LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021025\
Data File : BF141536.D
Acq On : 10 Feb 2025 15:57
Operator : RC/JU
Sample : Q1322-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MANHOLE

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-BF020625.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.758	107	113	124	rBV	19648	37881	1.32%	0.283%
2	3.799	284	290	298	rBV	20945	35456	1.23%	0.265%
3	5.404	558	563	582	rBV	382135	545513	18.94%	4.080%
4	6.422	729	736	746	rBV	241969	364076	12.64%	2.723%
5	6.787	793	798	803	rBV	358780	446968	15.52%	3.343%
6	7.351	887	894	904	rBV	953382	1302388	45.22%	9.742%
7	8.069	1011	1016	1033	rVB	456606	592676	20.58%	4.433%
8	9.145	1193	1199	1209	rBV	1847061	2354377	81.74%	17.611%
9	9.822	1309	1314	1328	rVB	541027	683351	23.73%	5.111%
10	10.034	1345	1350	1355	rBV2	19827	31617	1.10%	0.236%
11	10.533	1430	1435	1443	rBV	269277	339944	11.80%	2.543%
12	10.610	1443	1448	1465	rVV	886489	1150160	39.93%	8.603%
13	10.845	1482	1488	1498	rVB	18471	29799	1.03%	0.223%
14	11.310	1562	1567	1574	rBV	513434	669491	23.24%	5.008%
15	11.486	1592	1597	1605	rBV	83863	114687	3.98%	0.858%
16	11.839	1652	1657	1670	rBV2	194665	313562	10.89%	2.345%
17	12.545	1770	1777	1787	rBV	113215	224574	7.80%	1.680%
18	12.627	1787	1791	1803	rVB	51287	96518	3.35%	0.722%
19	12.898	1831	1837	1842	rBV	2215920	2880227	100.00%	21.544%
20	13.822	1986	1994	2006	rBV4	20752	73992	2.57%	0.553%
21	13.951	2010	2016	2022	rBV	418250	540873	18.78%	4.046%
22	15.416	2259	2265	2274	rVB	241714	393701	13.67%	2.945%
23	16.310	2411	2417	2441	rVB	29306	147255	5.11%	1.101%

Sum of corrected areas: 13369086

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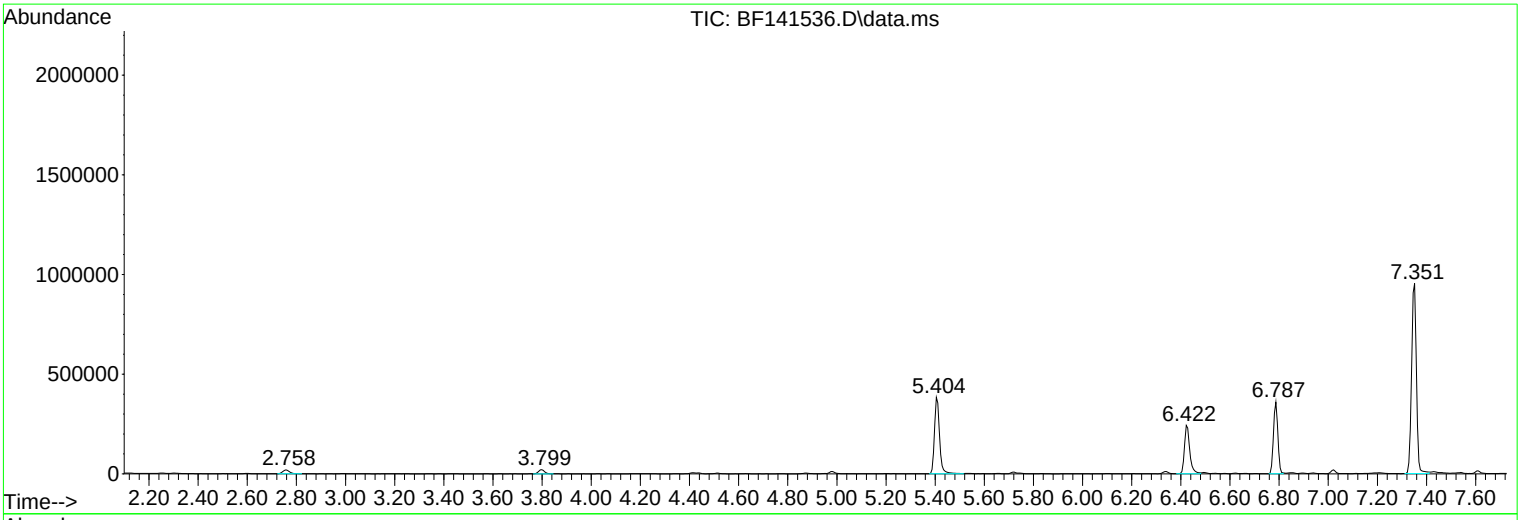
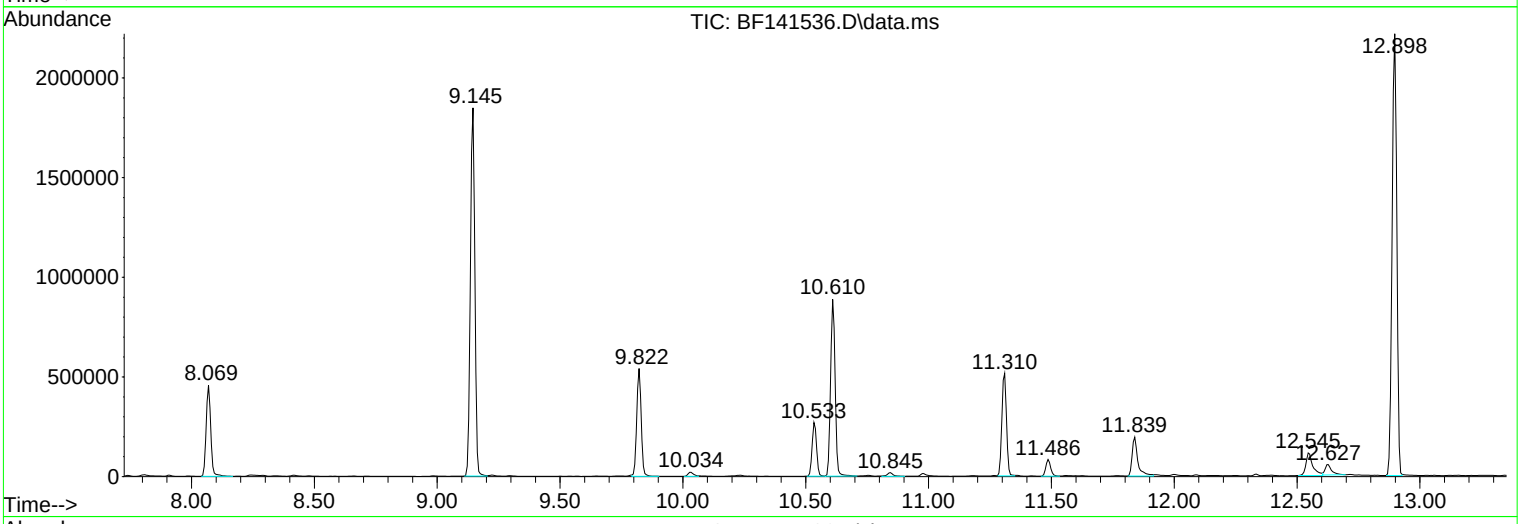
Sample : Q1322-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

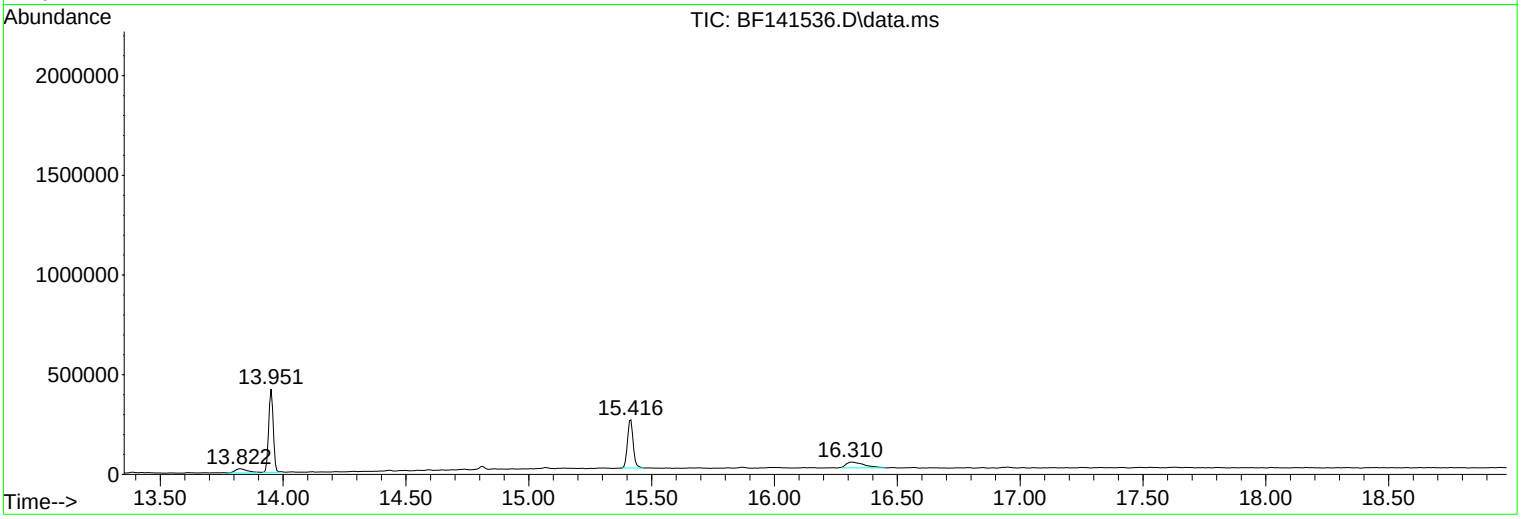
Instrument :
BNA_F
ClientSampleId :
MANHOLE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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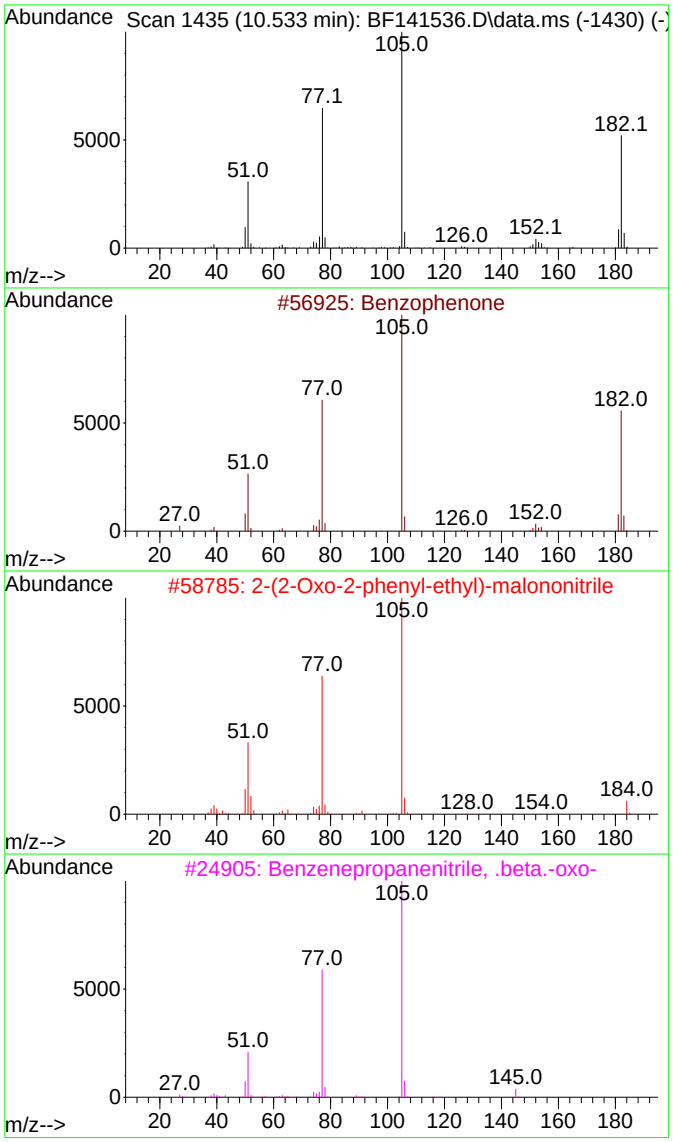
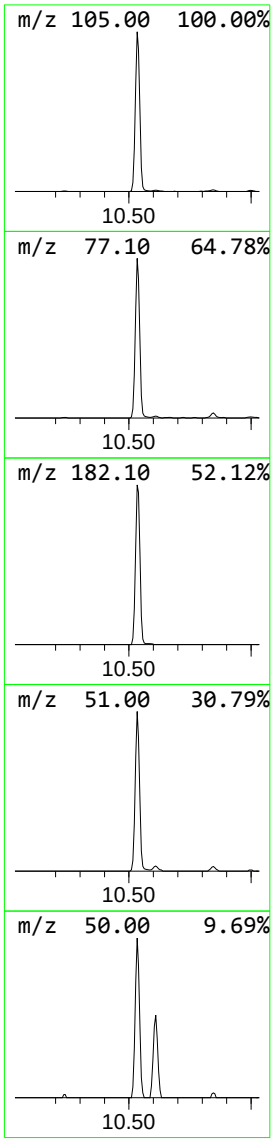
Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.534	9.95 ng	339944	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
4	Vinyl benzoate	148	C9H8O2	000769-78-8	50
5	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50





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Data File : BF141536.D
Acq On : 10 Feb 2025 15:57
Operator : RC/JU
Sample : Q1322-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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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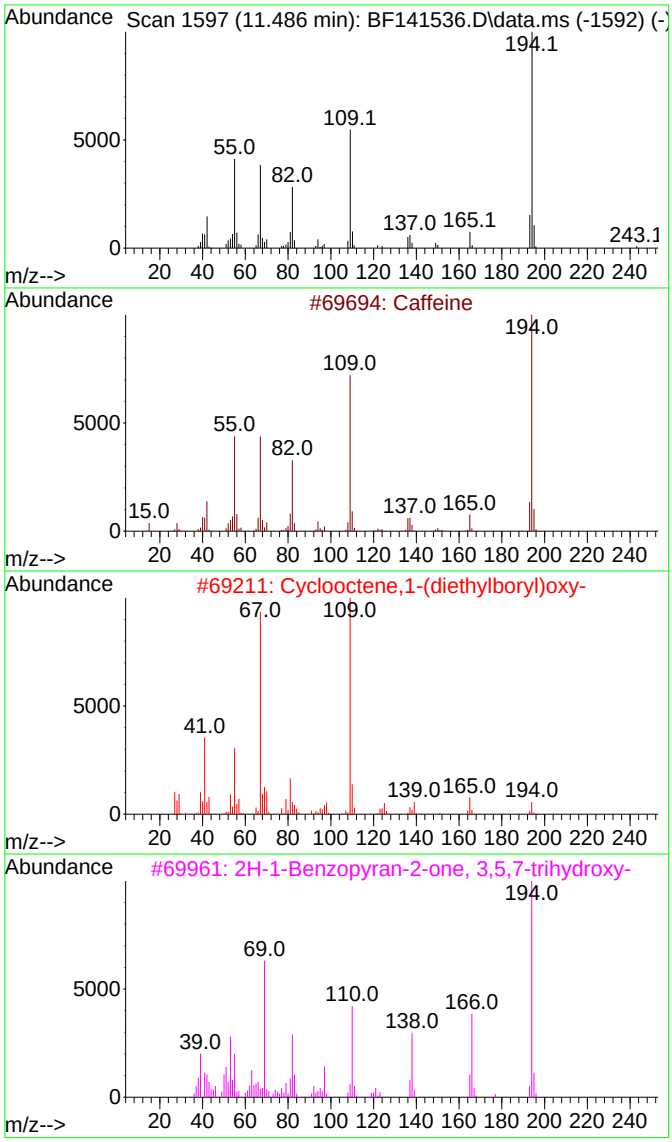
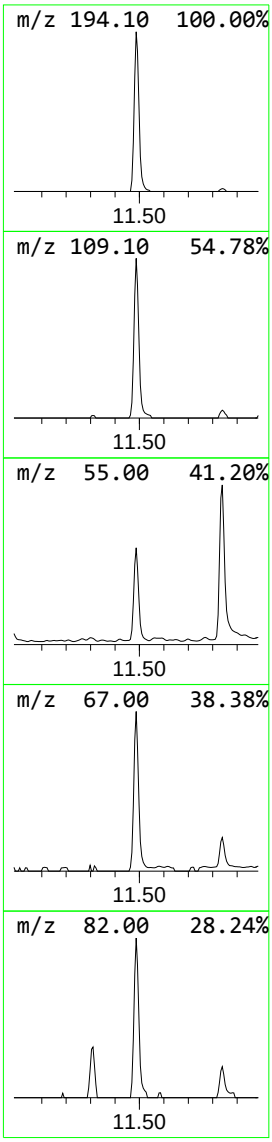
Peak Number 2 Caffeine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.486	3.43 ng	114687	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	98
2	Cyclooctene,1-(diethylboryl)oxy-	194	C12H23BO	057387-71-0	47
3	2H-1-Benzopyran-2-one, 3,5,7-tri...	194	C9H6O5	022065-07-2	43
4	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	43
5	2H-Pyrazol-3-ol, 5-(2,5-dimethyl...	194	C9H10N2OS	1000304-22-5	38





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Data File : BF141536.D
Acq On : 10 Feb 2025 15:57
Operator : RC/JU
Sample : Q1322-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MANHOLE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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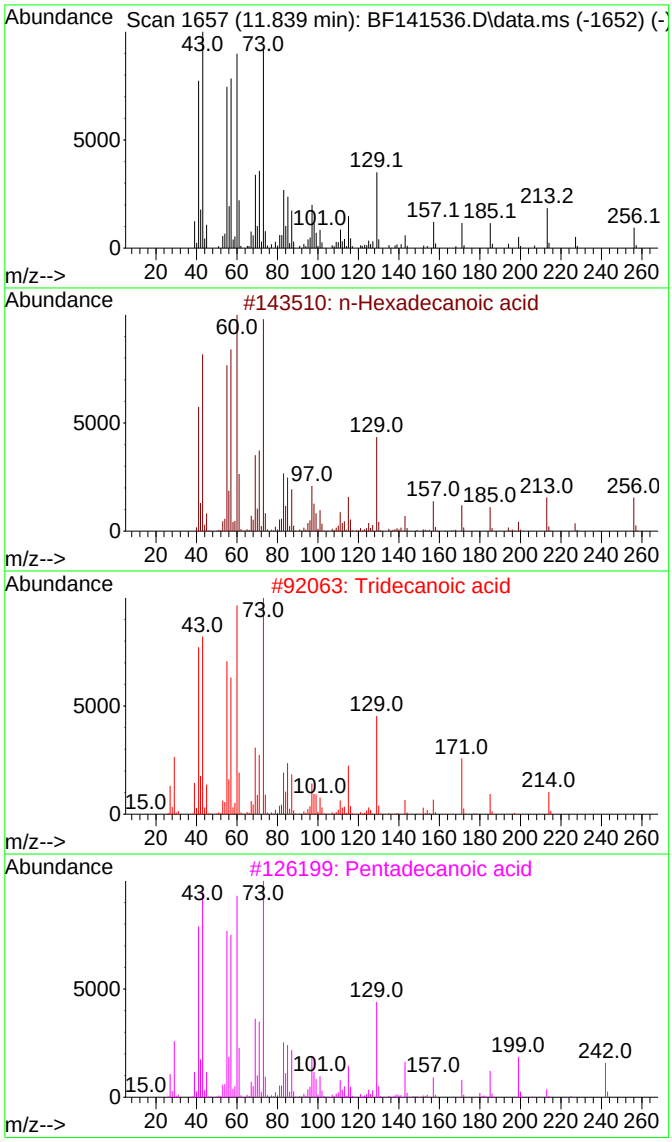
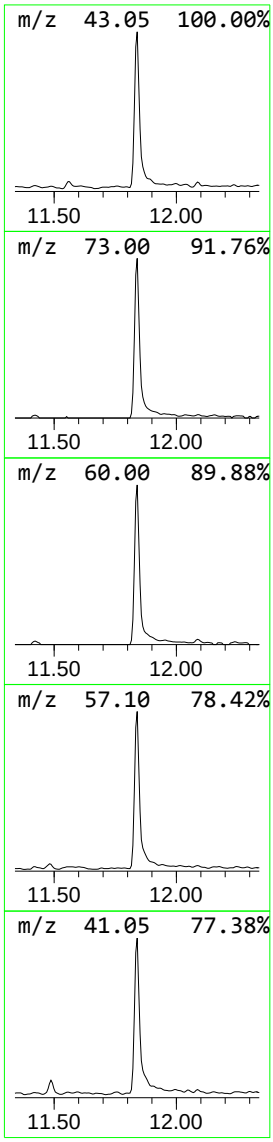
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	9.37 ng	313562	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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Data File : BF141536.D
Acq On : 10 Feb 2025 15:57
Operator : RC/JU
Sample : Q1322-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MANHOLE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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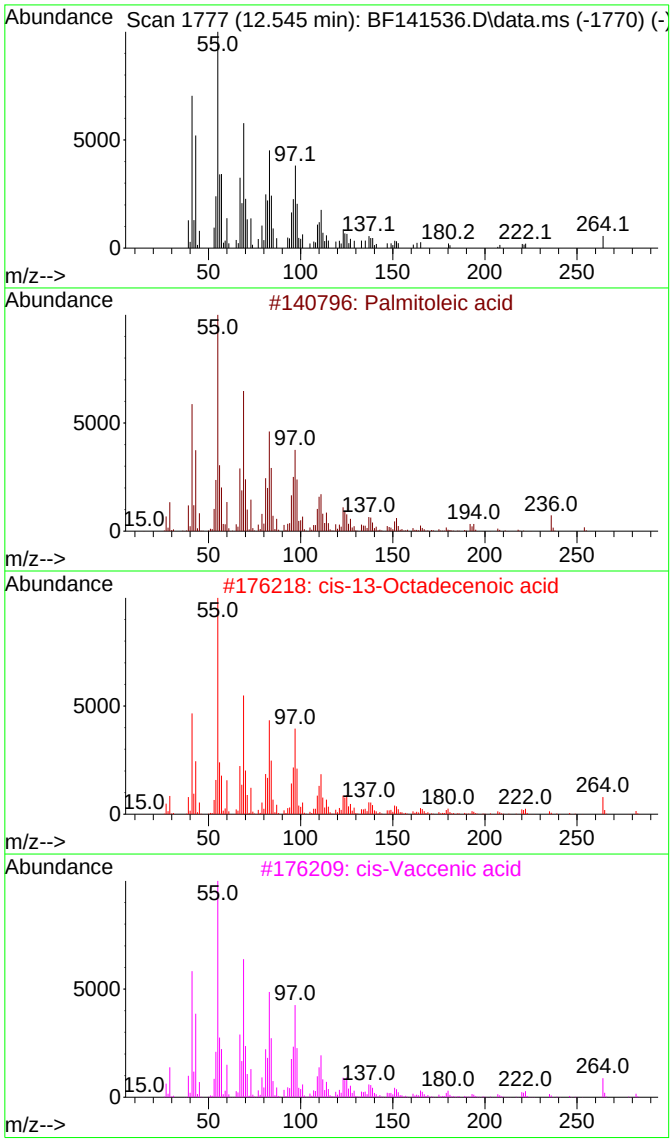
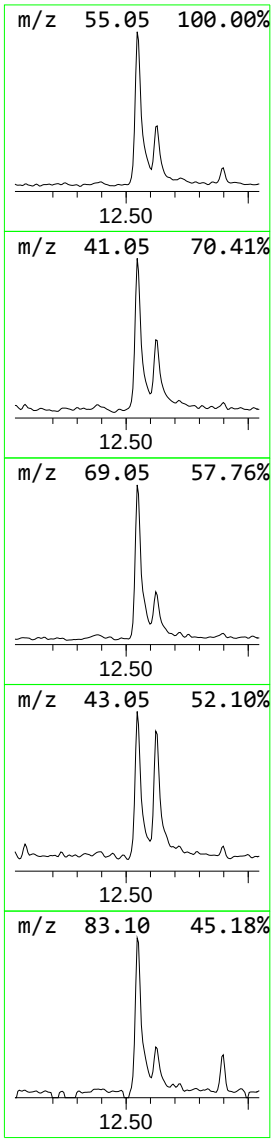
Peak Number 4 Palmitoleic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	6.71 ng	224574	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	91
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
5	Oleic Acid	282	C18H34O2	000112-80-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021025\
Data File : BF141536.D
Acq On : 10 Feb 2025 15:57
Operator : RC/JU
Sample : Q1322-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MANHOLE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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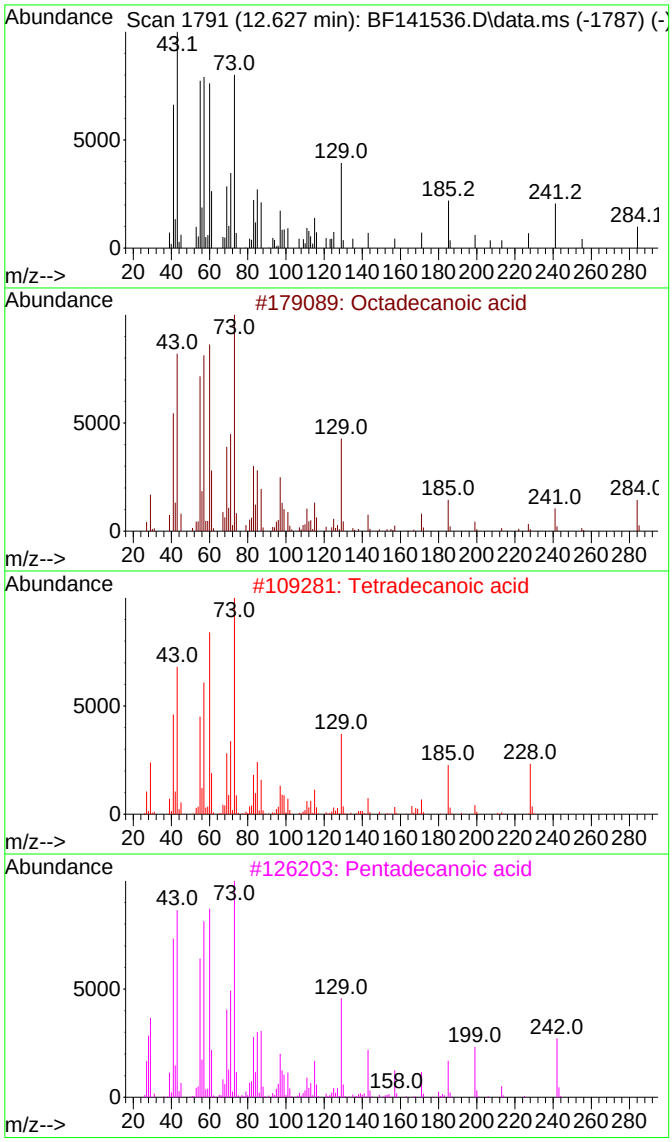
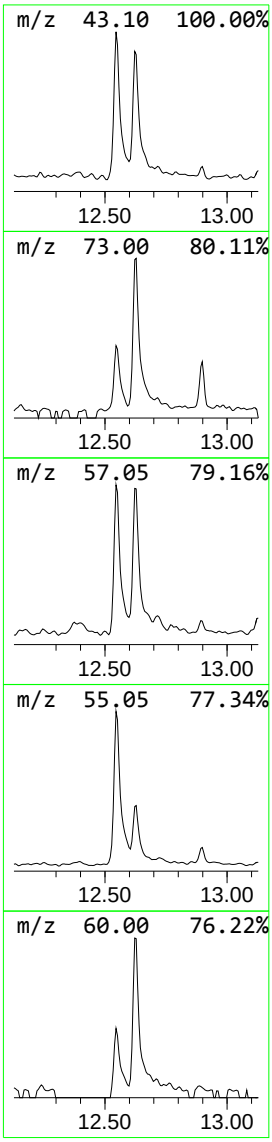
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.628	2.88 ng	96518	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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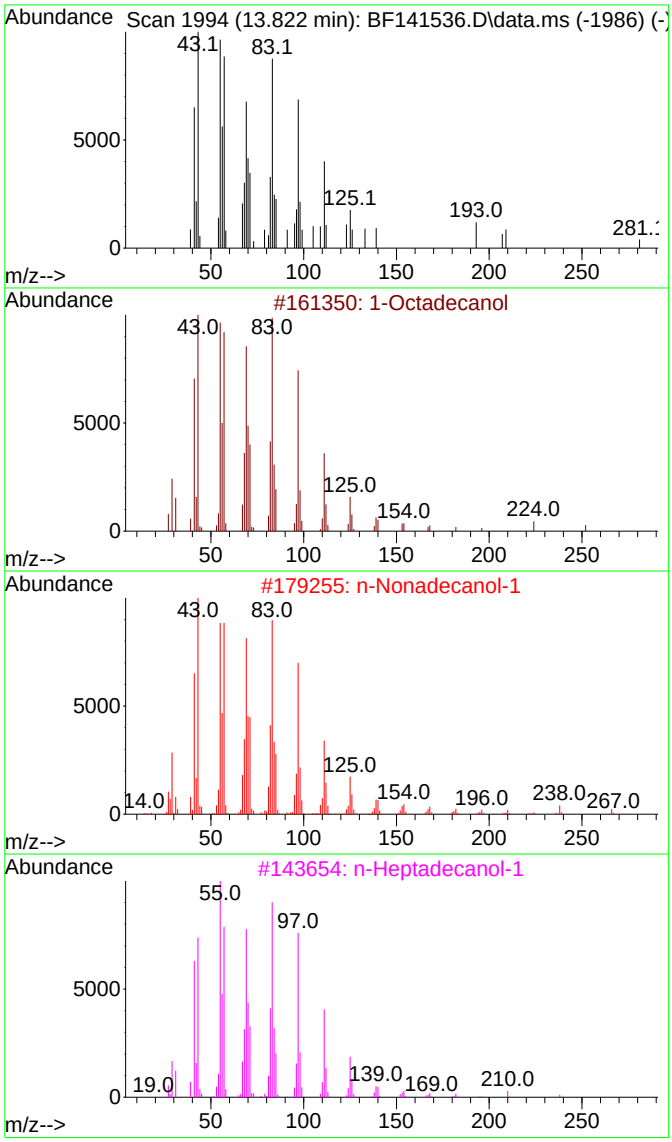
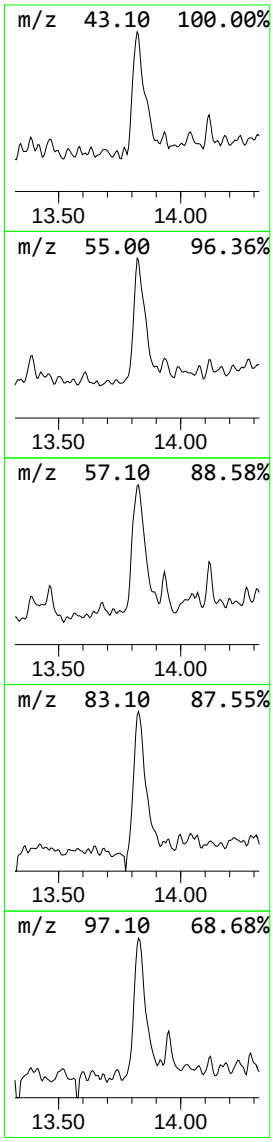
Peak Number 6 1-Octadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	2.74 ng	73992	Chrysene-d12	13.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	93
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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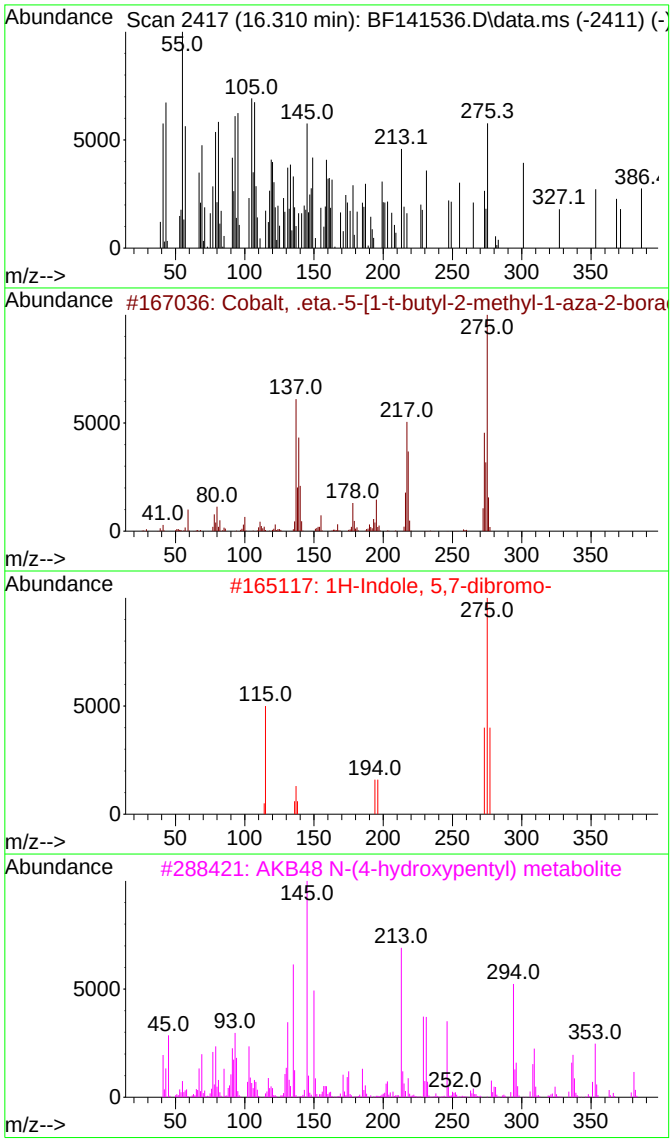
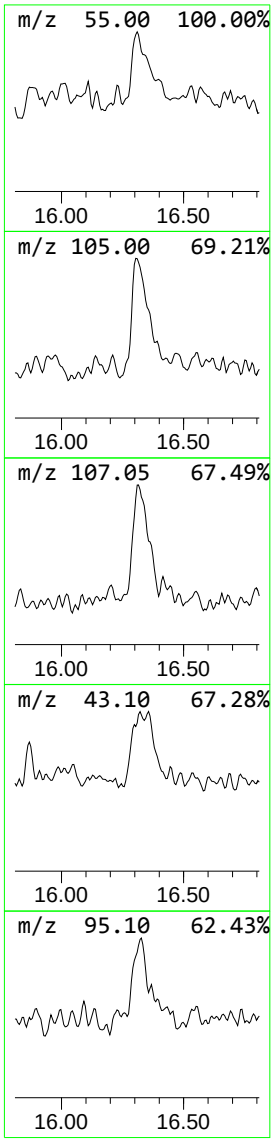
Peak Number 7 unknown16.310 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	7.48 ng	147255	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cobalt, .eta.-5-[1-t-butyl-2-met...	275	C14H23BCoN	1000161-32-7	10
2	1H-Indole, 5,7-dibromo-	273	C8H5Br2N	036132-08-8	9
3	AKB48 N-(4-hydroxypentyl) metabo...	381	C23H31N3O2	1843184-41-7	9
4	17.beta.-Hydroxy-4-propyl-3,4-se...	362	C23H38O3	059251-38-6	9
5	Cholest-5-ene, 3-(1-oxobuthoxy)-	456	C31H52O2	137036-79-4	9





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzophenone	10.534	9.9	ng	339944	3	9.822	683351	20.0
Caffeine	11.486	3.4	ng	114687	4	11.310	669491	20.0
n-Hexadecanoic ...	11.839	9.4	ng	313562	4	11.310	669491	20.0
Palmitoleic acid	12.545	6.7	ng	224574	4	11.310	669491	20.0
Octadecanoic acid	12.628	2.9	ng	96518	4	11.310	669491	20.0
1-Octadecanol	13.822	2.7	ng	73992	5	13.951	540873	20.0
unknown16.310	16.310	7.5	ng	147255	6	15.416	393701	20.0