LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GHL-SS-44

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: BF136831.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.869	298	303	312	rVB	4977	8756	1.18%	0.123%
2	5.010	494	497	501	rBV	11050	10869	1.47%	0.152%
3	5.422	564	567	577	rBV	563506	508551	68.82%	7.131%
4	6.228	700	704	712	rBV3	8351	11663	1.58%	0.164%
5	6.422	734	737	750	rBV	686959	640660	86.70%	8.984%
6	6.781	794	798	802	rBV	493334	380709	51.52%	5.339%
7	7.339	889	893	901	rBV	368717	301128	40.75%	4.223%
8	8.057	1011	1015	1018	rBV	625325	493823	66.83%	6.925%
9	9.133	1194	1198	1201	rBV	727954	564148	76.34%	7.911%
10	9.816	1310	1314	1326	rBV	667453	567682	76.82%	7.961%
11	10.604	1445	1448	1464	rBV	596952	561320	75.96%	7.871%
12	11.304	1563	1567	1571	rBV	644007	577633	78.17%	8.100%
13	11.839	1655	1658	1674	rBV3	41060	84291	11.41%	1.182%
14	12.092	1698	1701	1704	rVB	38462	30101	4.07%	0.422%
15	12.639	1791	1794	1803	rBV7	5470	12952	1.75%	0.182%
16	12.898	1834	1838	1842	rBV	856976	738958	100.00%	10.362%
17	13.127	1873	1877	1881	rBV3	23453	29543	4.00%	0.414%
18	13.251	1895	1898	1905	rBV3	7930	9347	1.26%	0.131%
19	13.480	1933	1937	1939	rBV5	10115	11846	1.60%	0.166%
20	13.710	1973	1976	1980	rBV4	7599	8245	1.12%	0.116%
21	13.810	1990	1993	1996	rBV	52075	43883	5.94%	0.615%
22	13.963	2007	2019	2029	rVB	405865	437696	59.23%	6.138%
23	14.057	2029	2035	2039	rVV3	14601	21211	2.87%	0.297%
24	14.127	2043	2047	2054	rVB2	16397	19397	2.62%	0.272%
25	14.274	2068	2072	2078	rVB	51923	47946	6.49%	0.672%
26	14.410	2092	2095	2097	rBV	29929	31411	4.25%	0.440%
27	14.433	2097	2099	2103	rVB	79962	69188	9.36%	0.970%
28	14.492	2106	2109	2113	rBV	100548	93051	12.59%	1.305%
29	14.592	2124	2126	2129	rVB4	11335	9142	1.24%	0.128%
30	14.745	2148	2152	2155	rVB3	18752	21616	2.93%	0.303%
31	14.815	2160	2164	2170	rVB4	22512	28131	3.81%	0.394%
32	15.086	2206	2210	2216	rVB	51316	59662	8.07%	0.837%
33	15.239	2233	2236	2240	rBV4	11592	18180	2.46%	0.255%
34	15.445	2266	2271	2280	rVB	247467	354335	47.95%	4.969%
35	15.686	2308	2312	2316	rVB5	10986	16869	2.28%	0.237%
36	15.745	2319	2322	2328	rVB8	10724	18984	2.57%	0.266%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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	15.921	2347	2352	2359	rVB2	32474	55366	7.49%	0.776%
38	16.051	2370	2374	2383	rVB9	9745	22825	3.09%	0.320%
39	16.180	2391	2396	2400	rBV8	7862	16010	2.17%	0.225%
40	16.356	2421	2426	2428	rBV6	7067	11929	1.61%	0.167%
41	16.745	2489	2492	2498	rVB7	9417	14693	1.99%	0.206%
42	17.062	2542	2546	2550	rBV6	8215	14790	2.00%	0.207%
43	17.251	2574	2578	2582	rVB7	7837	14777	2.00%	0.207%
44	17.386	2595	2601	2608	rBV3	50521	104045	14.08%	1.459%
45	18.115	2719	2725	2731	rVB9	11879	25143	3.40%	0.353%
46	18.598	2803	2807	2808	rBV4	6741	8700	1.18%	0.122%

Sum of corrected areas: 7131205

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
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Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
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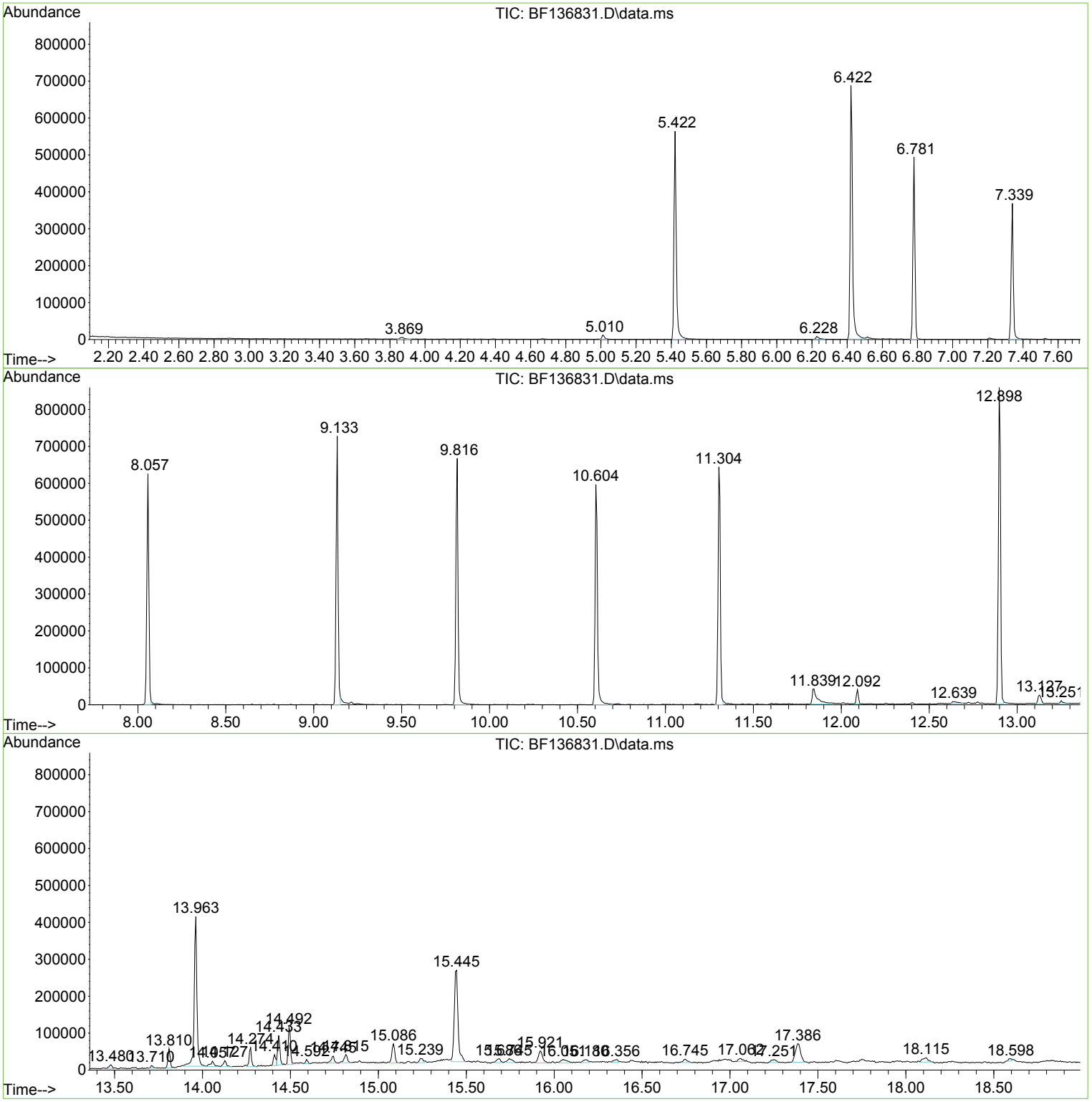
Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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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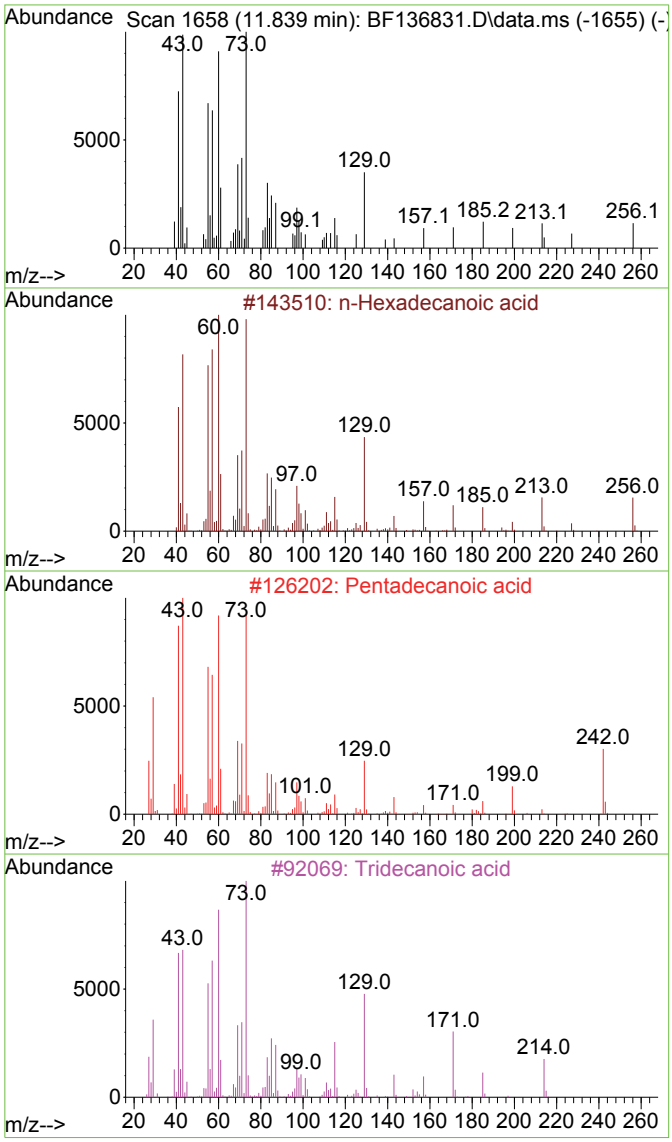
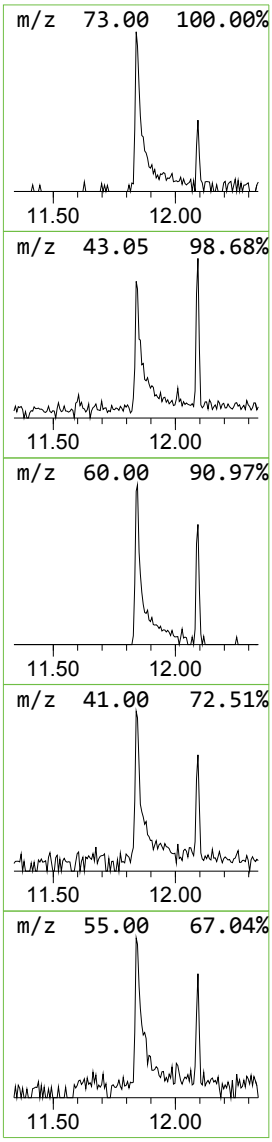
Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.92 ng	84291	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
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Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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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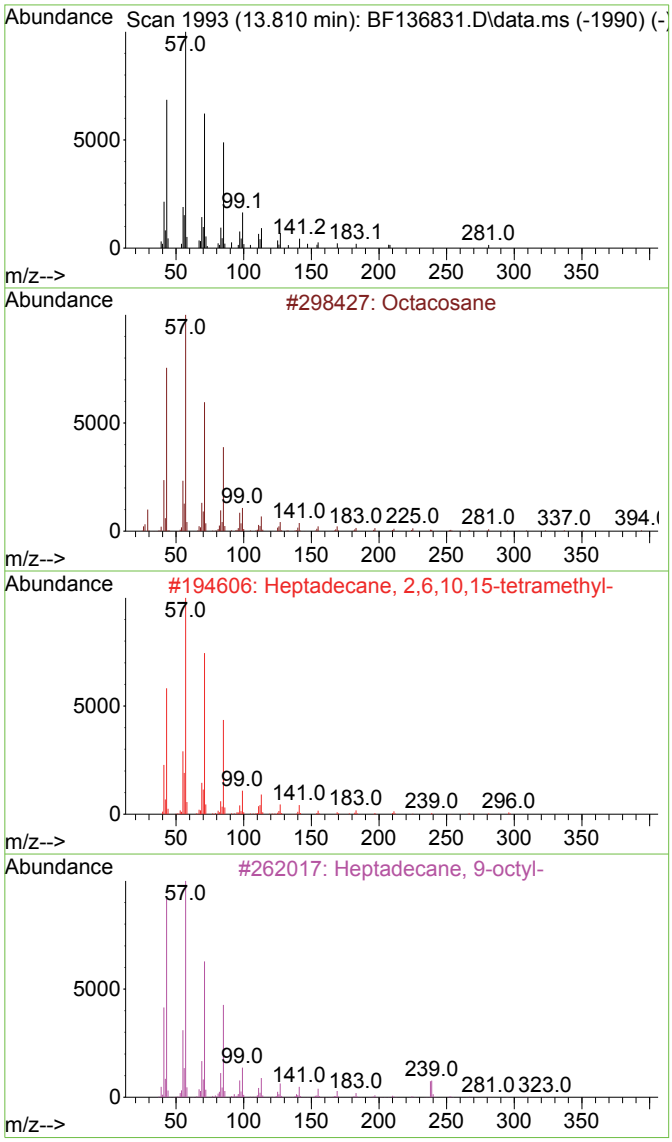
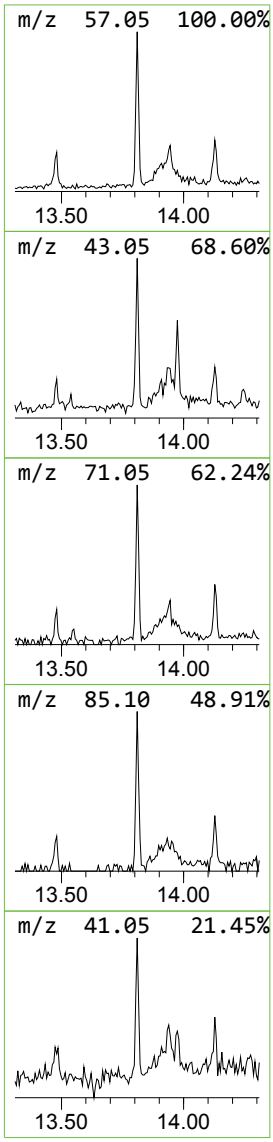
Peak Number 2 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	2.01 ng	43883	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Octadecane	254	C18H38	000593-45-3	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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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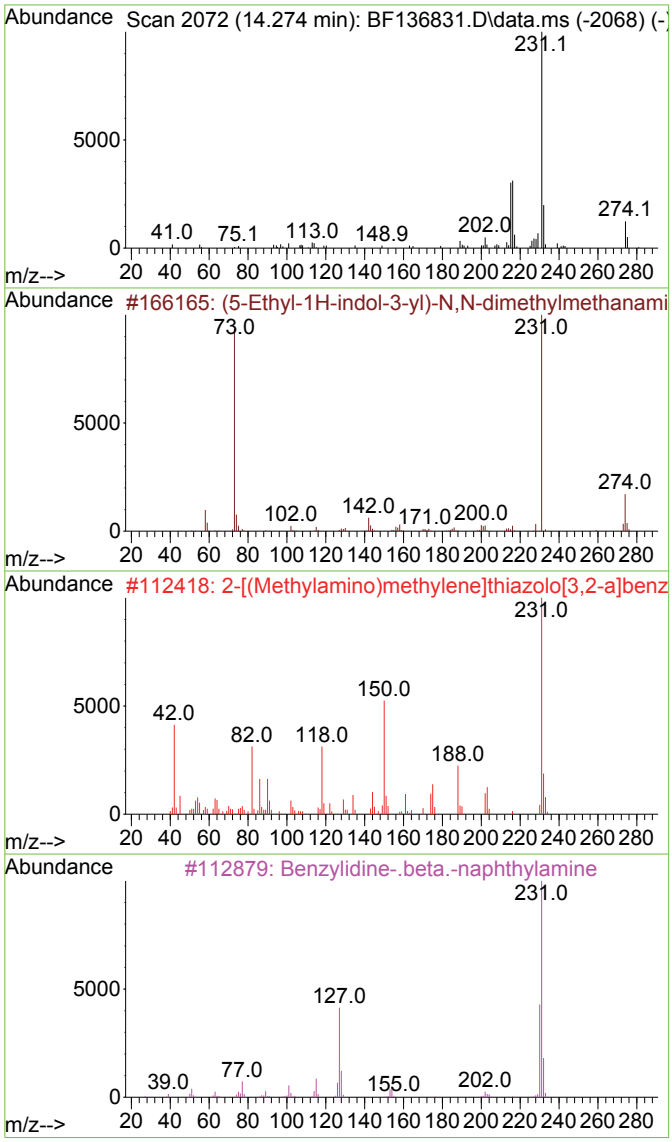
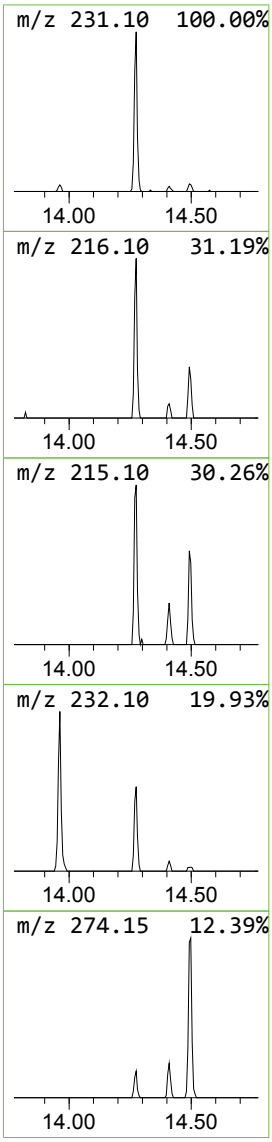
Peak Number 3 unknown14.274 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	2.19 ng	47946	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(5-Ethyl-1H-indol-3-yl)-N,N-dime...	274	C16H26N2Si	074367-52-5	47
2	2-[(Methylamino)methylene]thiazo...	231	C11H9N3OS	072740-41-1	47
3	Benzylidine-.beta.-naphthylamine	231	C17H13N	000891-32-7	47
4	Ethyl 1,2-dihydro-1-methyl-2-oxo...	231	C13H13NO3	027330-23-0	47
5	10H-Phenothiazine, 5,5-dioxide	231	C12H9NO2S	001209-66-1	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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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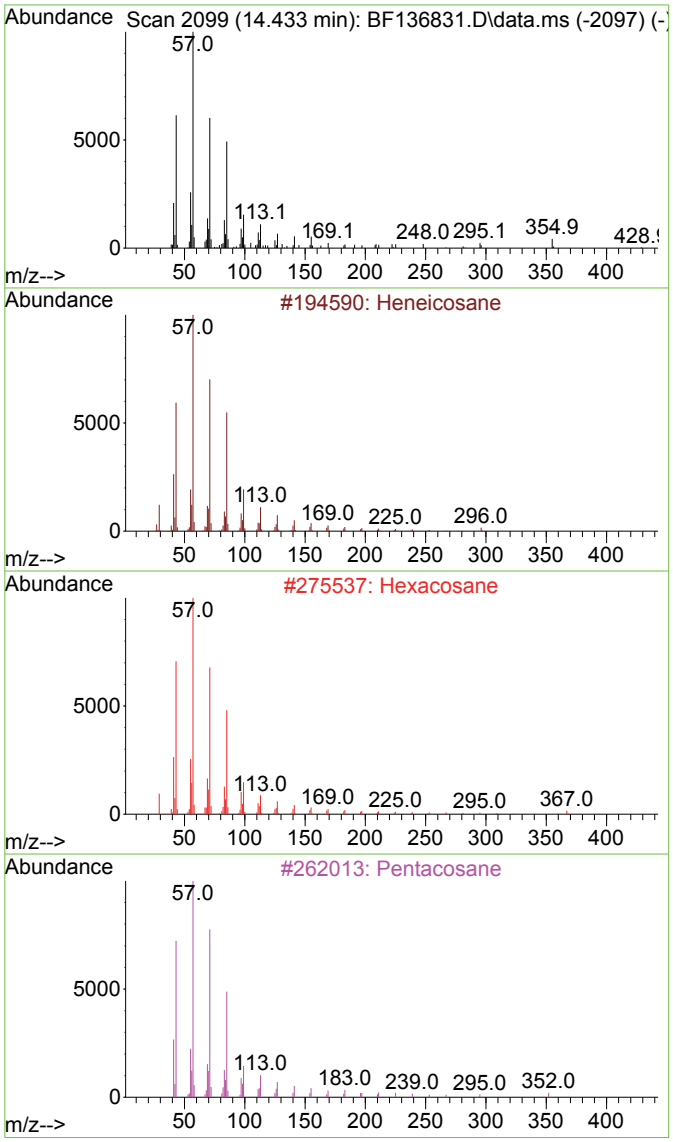
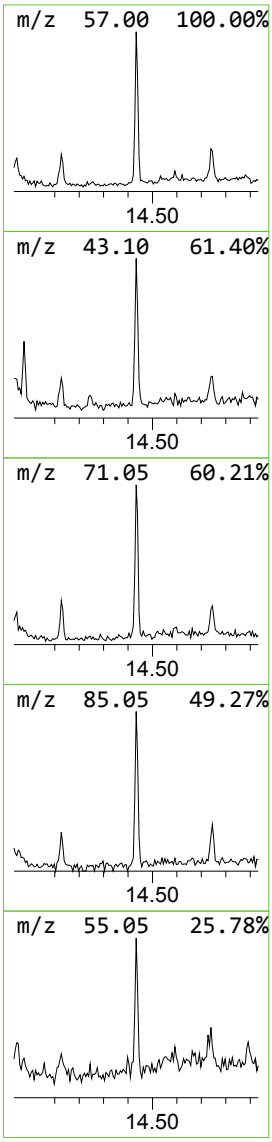
Peak Number 4 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	3.16 ng	69188	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Hexacosane	366	C26H54	000630-01-3	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Tetracosane	338	C24H50	000646-31-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

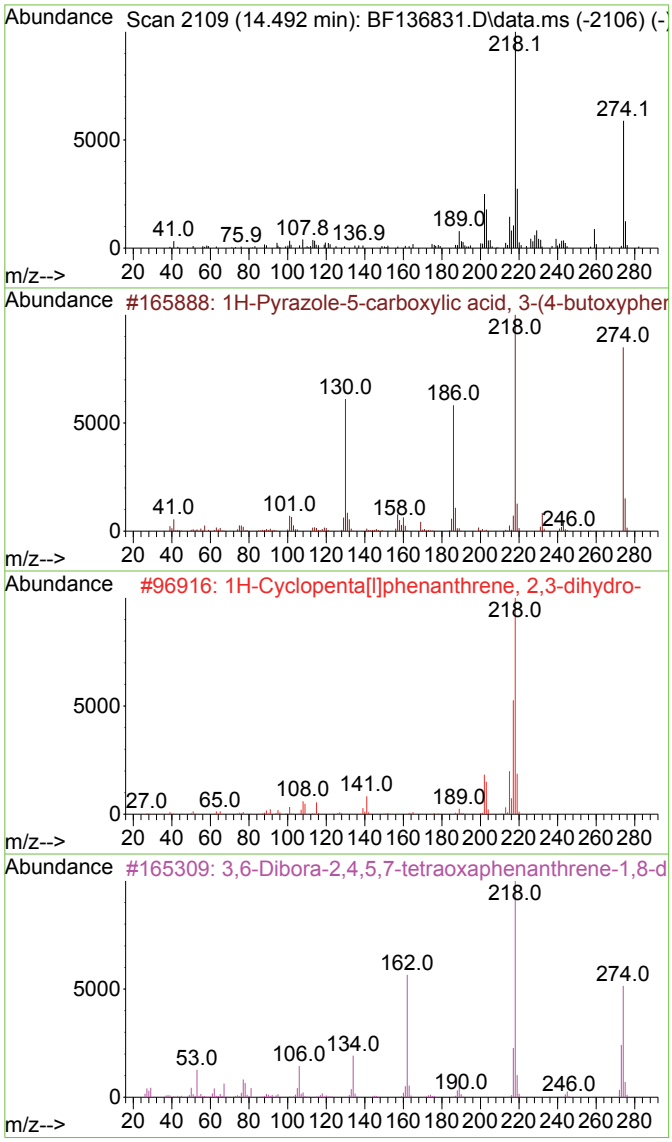
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

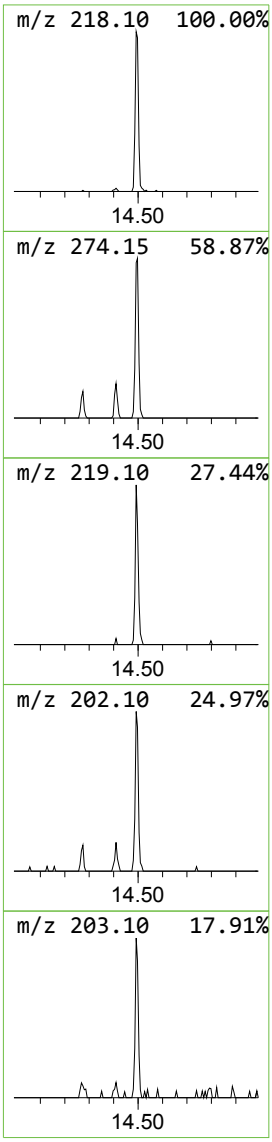
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Pyrazole-5-carboxylic ac... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	4.25 ng	93051	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-5-carboxylic acid, 3...	274	C15H18N2O3	1000319-72-5	58
2	1H-Cyclopenta[l]phenanthrene, 2,...	218	C17H14	000723-98-8	52
3	3,6-Dibora-2,4,5,7-tetraoxaphena...	274	C12H12B2O6	1000159-66-2	50
4	1,4-Methanonaphthalene, 1,4-dihy...	218	C17H14	055028-73-4	46
5	Naphthalene, 2-(phenylmethyl)-	218	C17H14	000613-59-2	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
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Acq On : 29 Dec 2023 16:11
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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

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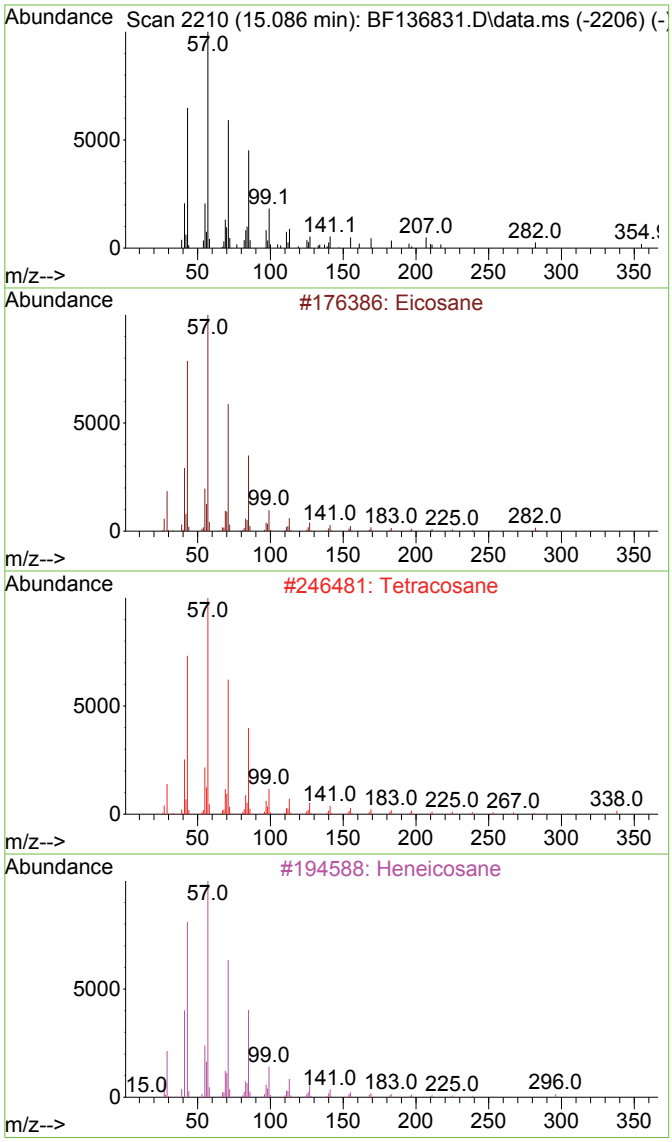
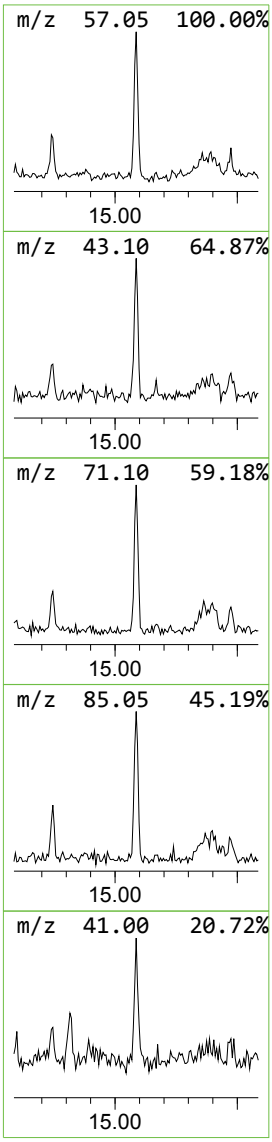
Peak Number 6 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.37 ng	59662	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetracosane	338	C24H50	000646-31-1	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetratetracontane	619	C44H90	007098-22-8	86
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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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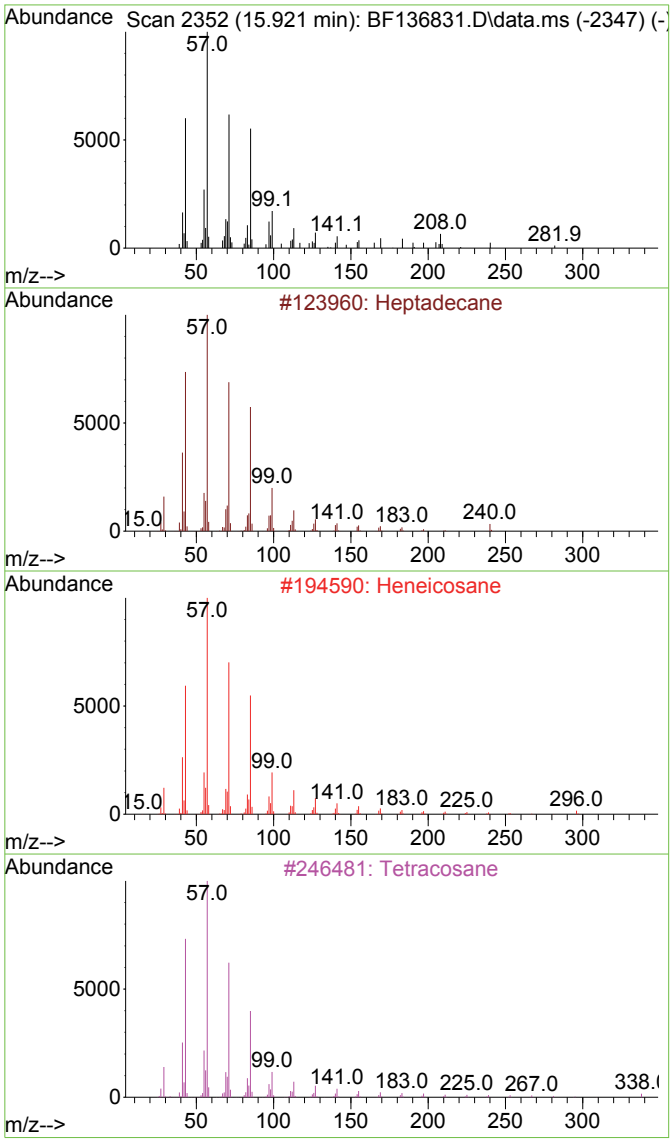
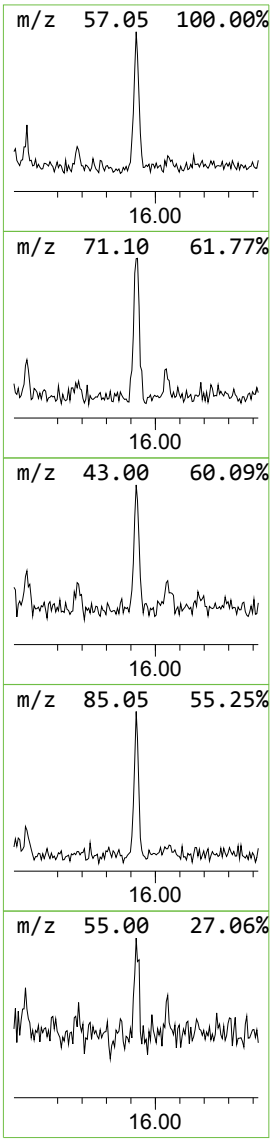
Peak Number 7 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.13 ng	55366	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetracosane	338	C24H50	000646-31-1	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Octacosane	394	C28H58	000630-02-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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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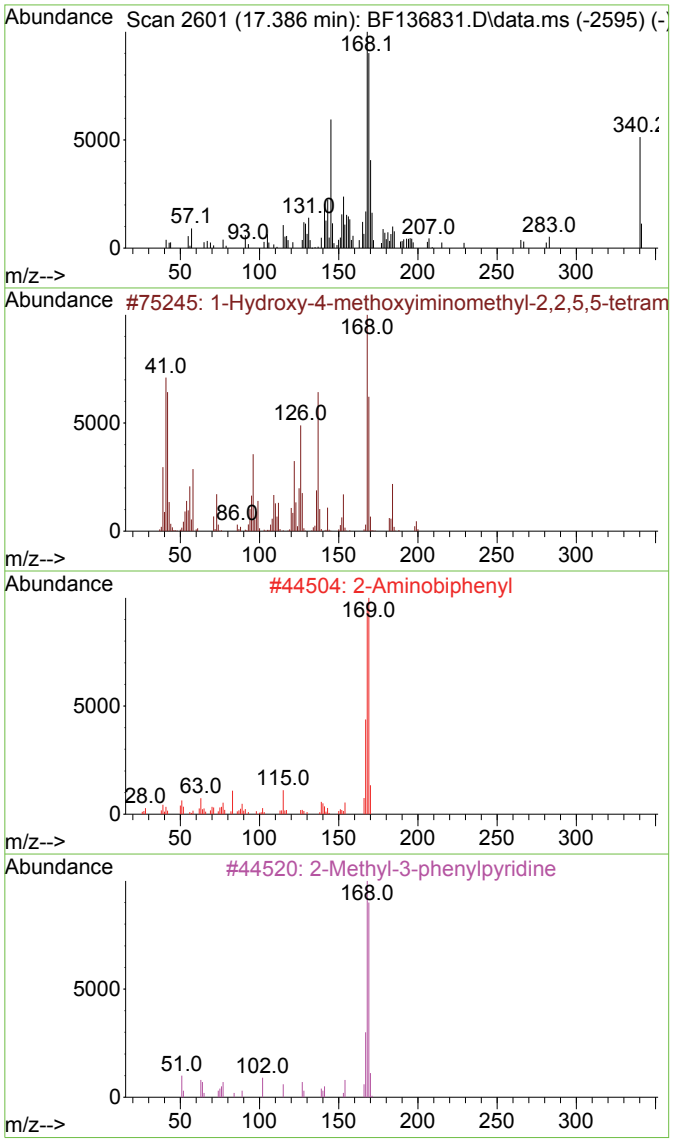
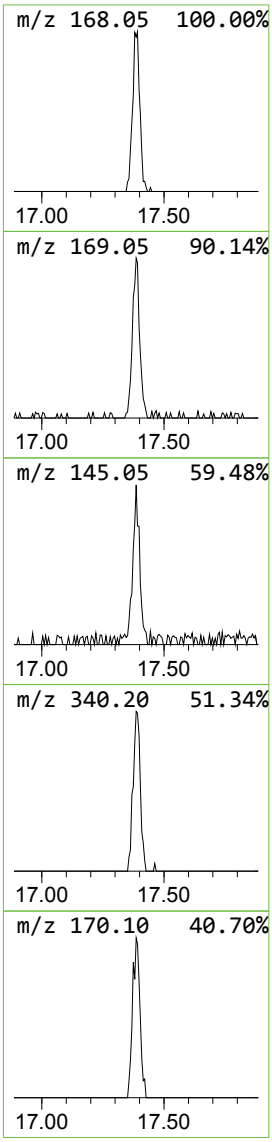
Peak Number 8 unknown17.386 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.386	5.87 ng	104045	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hydroxy-4-methoxyiminomethyl-2...	199	C9H17N3O2	344411-55-8	47
2	2-Aminobiphenyl	169	C12H11N	000090-41-5	38
3	2-Methyl-3-phenylpyridine	169	C12H11N	003256-89-1	38
4	N-(2-Naphthylmethylene)-methylamine	169	C12H11N	1000433-45-5	38
5	Pyridine, 3-(phenylmethyl)-	169	C12H11N	000620-95-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136831.D
Acq On : 29 Dec 2023 16:11
Operator : CG\JU
Sample : 05909-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-44

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
n-Hexadecanoic ...	11.839	2.9	ng	84291	4	11.304	577633	20.0
Octacosane	13.810	2.0	ng	43883	5	13.963	437696	20.0
unknown14.274	14.274	2.2	ng	47946	5	13.963	437696	20.0
Heneicosane	14.433	3.2	ng	69188	5	13.963	437696	20.0
1H-Pyrazole-5-c...	14.492	4.3	ng	93051	5	13.963	437696	20.0
Eicosane	15.086	3.4	ng	59662	6	15.445	354335	20.0
Heptadecane	15.921	3.1	ng	55366	6	15.445	354335	20.0
unknown17.386	17.386	5.9	ng	104045	6	15.445	354335	20.0