LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130541.D
Acq On : 05 Oct 2022 21:16
Operator : CG\JU
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 257248-6

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130541.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.798	458	461	473	rBV	131412	156931	6.18%	1.029%
2	5.234	532	535	546	rBV	806537	822588	32.42%	5.392%
3	6.275	709	712	732	rVB	450265	464595	18.31%	3.046%
4	6.634	769	773	778	rBV	565692	500608	19.73%	3.282%
5	7.204	865	870	872	rBV	1426728	1386846	54.66%	9.091%
6	7.845	974	979	987	rBV4	50729	160036	6.31%	1.049%
7	7.916	987	991	999	rVB	553694	512517	20.20%	3.360%
8	8.551	1096	1099	1107	rBV	37749	48172	1.90%	0.316%
9	8.992	1170	1174	1177	rBV	3007432	2279658	89.84%	14.944%
10	9.628	1279	1282	1285	rBV	424739	446443	17.59%	2.927%
11	9.663	1285	1288	1296	rVB	562129	486904	19.19%	3.192%
12	10.451	1418	1422	1435	rBV	1333726	1196782	47.17%	7.845%
13	10.598	1444	1447	1459	rVB	671639	558218	22.00%	3.659%
14	10.716	1464	1467	1474	rBV	128001	133508	5.26%	0.875%
15	11.145	1536	1540	1546	rBV	503115	424813	16.74%	2.785%
16	11.474	1593	1596	1599	rBV	85162	71290	2.81%	0.467%
17	11.563	1605	1611	1629	rBV	381001	438897	17.30%	2.877%
18	11.692	1629	1633	1635	rBV	392924	371119	14.63%	2.433%
19	11.716	1635	1637	1640	rVB	697466	528180	20.82%	3.462%
20	12.333	1738	1742	1750	rBV2	231562	316395	12.47%	2.074%
21	12.468	1762	1765	1769	rBV	125392	138592	5.46%	0.909%
22	12.733	1805	1810	1813	rBV	3010117	2537422	100.00%	16.634%
23	13.098	1869	1872	1879	rVB	99563	84448	3.33%	0.554%
24	13.486	1930	1938	1939	rBV3	20054	40246	1.59%	0.264%
25	13.774	1983	1987	1995	rBV	576239	563178	22.19%	3.692%
26	14.345	2076	2084	2093	rBV9	19629	74968	2.95%	0.491%
27	15.162	2219	2223	2228	rBV	312691	375559	14.80%	2.462%
28	15.421	2263	2267	2273	rVB6	19881	31182	1.23%	0.204%
29	16.551	2456	2459	2465	rVB6	25704	46622	1.84%	0.306%
30	17.292	2580	2585	2594	rVB7	21715	57951	2.28%	0.380%

Sum of corrected areas: 15254668

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130541.D
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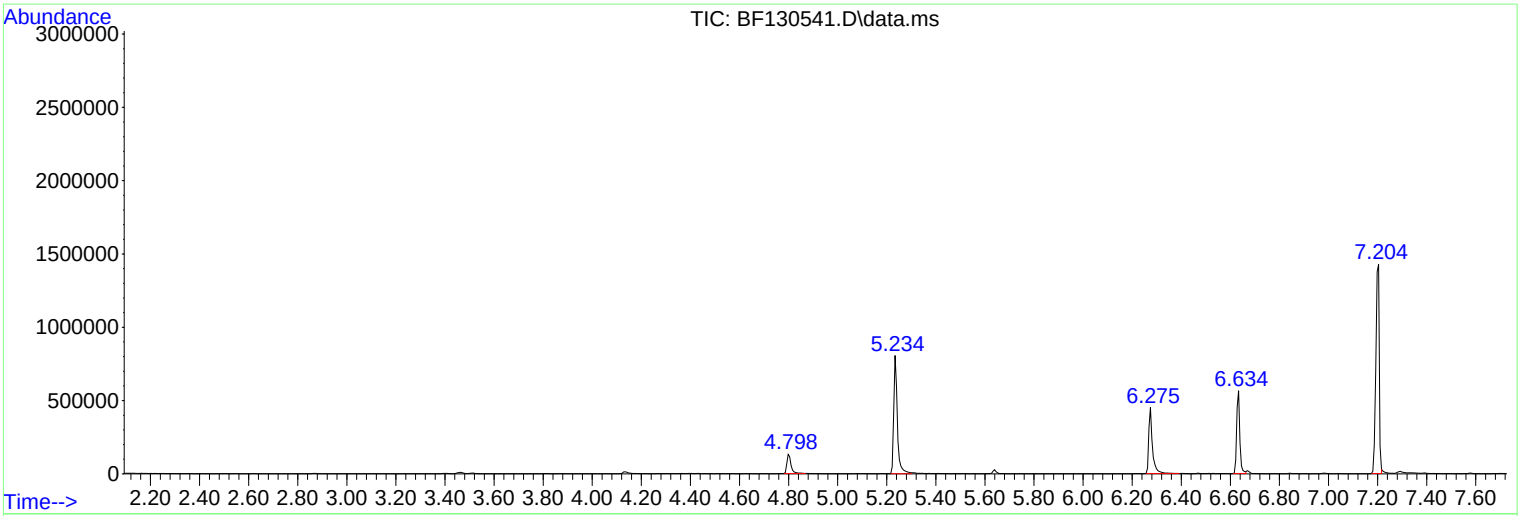
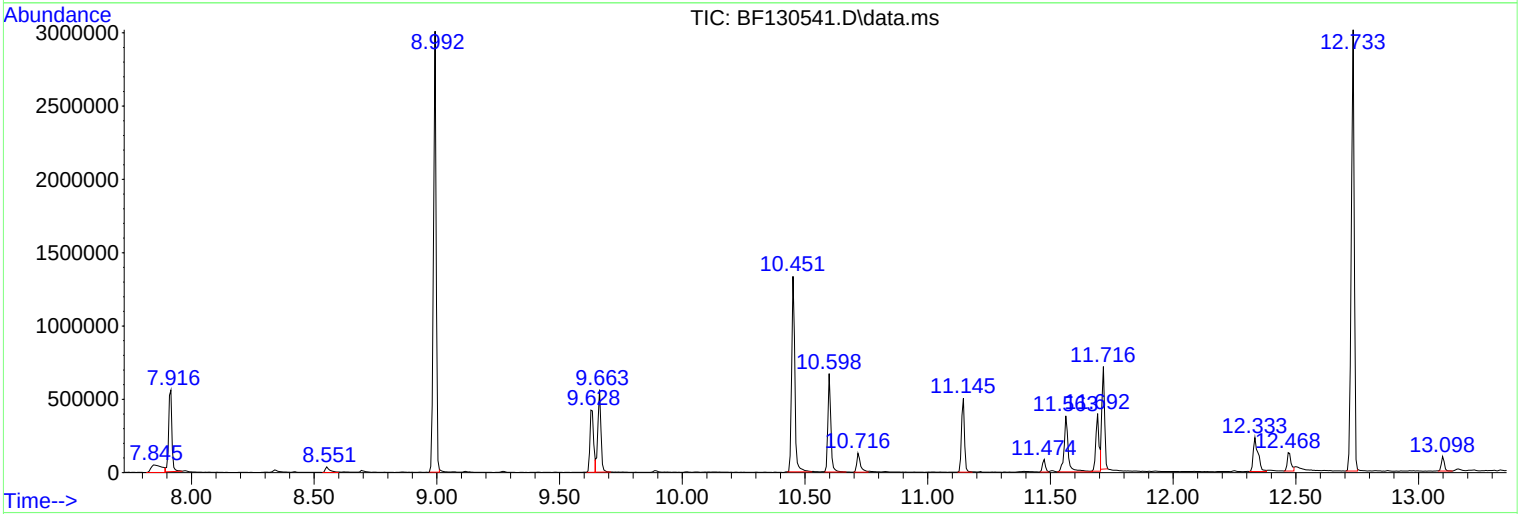
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

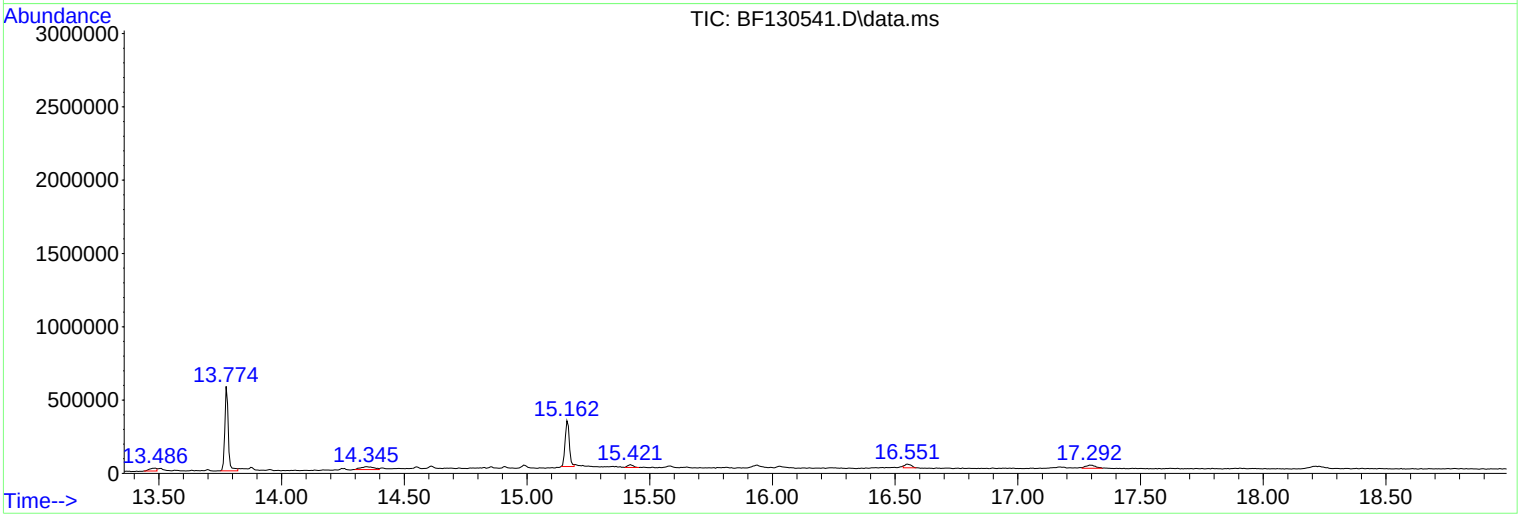
Instrument :
BNA_F
ClientSampleId :
257248-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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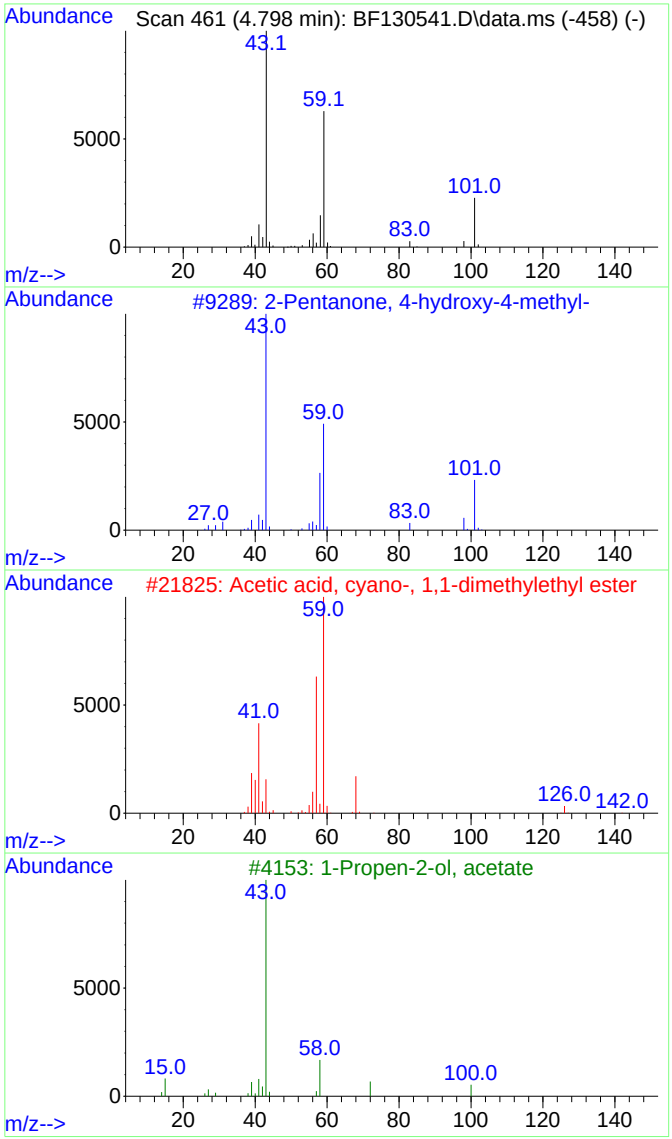
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

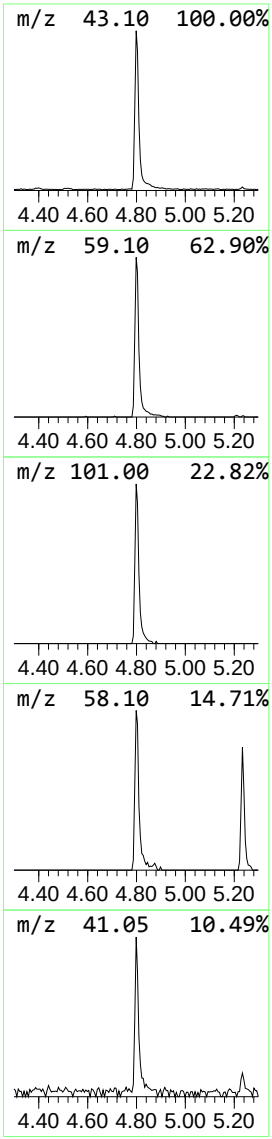
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.798	6.27 ng	156931	1,4-Dichlorobenzene-d4	6.634

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	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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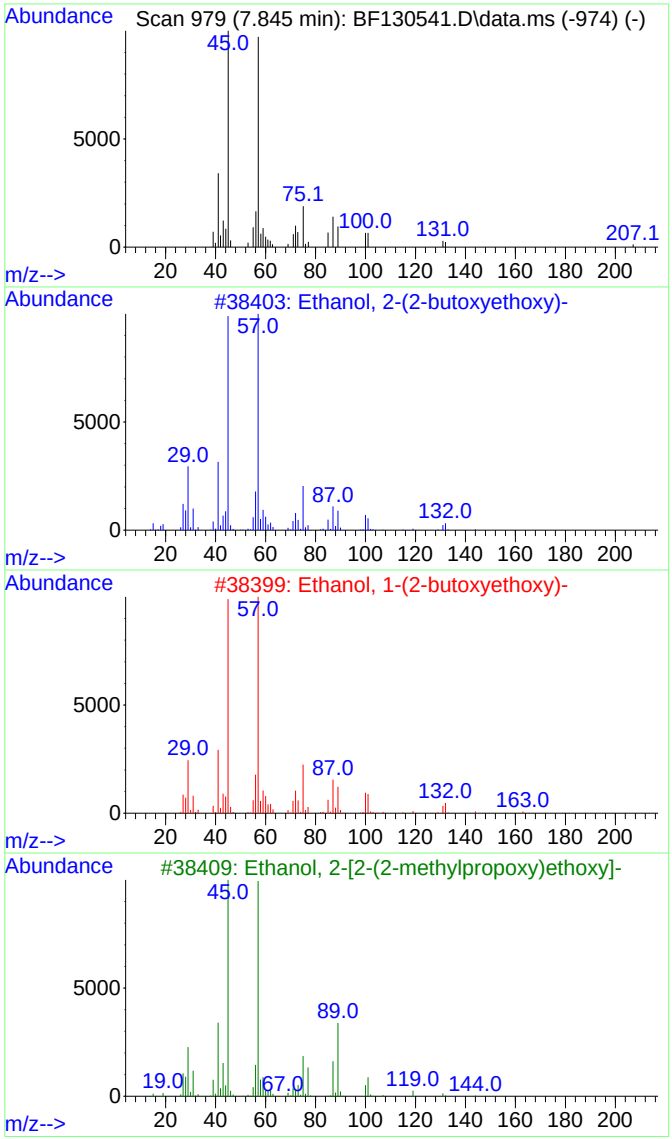
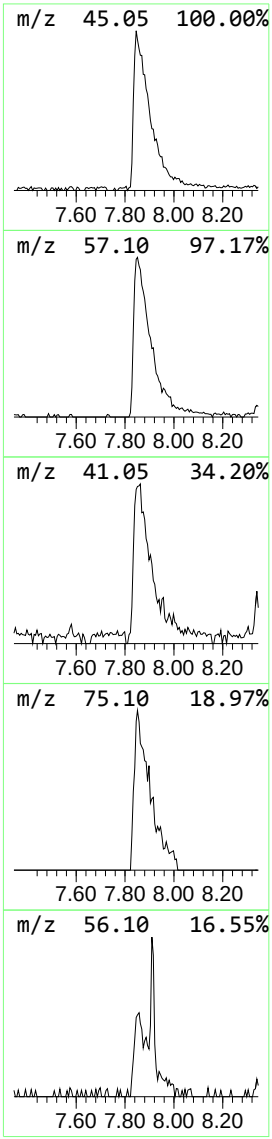
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.845	6.25 ng	160036	Naphthalene-d8	7.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	50





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Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
257248-6

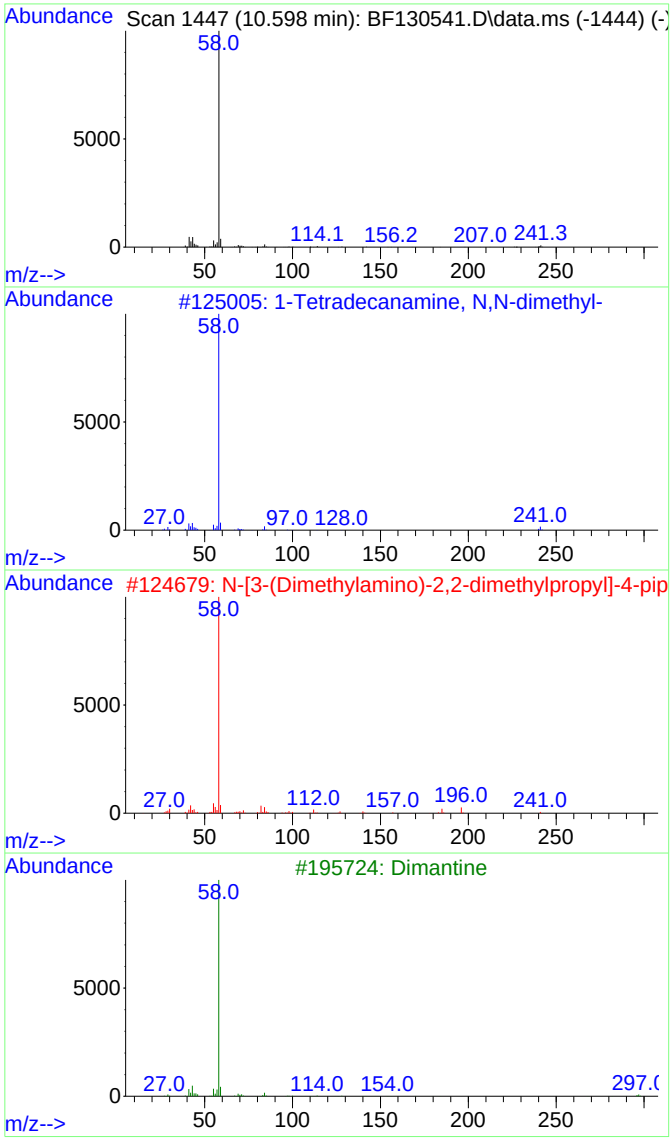
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

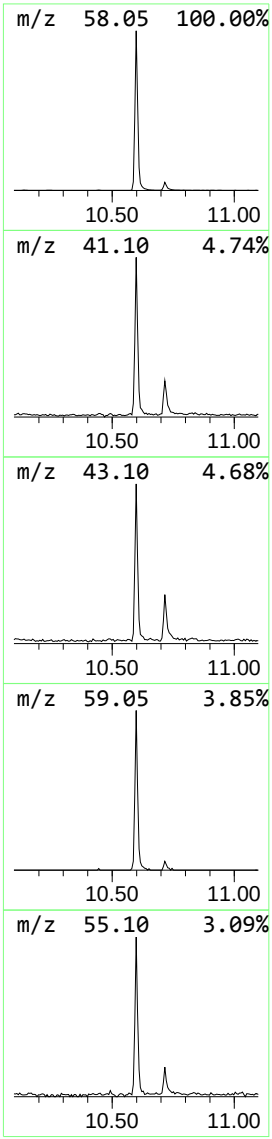
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Tetradecanamine, N,N-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	26.28 ng	558218	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	90
2	N-[3-(Dimethylamino)-2,2-dimethy...	241	C13H27N3O	728932-41-0	78
3	Dimantine	297	C20H43N	000124-28-7	78
4	Dimethyl palmitamine	269	C18H39N	000112-69-6	78
5	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	72





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Instrument :
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ClientSampleId :
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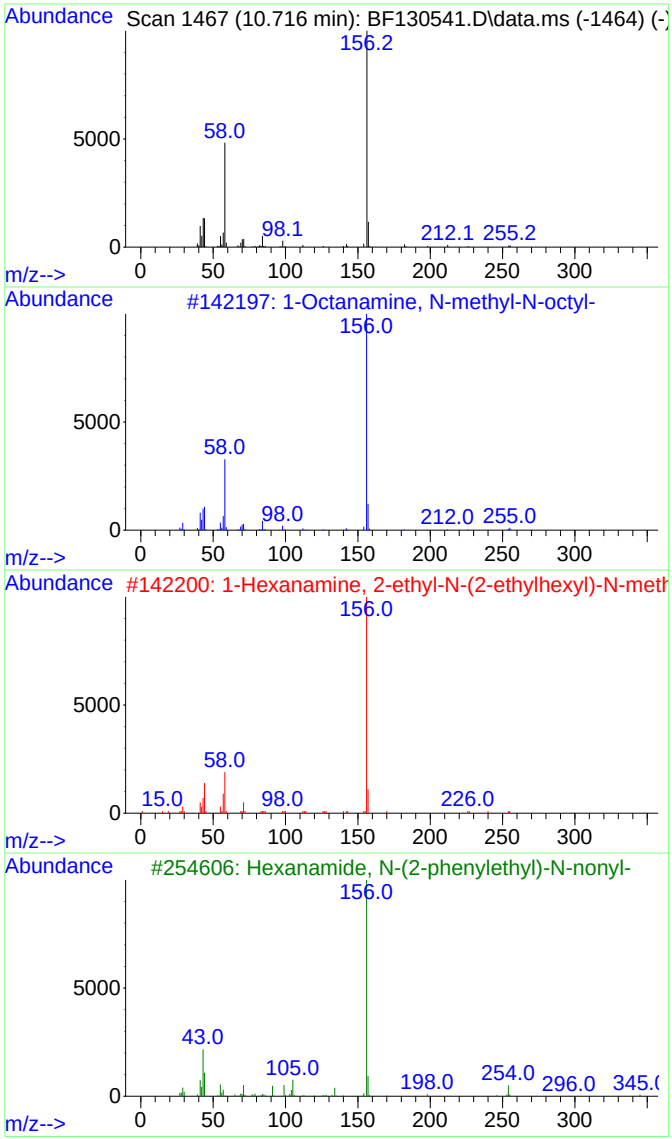
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

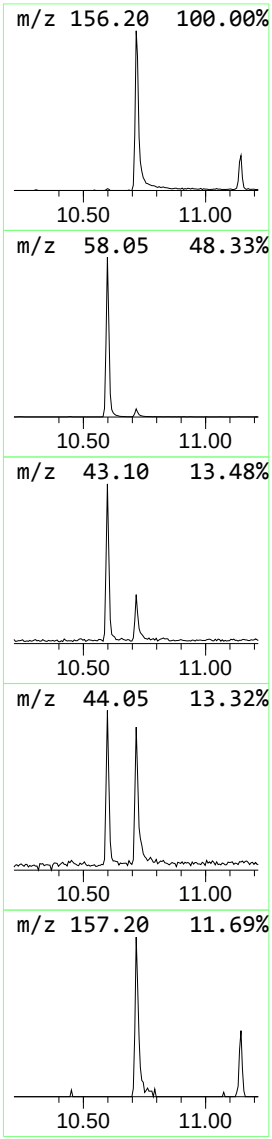
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Octanamine, N-methyl-N-oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.716	6.29 ng	133508	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanamine, N-methyl-N-octyl-	255	C17H37N	004455-26-9	95
2	1-Hexanamine, 2-ethyl-N-(2-ethyl...	255	C17H37N	039168-98-4	56
3	Hexanamide, N-(2-phenylethyl)-N-...	345	C23H39NO	1000451-18-1	50
4	l-Norvaline, N-allyloxycarbonyl-...	369	C21H39NO4	1000320-75-2	43
5	l-Valine, N-allyloxycarbonyl-, d...	341	C19H35NO4	1000323-39-3	43





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
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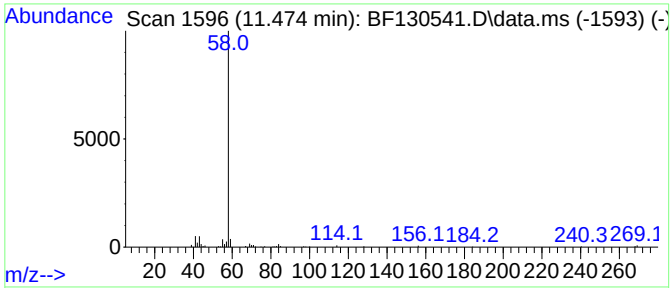
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

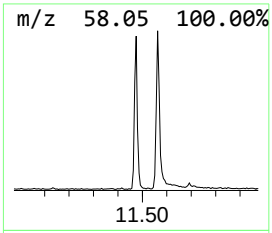
****

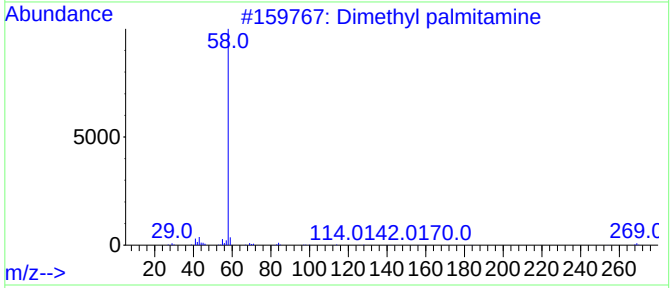
Peak Number 5 Dimethyl palmitamine Concentration Rank 8

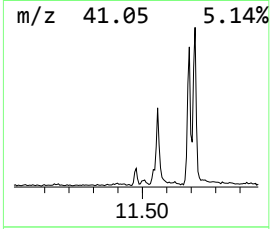
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.474	3.36 ng	71290	Phenanthrene-d10	11.145

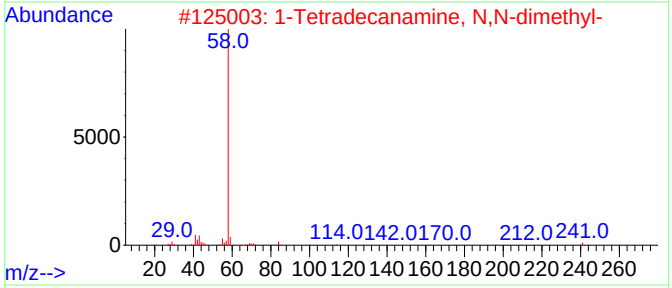
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl palmitamine	269	C18H39N	000112-69-6	90
2	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	78
3	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	78
4	1-Pentadecanamine, N,N-dimethyl-	255	C17H37N	017678-60-3	72
5	Docosylamine, N,N-dimethyl-	353	C24H51N	1000406-30-6	72

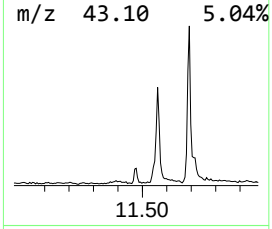


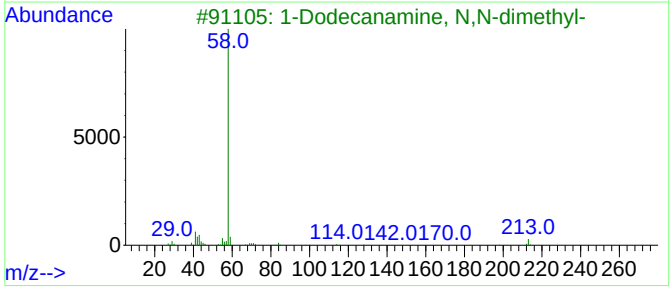


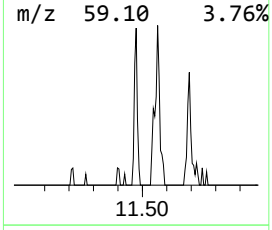


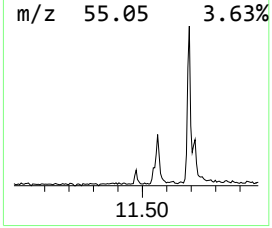












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

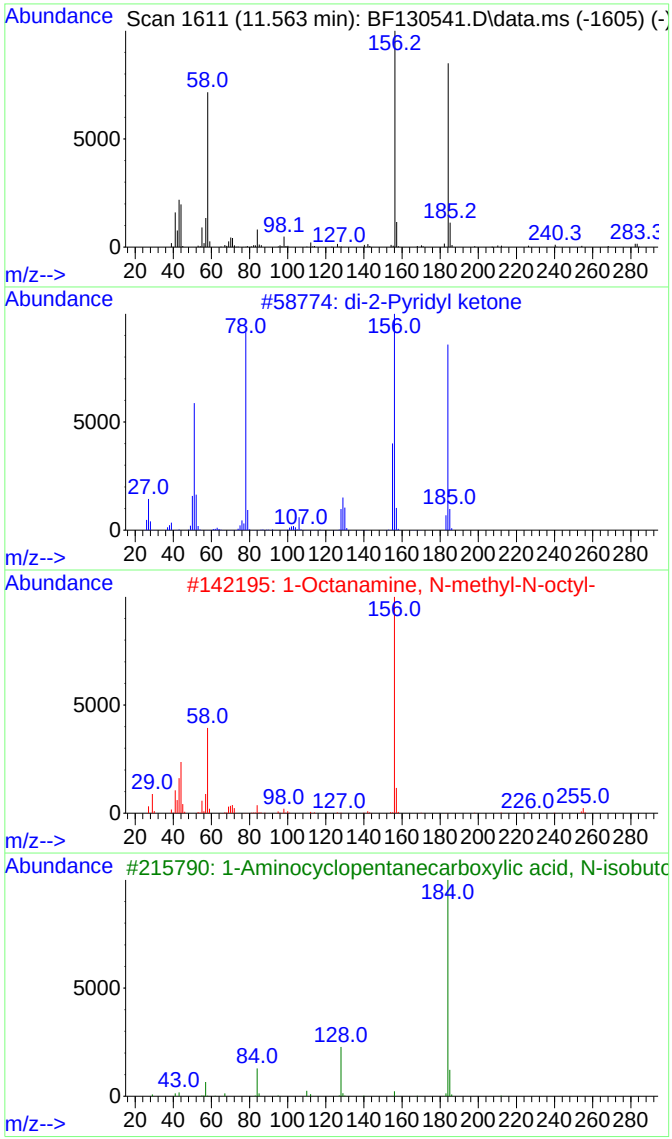
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

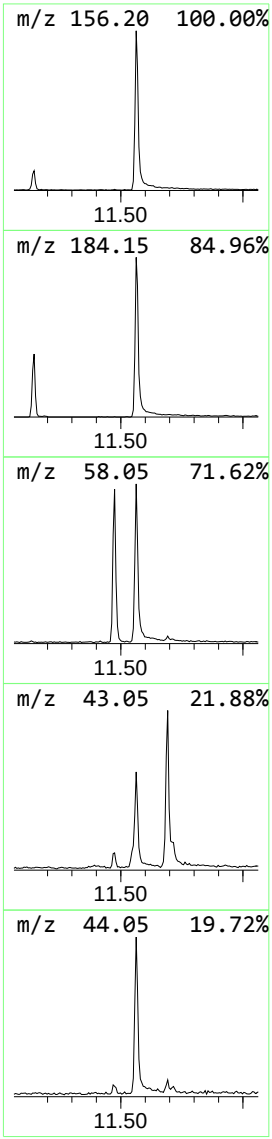
****

Peak Number 6 di-2-Pyridyl ketone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.563	20.66 ng	438897	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-2-Pyridyl ketone	184	C11H8N2O	019437-26-4	53
2	1-Octanamine, N-methyl-N-octyl-	255	C17H37N	004455-26-9	38
3	1-Aminocyclopentanecarboxylic ac...	313	C17H31NO4	1010329-10-1	22
4	Pipecolic acid, N-isobutoxycarbo...	369	C21H39NO4	1000393-02-3	22
5	Pipecolic acid, N-ethoxycarbonyl...	299	C16H29NO4	1000393-07-4	22





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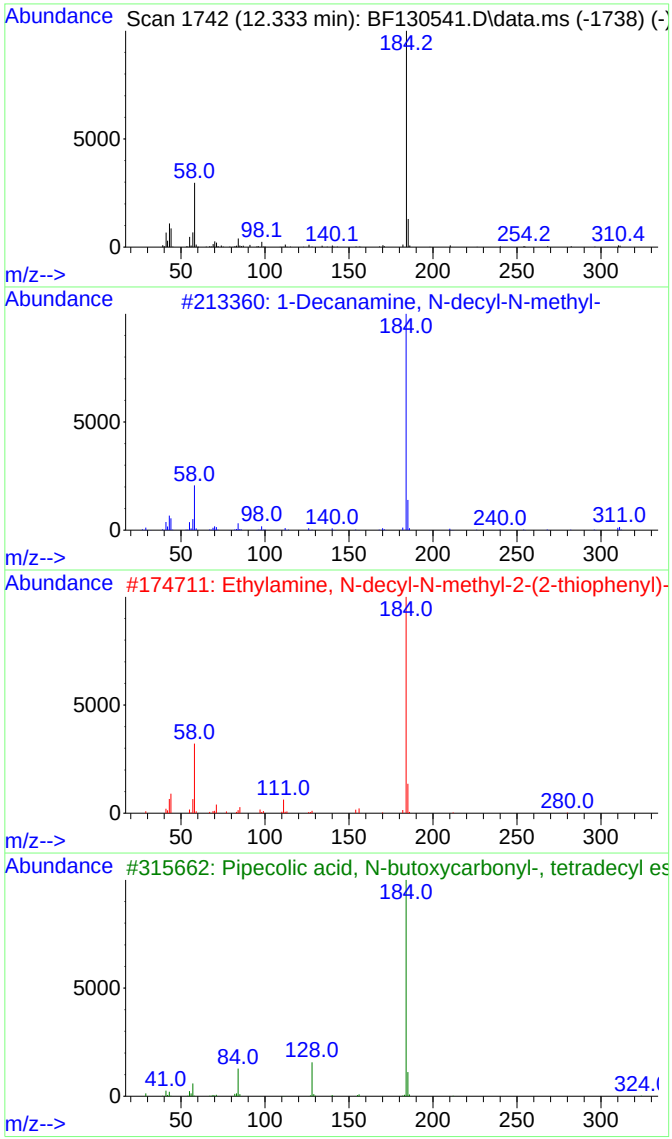
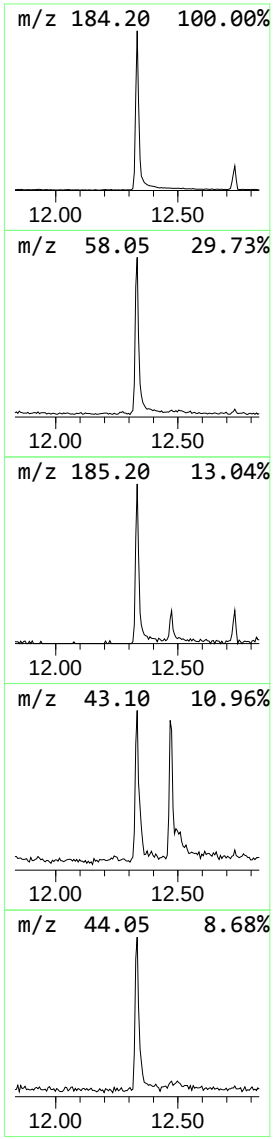
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Decanamine, N-decyl-N-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.333	14.90 ng	316395	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanamine, N-decyl-N-methyl-	311	C21H45N	007396-58-9	95
2	Ethylamine, N-decyl-N-methyl-2-(...	281	C17H31NS	1000310-34-4	56
3	Pipecolic acid, N-butoxycarbonyl...	425	C25H47NO4	1000393-05-9	53
4	D-Alanine, N-(2,5-difluorobenzoy...	411	C23H35F2NO3	1000348-47-0	53
5	1-Aminocyclopentanecarboxylic ac...	439	C26H49NO4	1000329-11-0	53





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Operator : CG\JU
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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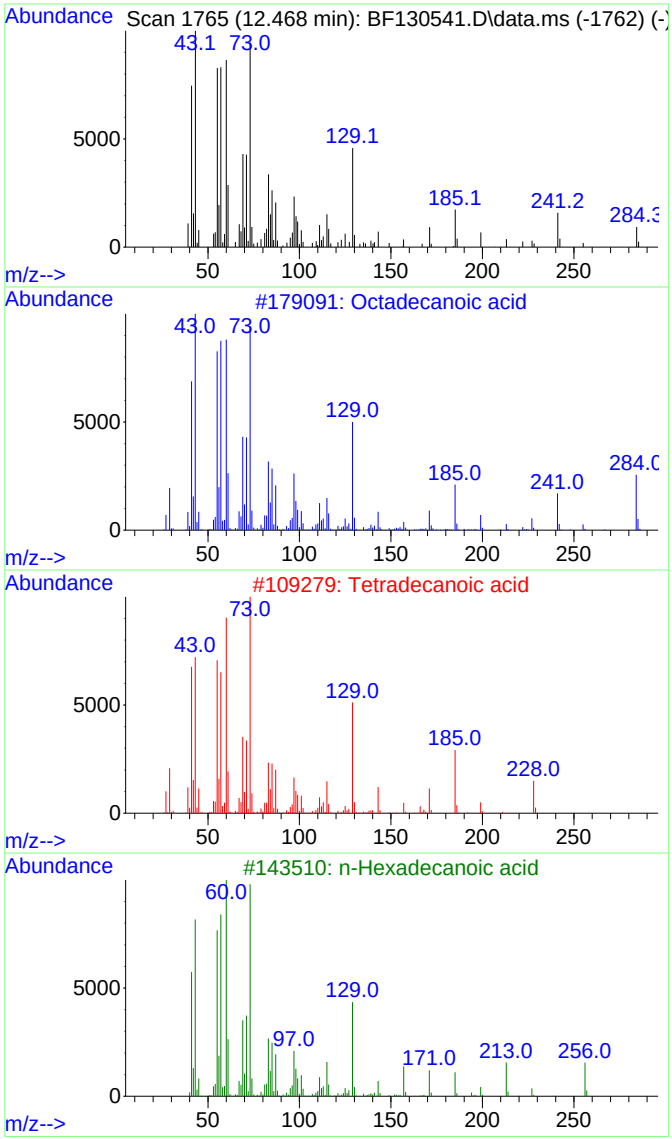
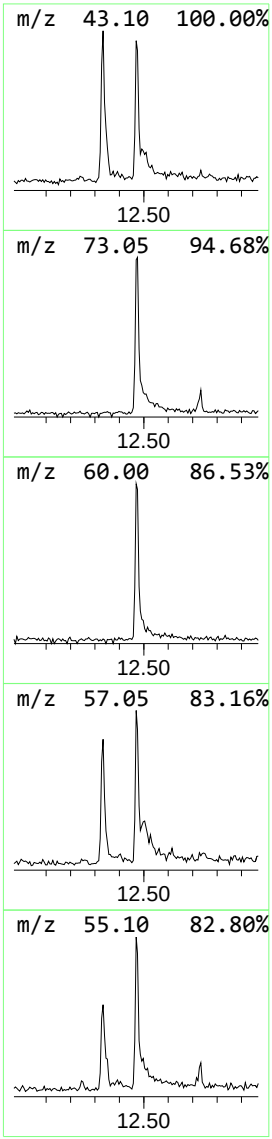
Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	4.92 ng	138592	Chrysene-d12	13.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Data File : BF130541.D
Acq On : 05 Oct 2022 21:16
Operator : CG\JU
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
257248-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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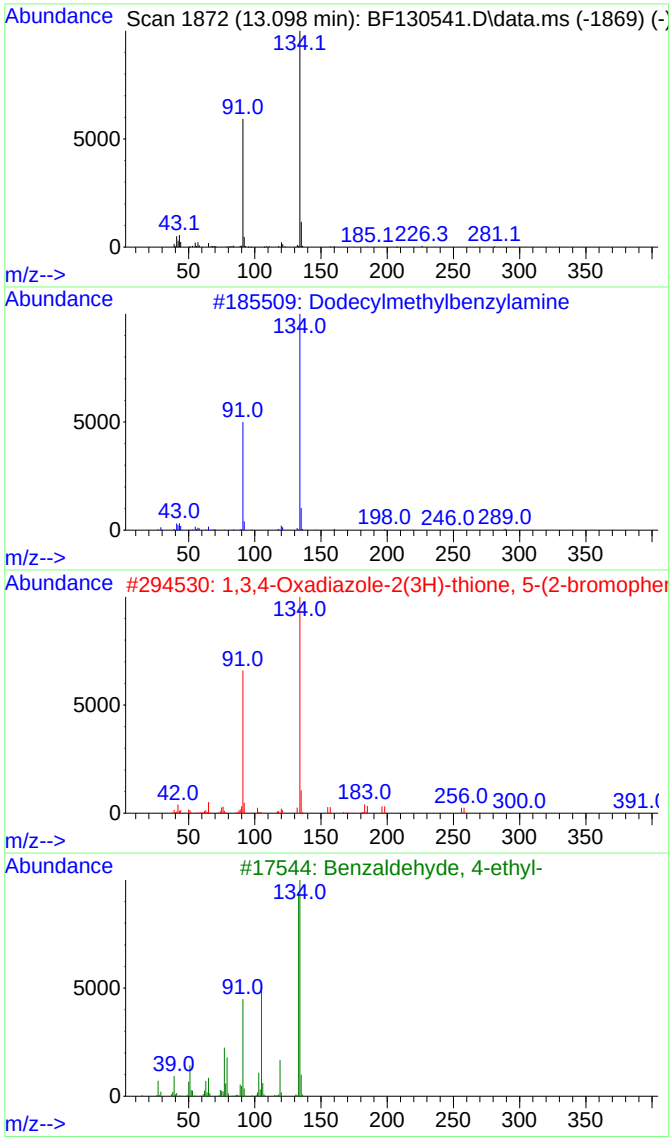
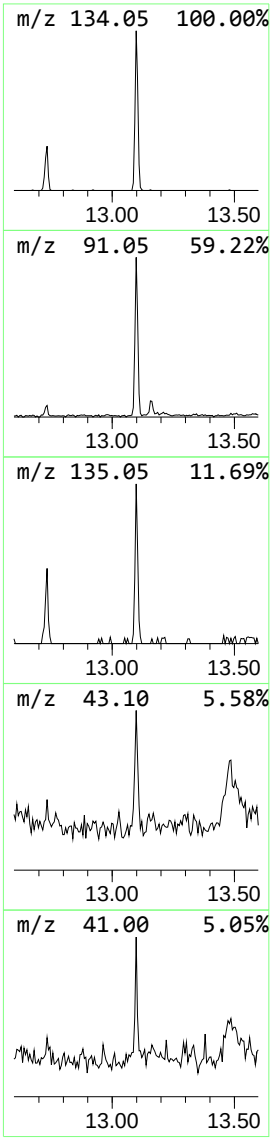
Peak Number 9 Dodecylmethylbenzylamine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	3.00 ng	84448	Chrysene-d12	13.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecylmethylbenzylamine	289	C20H35N	068397-57-9	86
2	1,3,4-Oxadiazole-2(3H)-thione, 5...	389	C17H16BrN3OS	1010271-07-7	64
3	Benzaldehyde, 4-ethyl-	134	C9H10O	004748-78-1	64
4	N-Methyl-N-benzyltetradecanamine	317	C22H39N	083690-72-6	56
5	Benzene, 1-ethenyl-3-methoxy-	134	C9H10O	000626-20-0	40





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Operator : CG\JU
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
257248-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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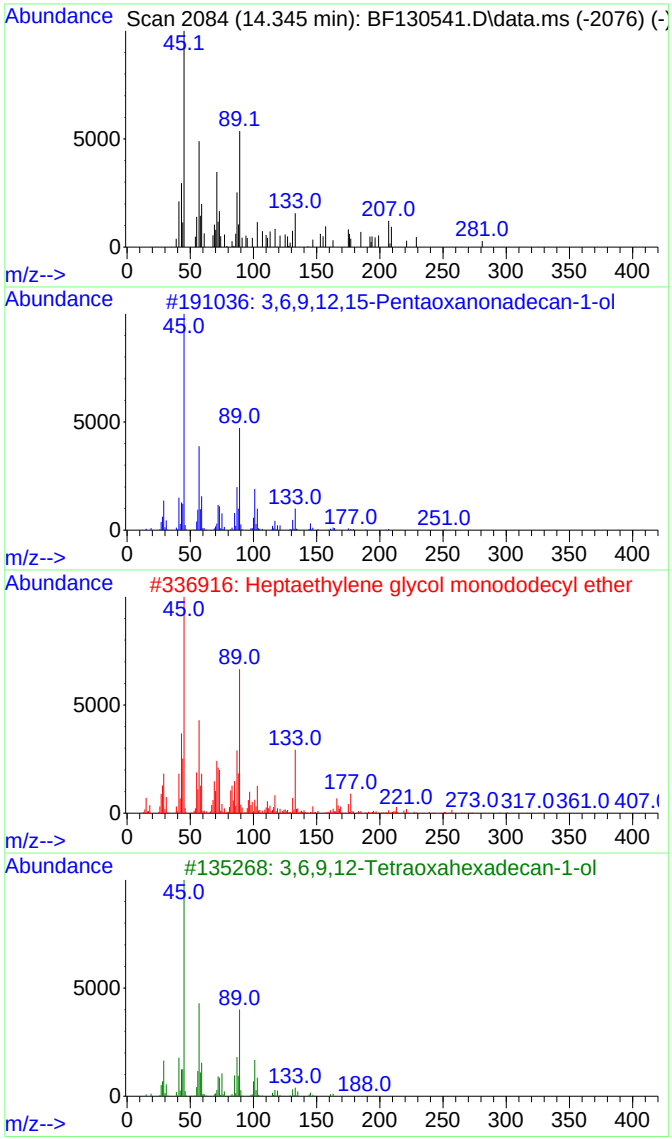
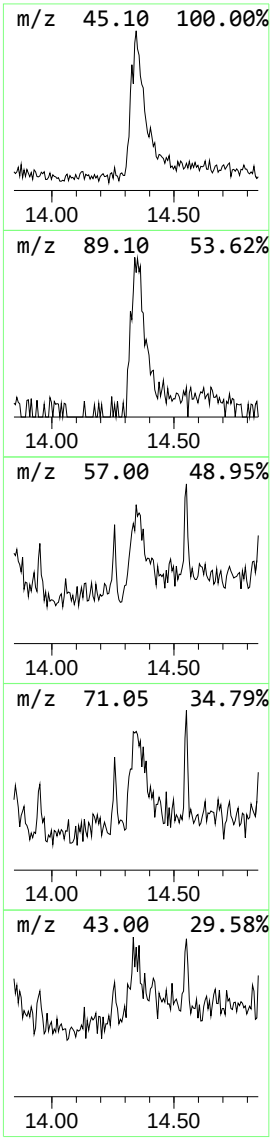
Peak Number 10 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	2.66 ng	74968	Chrysene-d12	13.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	64
2	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	59
3	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	59
4	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	59
5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	59





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Operator : CG\JU
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
257248-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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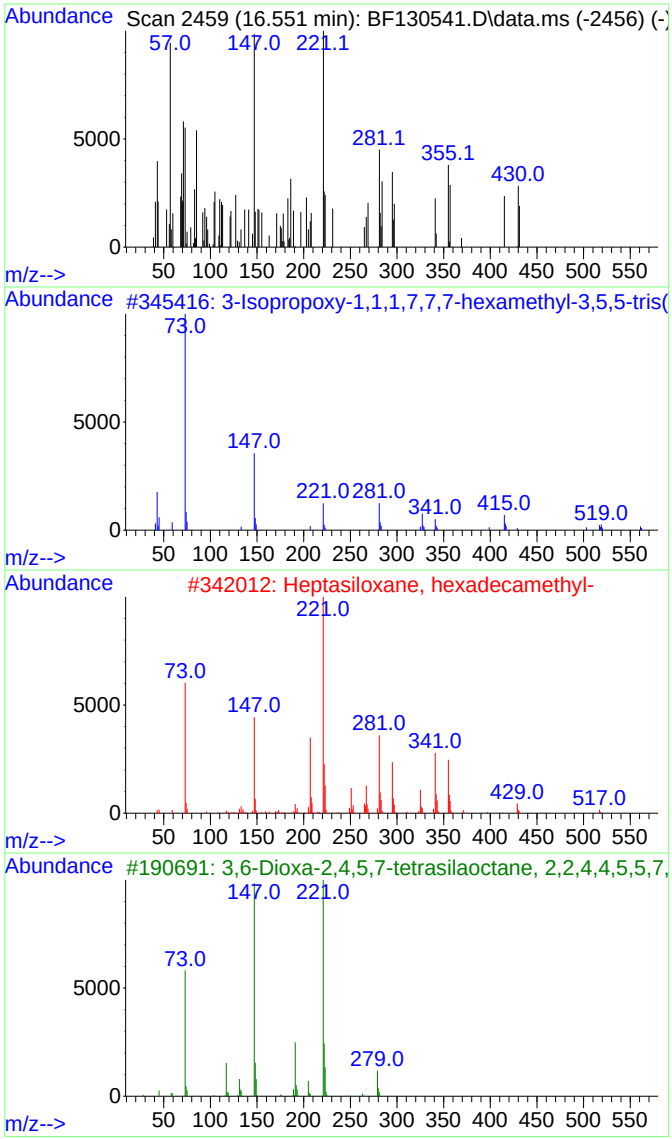
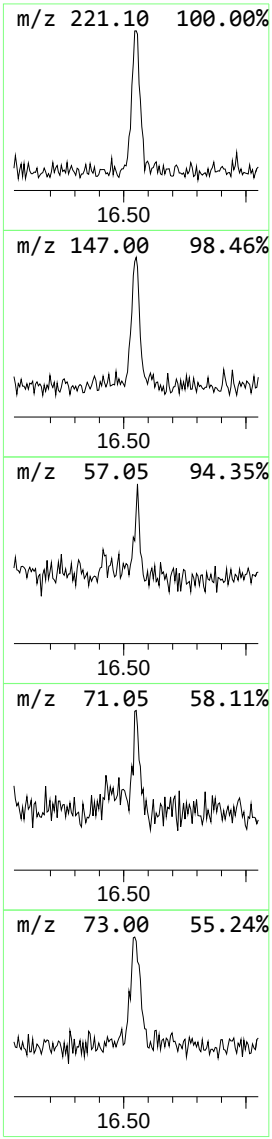
Peak Number 11 unknown16.551 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	2.48 ng	46622	Perylene-d12	15.162

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	43
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	37
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
4	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
5	benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	14





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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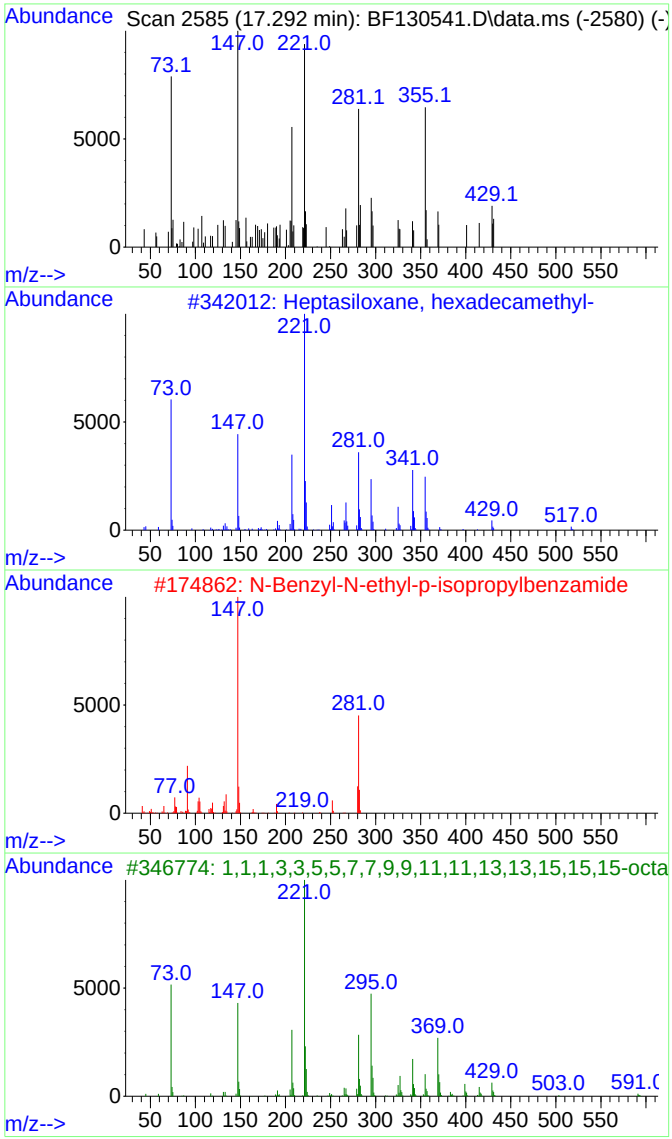
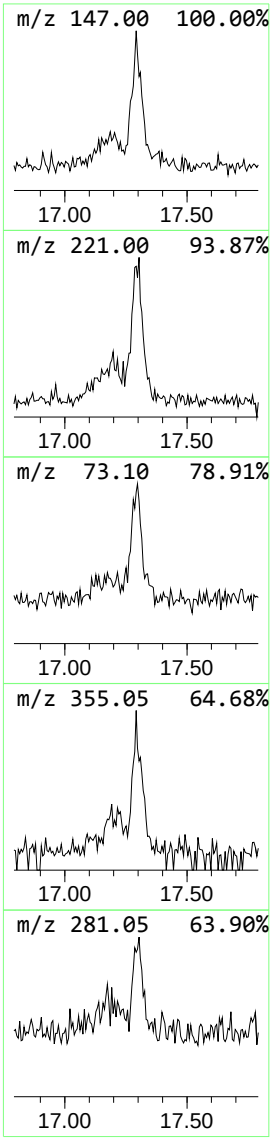
Peak Number 12 unknown17.292 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.292	3.09 ng	57951	Perylene-d12	15.162

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
2	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	14
4	1,2-Dibenzoyl-3-phenylcyclopropane	326	C23H18O2	029128-64-1	11
5	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130541.D
Acq On : 05 Oct 2022 21:16
Operator : CG\JU
Sample : N4974-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
257248-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.798	6.3	ng	156931	1	6.634	500608	20.0
Ethanol, 2-(2-b...	7.845	6.3	ng	160036	2	7.916	512517	20.0
1-Tetradecanami...	10.598	26.3	ng	558218	4	11.145	424813	20.0
1-Octanamine, N...	10.716	6.3	ng	133508	4	11.145	424813	20.0
Dimethyl palmit...	11.474	3.4	ng	71290	4	11.145	424813	20.0
di-2-Pyridyl ke...	11.563	20.7	ng	438897	4	11.145	424813	20.0
1-Decanamine, N...	12.333	14.9	ng	316395	4	11.145	424813	20.0
Octadecanoic acid	12.469	4.9	ng	138592	5	13.774	563178	20.0
Dodecylmethylbe...	13.098	3.0	ng	84448	5	13.774	563178	20.0
3,6,9,12,15-Pen...	14.345	2.7	ng	74968	5	13.774	563178	20.0
unknown16.551	16.551	2.5	ng	46622	6	15.162	375559	20.0
unknown17.292	17.292	3.1	ng	57951	6	15.162	375559	20.0