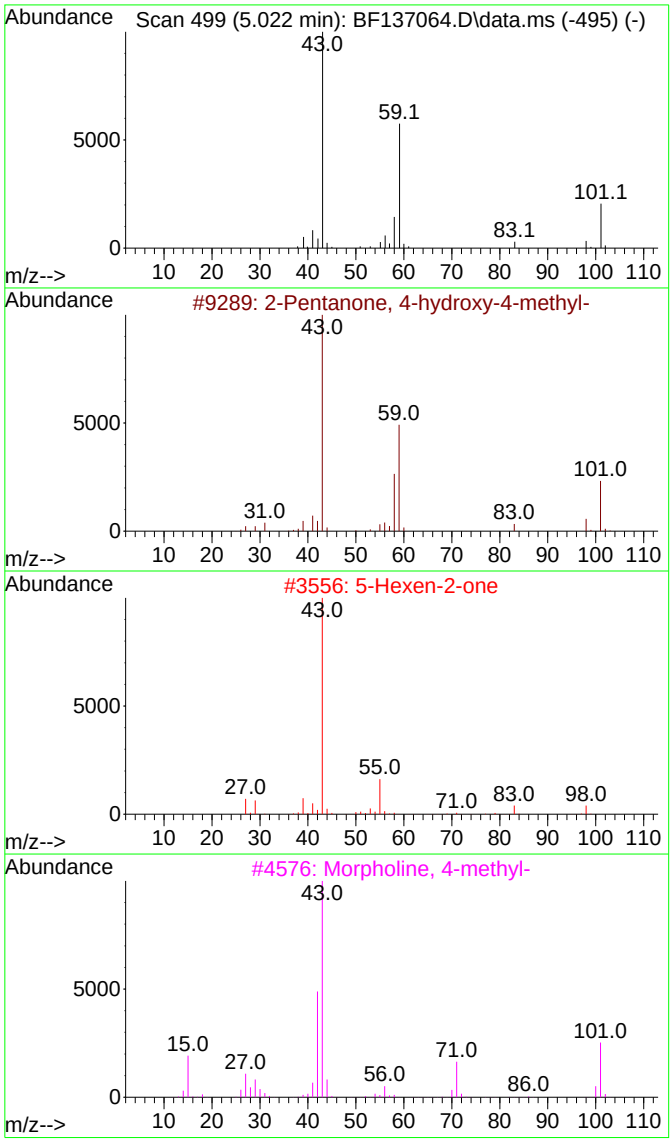
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

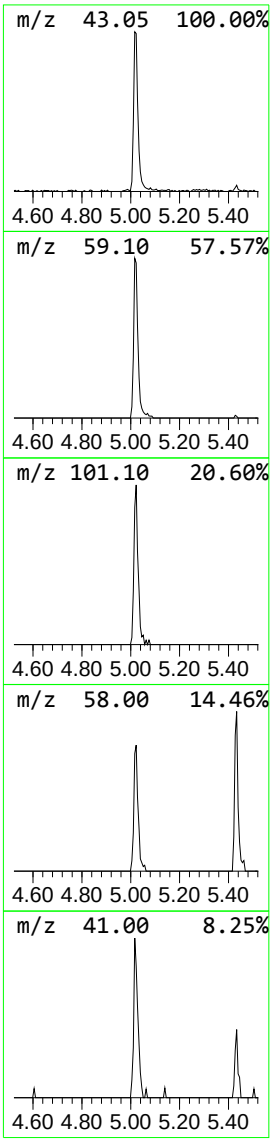
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	6.86 ng	86083	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

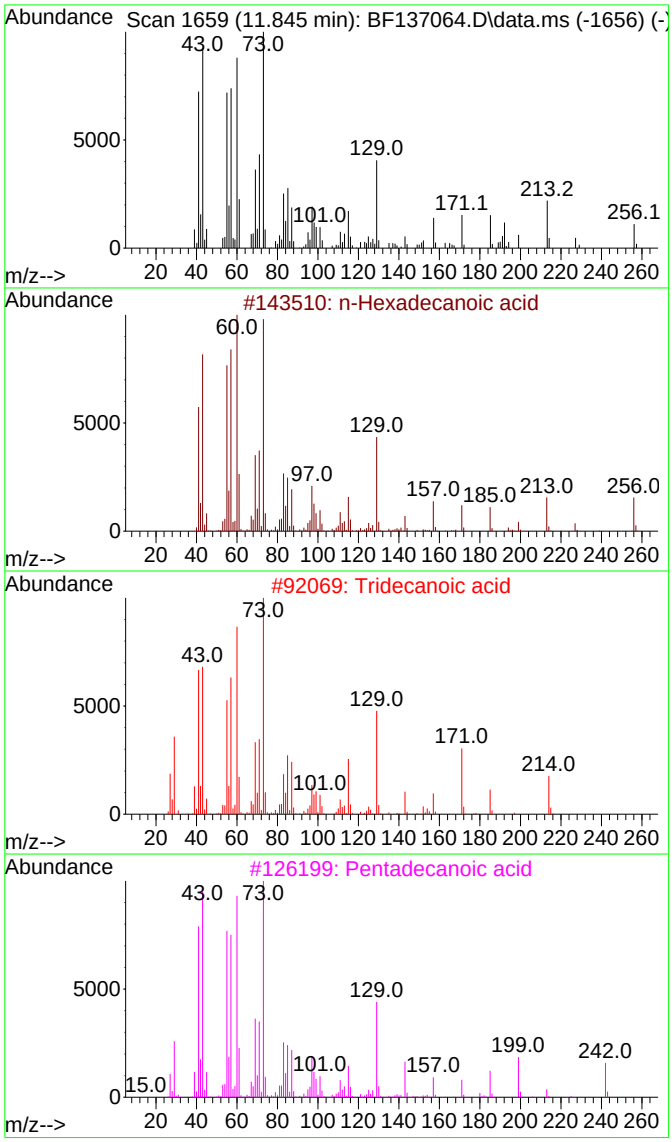
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

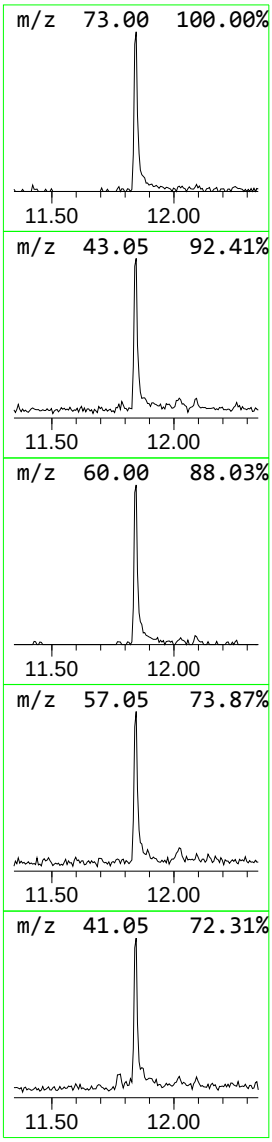
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	9.83 ng	162320	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

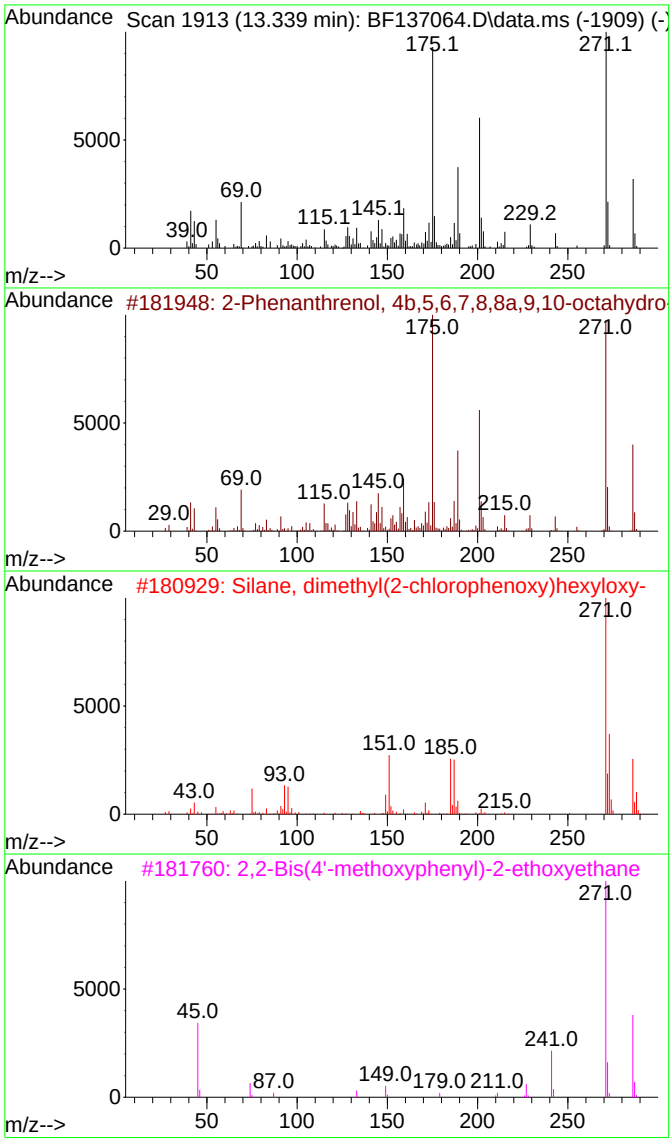
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

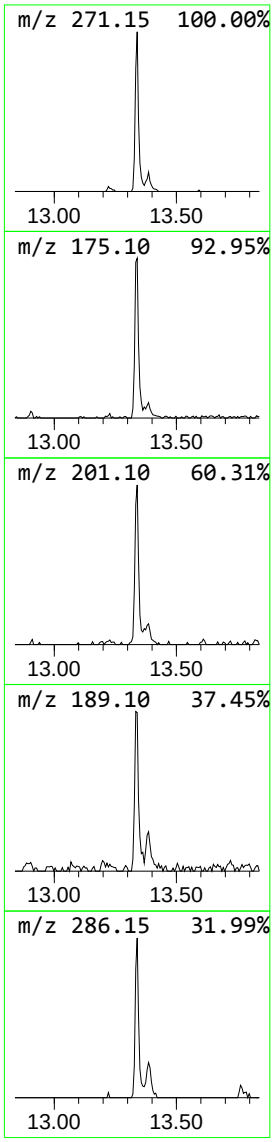
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.339	9.92 ng	209271	Chrysene-d12	13.968

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	Silane, dimethyl(2-chlorophenoxy...	286	C14H23ClO2Si	1000347-07-3	35
3	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	30
4	Silane, methylvinyl(hept-3-yloxy...	386	C20H42O3Si2	1000421-69-5	27
5	4-Hydroxy-4'-methyldiphenylamine...	271	C16H21NOSi	1000417-59-7	22





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Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

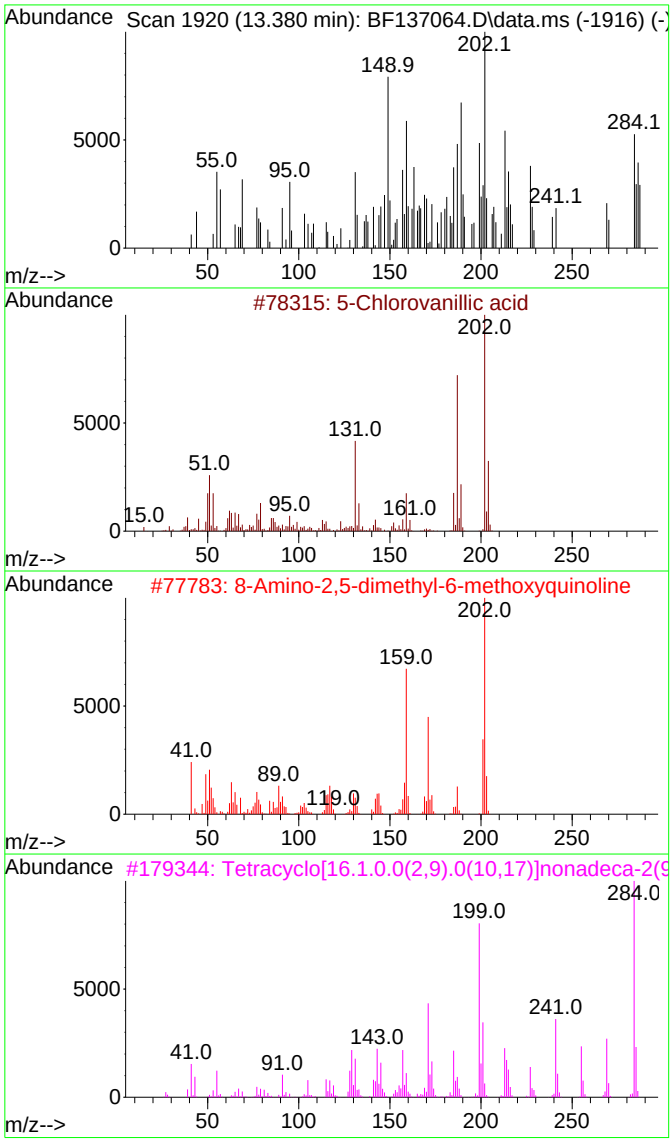
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

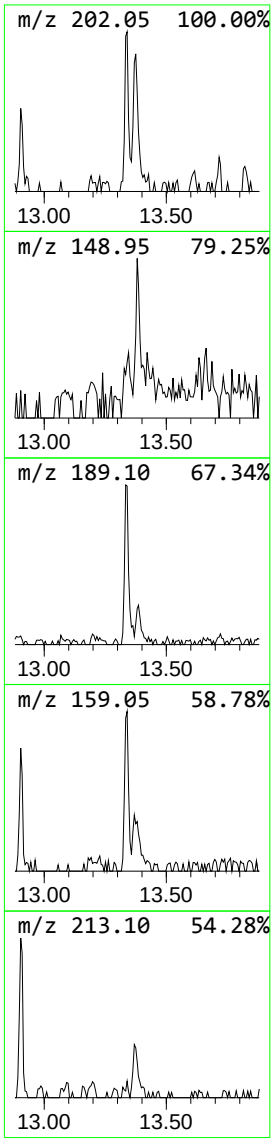
****

Peak Number 5 unknown13.380 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.380	4.19 ng	88345	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Chlorovanillic acid	202	C8H7ClO4	062936-23-6	14
2	8-Amino-2,5-dimethyl-6-methoxyqu...	202	C12H14N2O	1000214-69-9	11
3	Tetracyclo[16.1.0.0(2,9).0(10,17...	284	C21H32	1000163-57-5	10
4	6,6,8-Trimethyl-5,6-dihydro-[1,3...	217	C13H15NO2	136870-77-4	10
5	Stannane, diethenyldimethyl-	204	C6H12Sn	020204-11-9	10





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Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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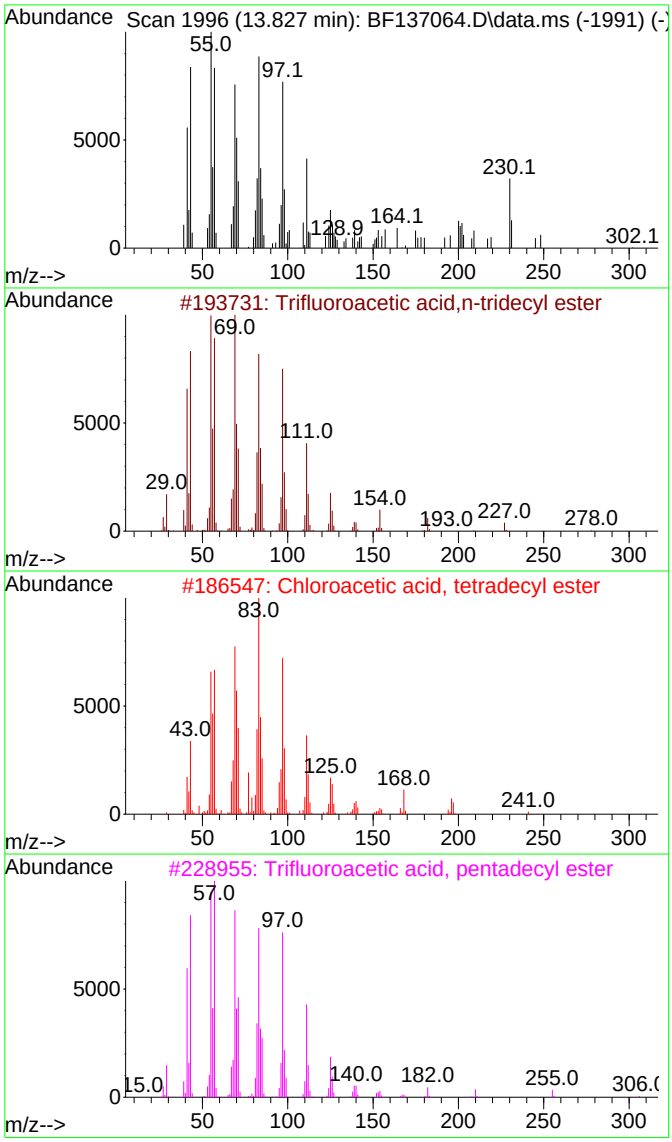
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

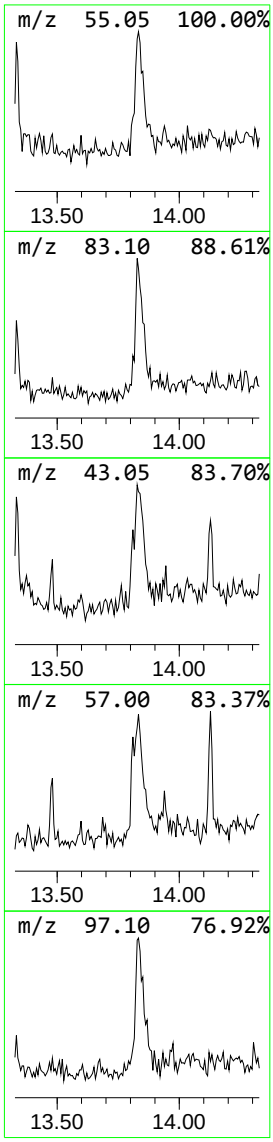
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Trifluoroacetic acid,n-trid... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	5.20 ng	109646	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	93
2	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	91
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4	1-Tricosene	322	C23H46	018835-32-0	87
5	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

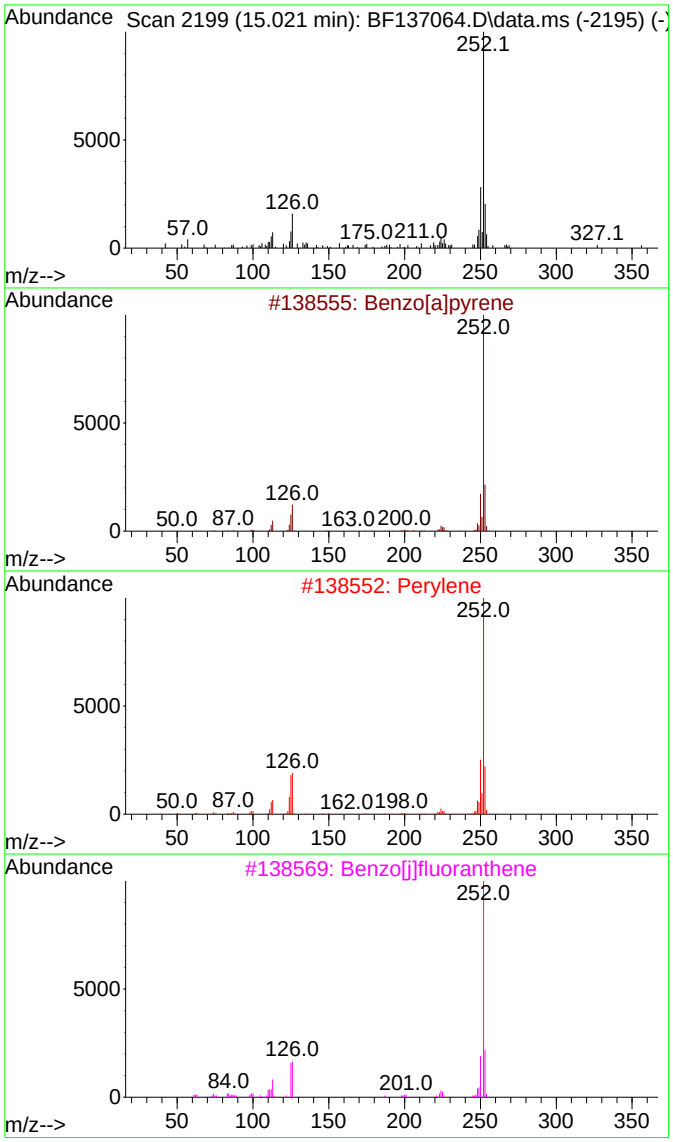
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

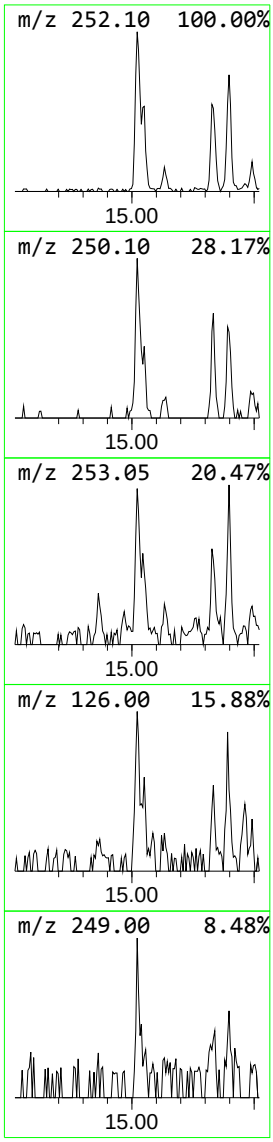
****

Peak Number 7 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	3.01 ng	64512	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	93
2	Perylene	252	C20H12	000198-55-0	90
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81





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Data File : BF137064.D
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Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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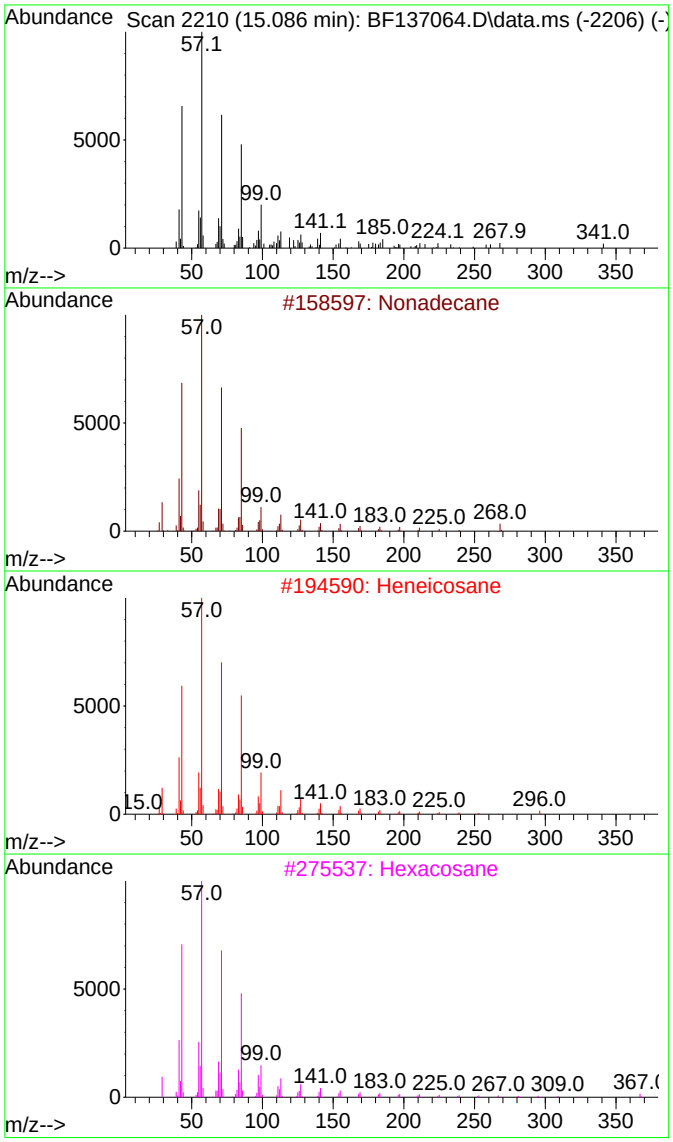
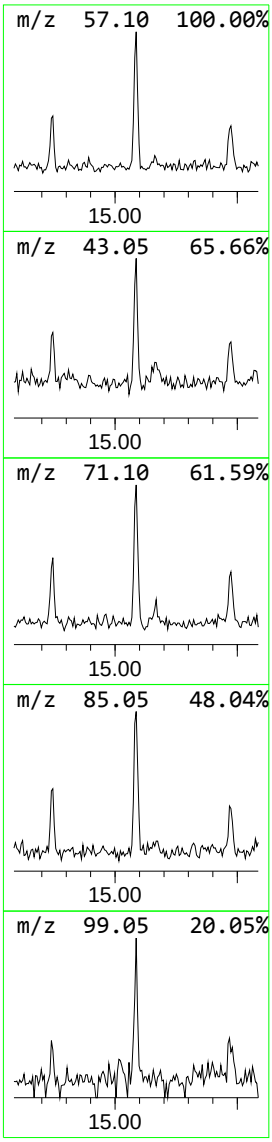
Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.05 ng	65327	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	92
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	81
4	Tetracosane	338	C24H50	000646-31-1	81
5	Octacosane	394	C28H58	000630-02-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

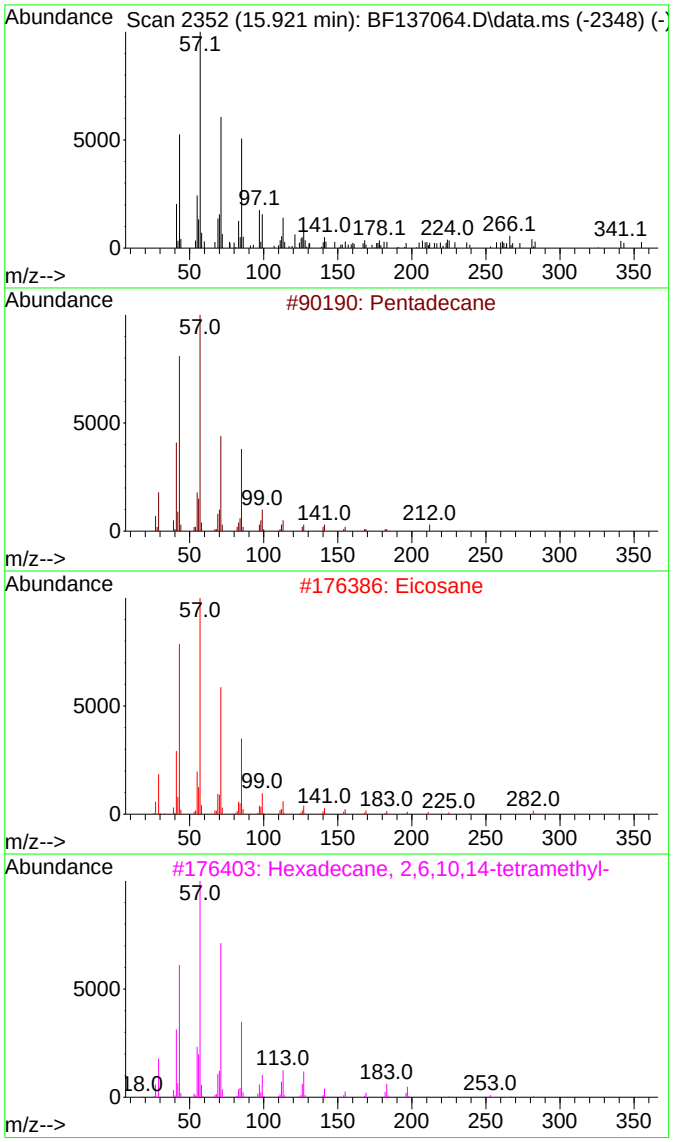
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

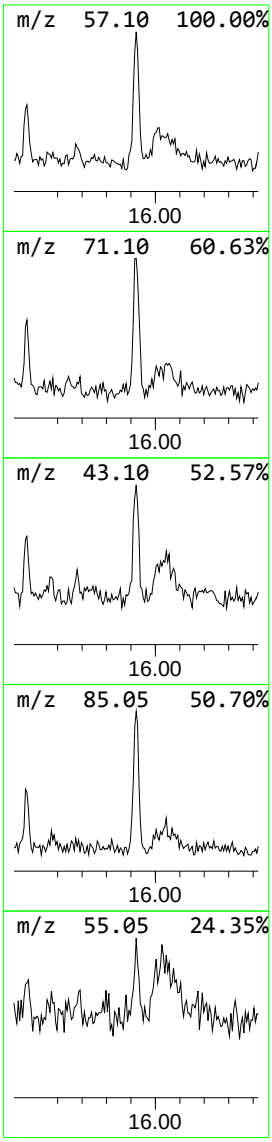
****

Peak Number 9 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.52 ng	53844	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
4	Octacosane	394	C28H58	000630-02-4	83
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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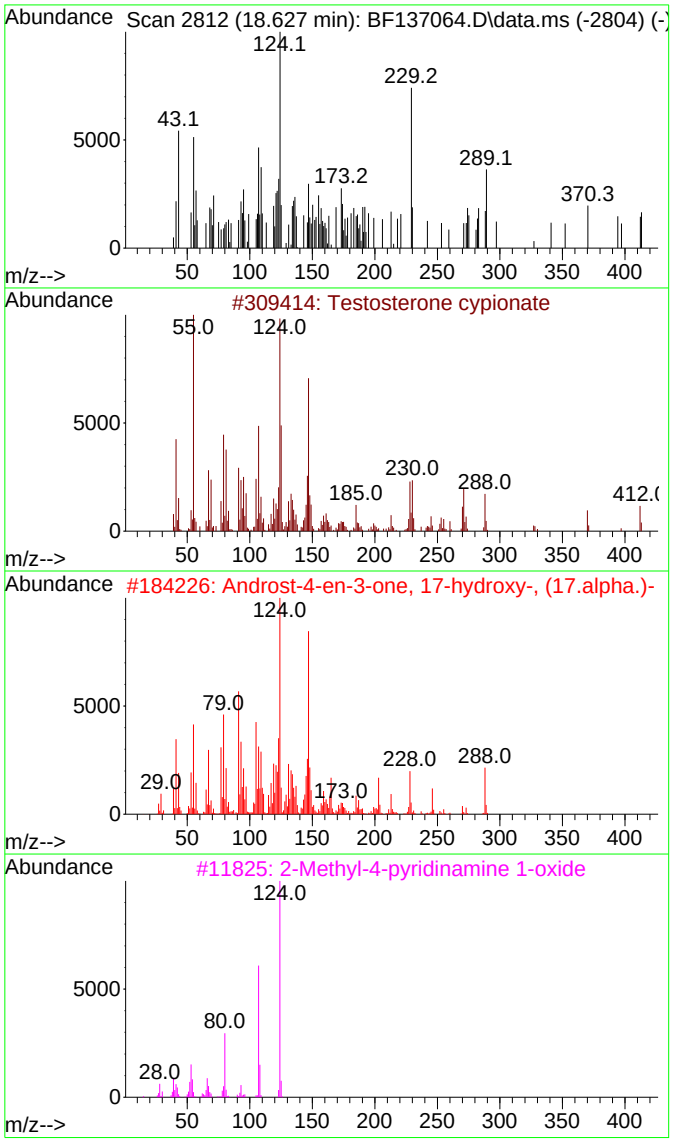
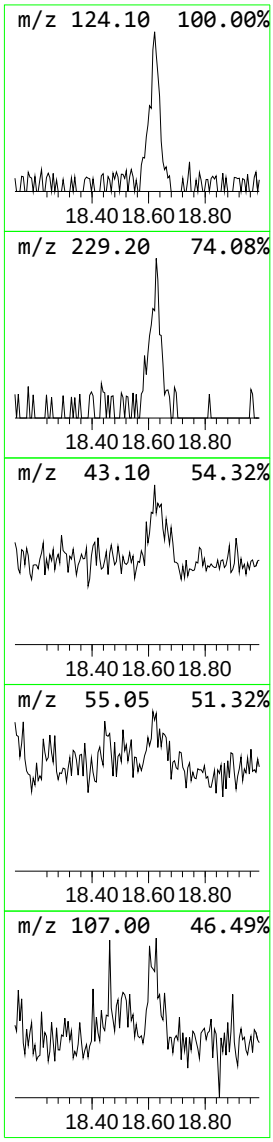
Peak Number 10 unknown18.627 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.627	4.46 ng	95396	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Testosterone cypionate	412	C27H40O3	000058-20-8	43
2	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	42
3	2-Methyl-4-pyridinamine 1-oxide	124	C6H8N2O	014045-17-1	27
4	Cholest-5-en-3-one, 4,4-dimethyl-	412	C29H48O	002220-42-0	22
5	Testosterone	288	C19H28O2	000058-22-0	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137064.D
Acq On : 15 Jan 2024 15:41
Operator : CG\JU
Sample : P1132-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	6.9	ng	86083	1	6.787	250921	20.0
n-Hexadecanoic ...	11.845	9.8	ng	162320	4	11.310	330187	20.0
2-Phenanthrenol...	13.339	9.9	ng	209271	5	13.968	421810	20.0
unknown13.380	13.380	4.2	ng	88345	5	13.968	421810	20.0
Trifluoroacetic...	13.827	5.2	ng	109646	5	13.968	421810	20.0
Perylene	15.021	3.0	ng	64512	6	15.462	428032	20.0
Nonadecane	15.086	3.0	ng	65327	6	15.462	428032	20.0
Pentadecane	15.921	2.5	ng	53844	6	15.462	428032	20.0
unknown18.627	18.627	4.5	ng	95396	6	15.462	428032	20.0