LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128603.D
Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BB-8

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	468	471	478	rVB	32714	32120	1.40%	0.160%
2	5.498	542	546	562	rVB	2141629	2216304	96.64%	11.056%
3	5.610	562	565	569	rBV	34069	28947	1.26%	0.144%
4	6.528	716	721	729	rBV	2099735	2114345	92.19%	10.547%
5	6.586	729	731	734	rVB	45486	36205	1.58%	0.181%
6	6.839	771	774	778	rBV	741835	656913	28.64%	3.277%
7	7.410	865	871	874	rBV	1553031	1496601	65.26%	7.466%
8	8.128	989	993	996	rBV	953134	787388	34.33%	3.928%
9	9.204	1170	1176	1179	rBV	2894110	2293351	100.00%	11.440%
10	9.880	1288	1291	1295	rBV	950172	793079	34.58%	3.956%
11	10.680	1423	1427	1438	rBV	1211754	1222467	53.30%	6.098%
12	10.780	1442	1444	1453	rVB7	42253	100181	4.37%	0.500%
13	11.016	1477	1484	1492	rVB7	51842	122778	5.35%	0.612%
14	11.369	1540	1544	1547	rBV	855187	697634	30.42%	3.480%
15	11.721	1601	1604	1607	rBV4	27200	31596	1.38%	0.158%
16	11.933	1634	1640	1643	rBV6	60791	143189	6.24%	0.714%
17	11.986	1646	1649	1654	rVV6	85971	177091	7.72%	0.883%
18	12.045	1657	1659	1662	rVV3	60422	83928	3.66%	0.419%
19	12.098	1665	1668	1671	rVV4	68742	99123	4.32%	0.494%
20	12.133	1671	1674	1684	rVB4	90637	189975	8.28%	0.948%
21	12.321	1704	1706	1713	rVB7	25873	44210	1.93%	0.221%
22	12.574	1745	1749	1755	rVB3	450215	665193	29.01%	3.318%
23	12.710	1768	1772	1781	rBV3	65908	154629	6.74%	0.771%
24	12.815	1787	1790	1792	rBV	50205	53882	2.35%	0.269%
25	12.957	1810	1814	1818	rBV	1904130	1674440	73.01%	8.353%
26	13.351	1877	1881	1885	rVB	304667	384407	16.76%	1.918%
27	13.598	1918	1923	1930	rVB	603315	909823	39.67%	4.539%
28	14.010	1990	1993	1997	rBV	570922	584308	25.48%	2.915%
29	14.062	1998	2002	2005	rVV3	282315	391351	17.06%	1.952%
30	14.115	2008	2011	2020	rVB	251789	306619	13.37%	1.530%
31	14.292	2037	2041	2045	rVB	303001	401728	17.52%	2.004%
32	14.721	2110	2114	2121	rBV3	204749	294165	12.83%	1.467%
33	14.974	2153	2157	2166	rVB2	195860	393291	17.15%	1.962%
34	15.486	2240	2244	2253	rVB	357763	465205	20.28%	2.321%

Sum of corrected areas: 20046466

Instrument :
BNA_F
ClientSampleId :
BB-8

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Instrument :
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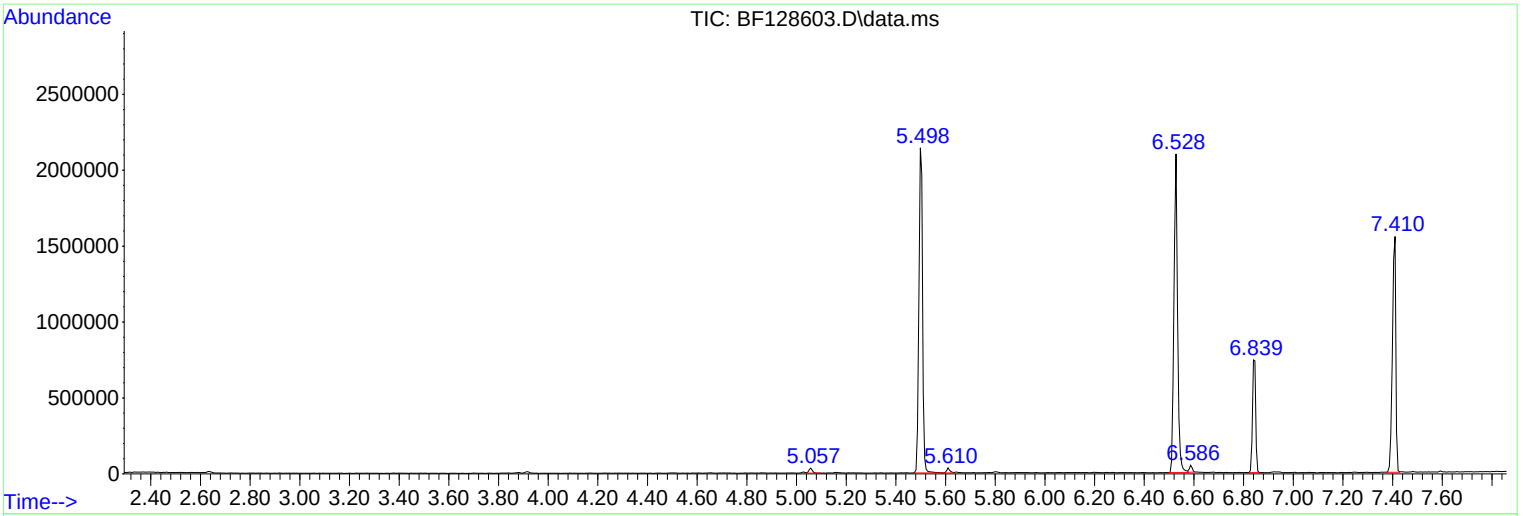
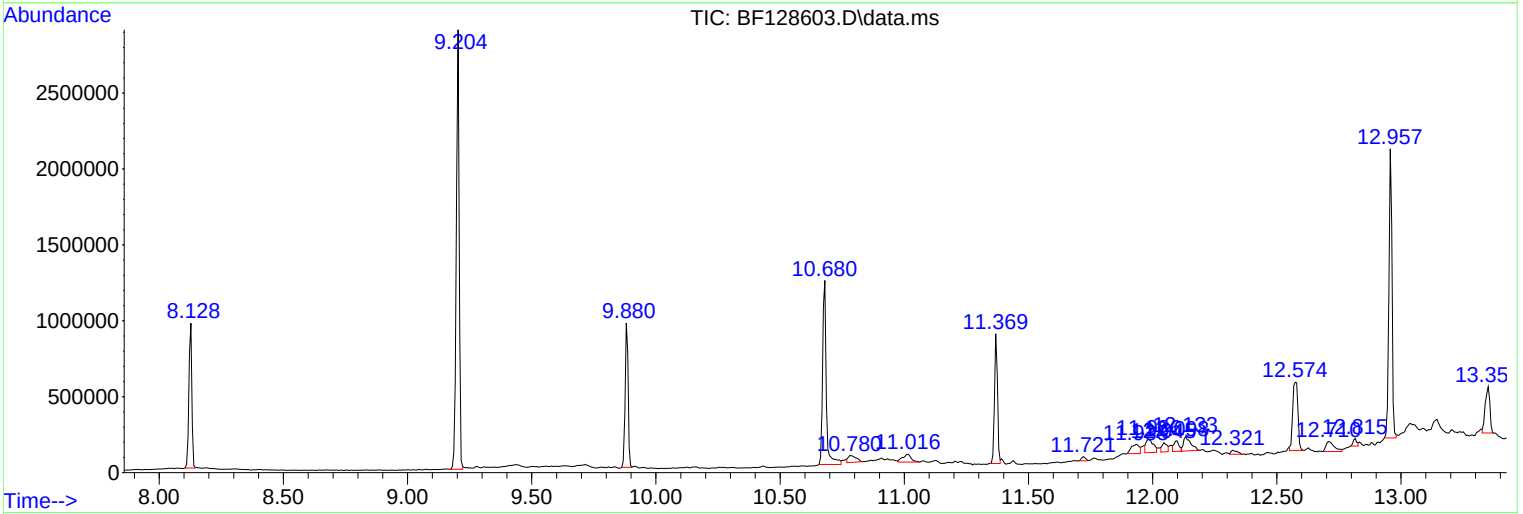
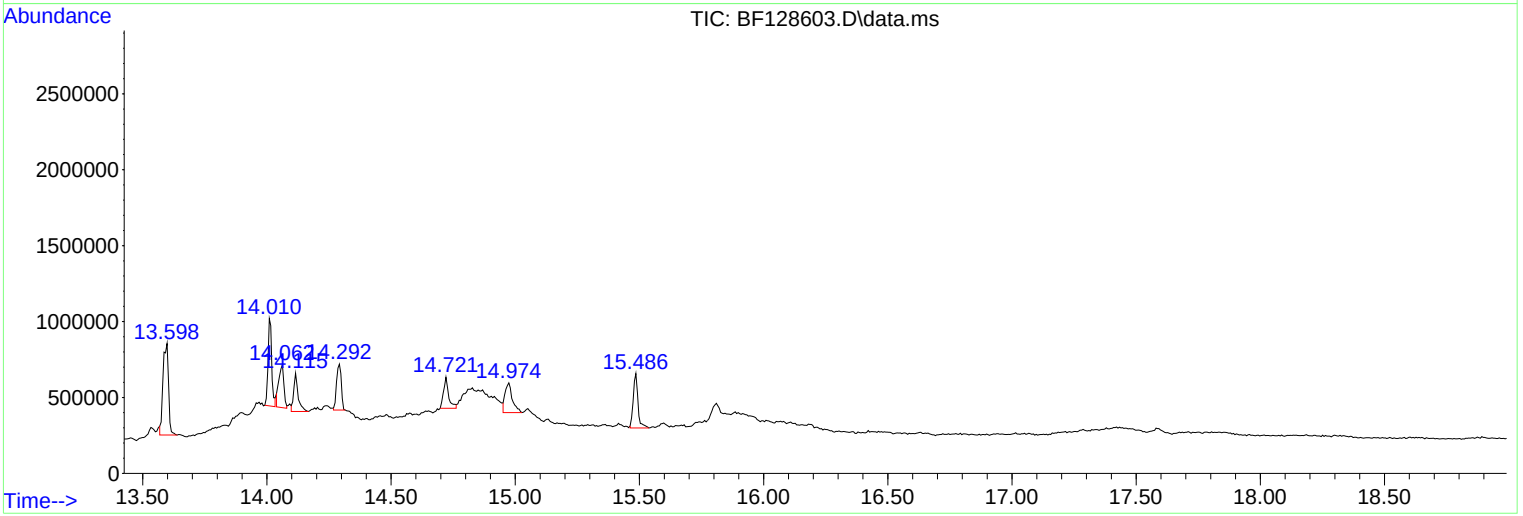
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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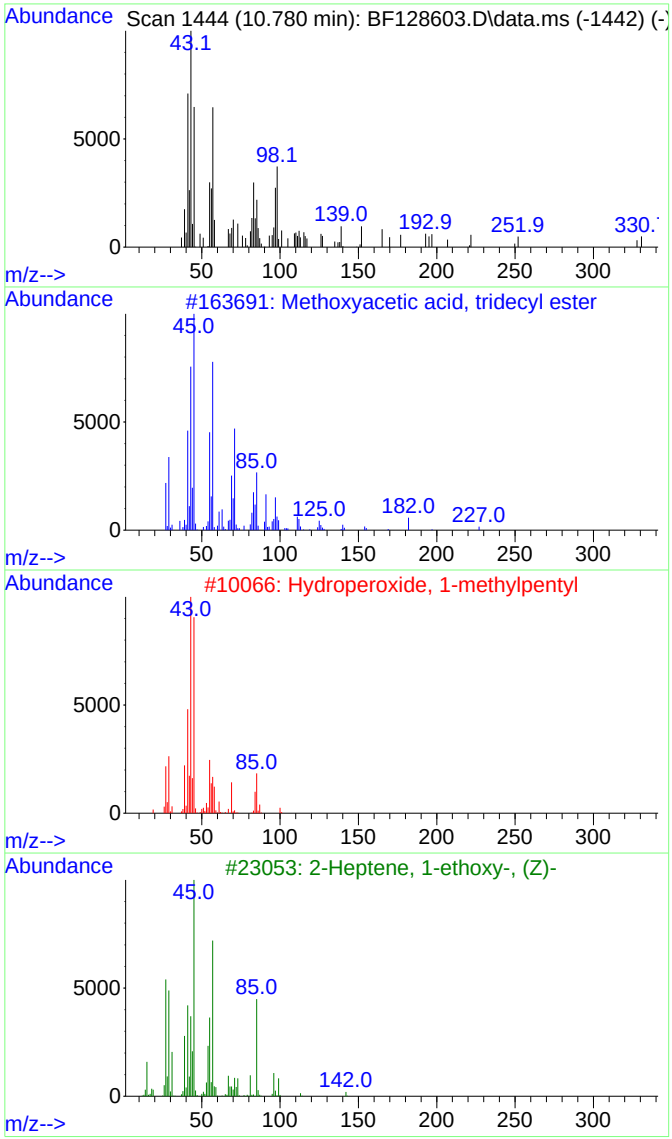
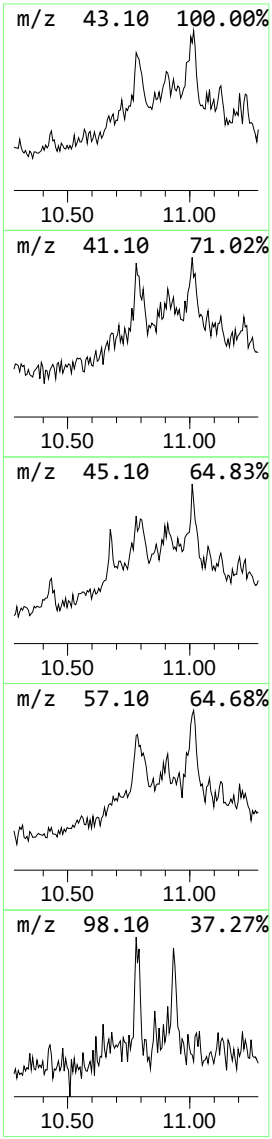
Peak Number 1 unknown10.780 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.780	2.87 ng	100181	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, tridecyl ester	272	C16H32O3	1000281-82-0	38
2	Hydroperoxide, 1-methylpentyl	118	C6H14O2	024254-55-5	27
3	2-Heptene, 1-ethoxy-, (Z)-	142	C9H18O	051149-74-7	27
4	2-Octanol	130	C8H18O	000123-96-6	22
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	22





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TIC Library : C:\Database\NIST20.L
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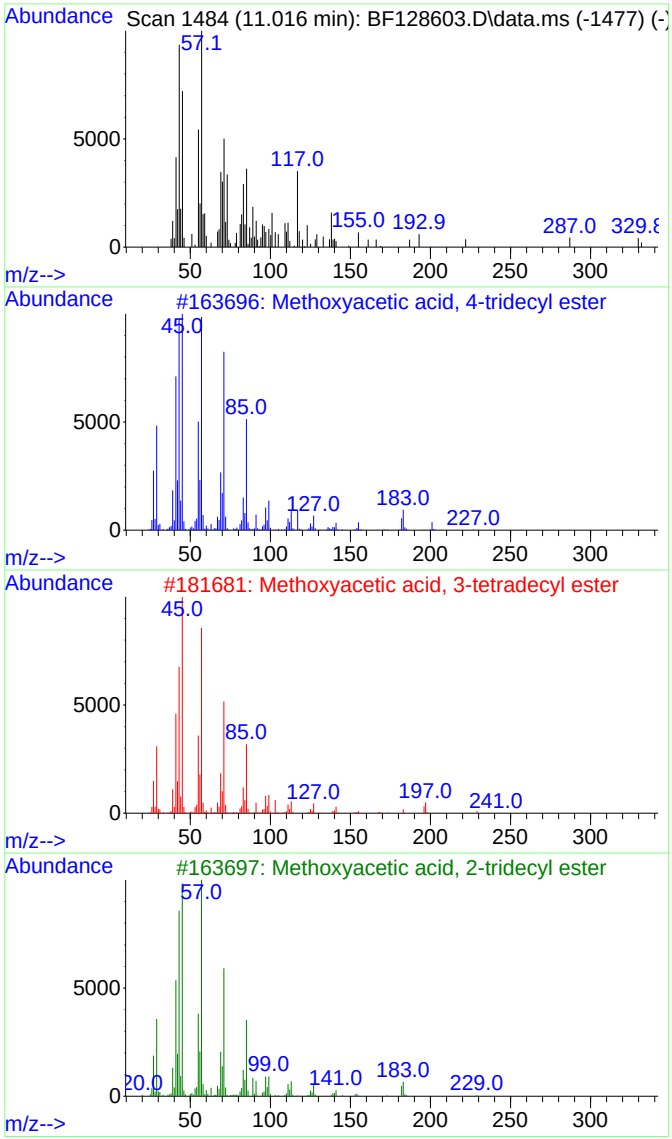
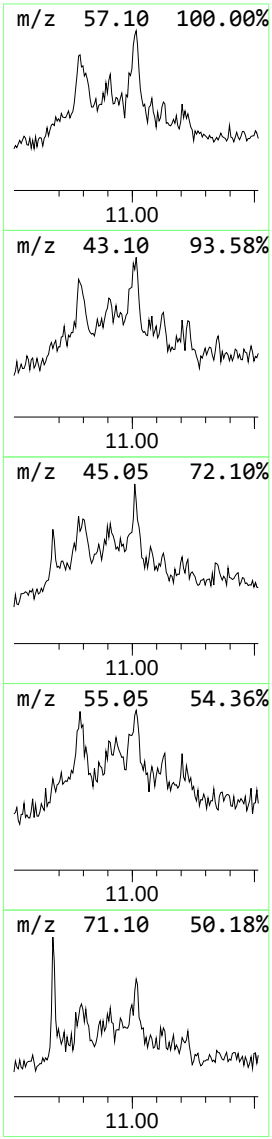
Peak Number 2 unknown11.016 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.016	3.52 ng	122778	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 4-tridecyl e...	272	C16H32O3	1000282-04-7	47
2	Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	43
3	Methoxyacetic acid, 2-tridecyl e...	272	C16H32O3	1000282-04-5	43
4	1-Butanamine, 4-methoxy-	103	C5H13NO	034039-36-6	27
5	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	25





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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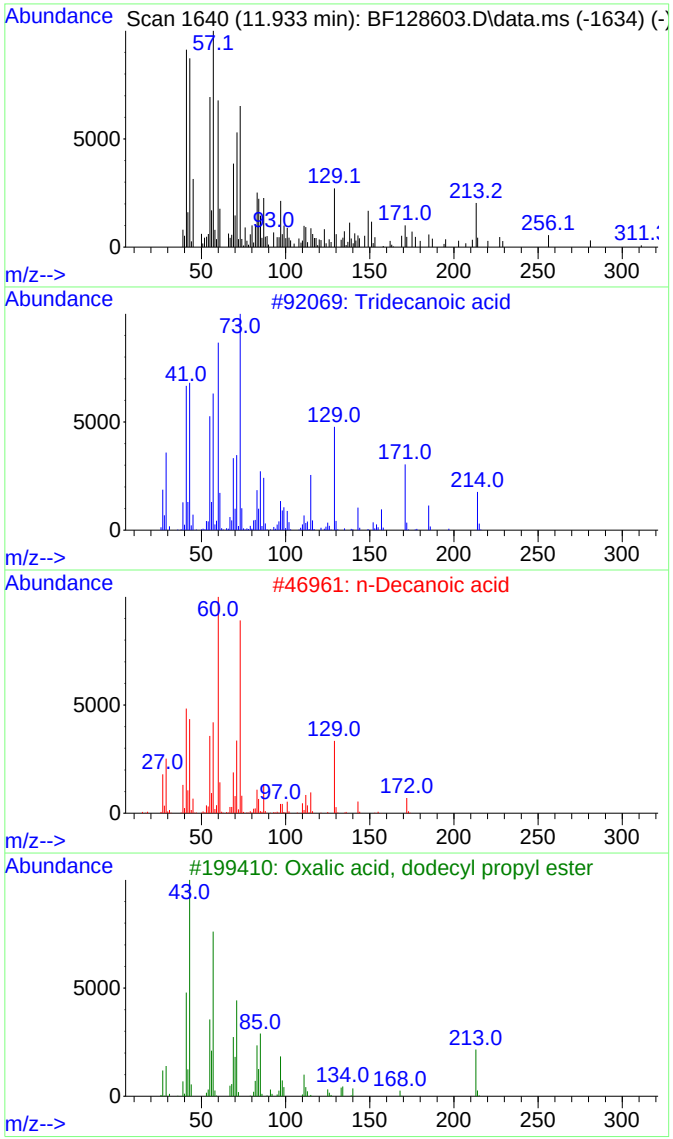
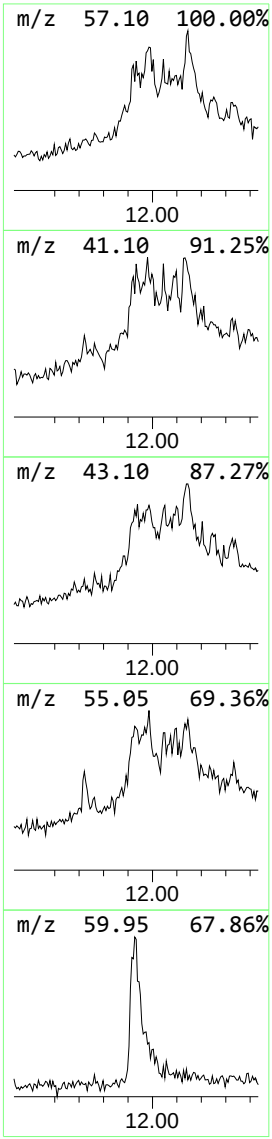
Peak Number 3 unknown11.933 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.10 ng	143189	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	46
2	n-Decanoic acid	172	C10H20O2	000334-48-5	46
3	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	38
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	27





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
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TIC Library : C:\Database\NIST20.L
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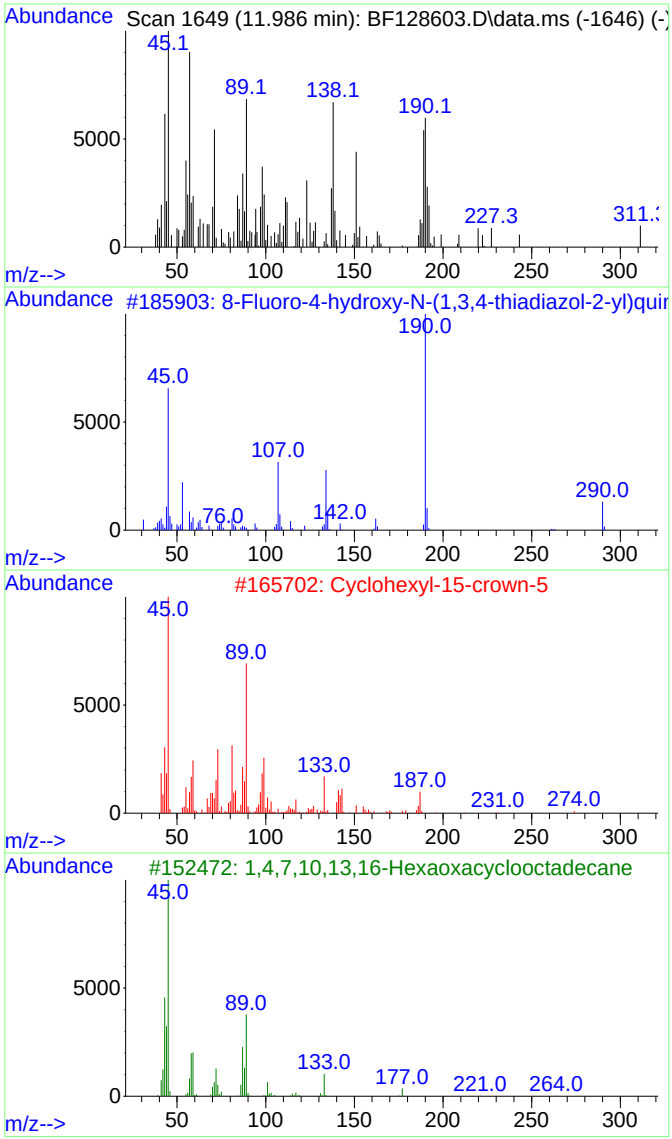
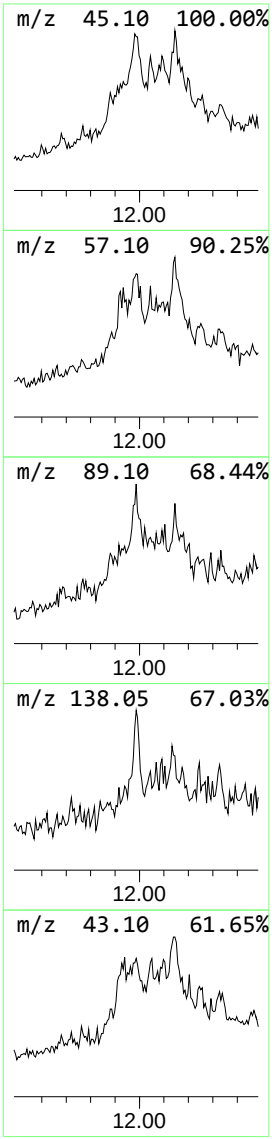
Peak Number 4 unknown11.986 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	5.08 ng	177091	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Fluoro-4-hydroxy-N-(1,3,4-thia...	290	C12H7FN4O2S	1000435-83-4	35
2	Cyclohexyl-15-crown-5	274	C14H26O5	017454-48-7	14
3	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	14
4	1,3,4-Trimethoxy-butan-2-ol	164	C7H16O4	033469-04-4	14
5	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	14





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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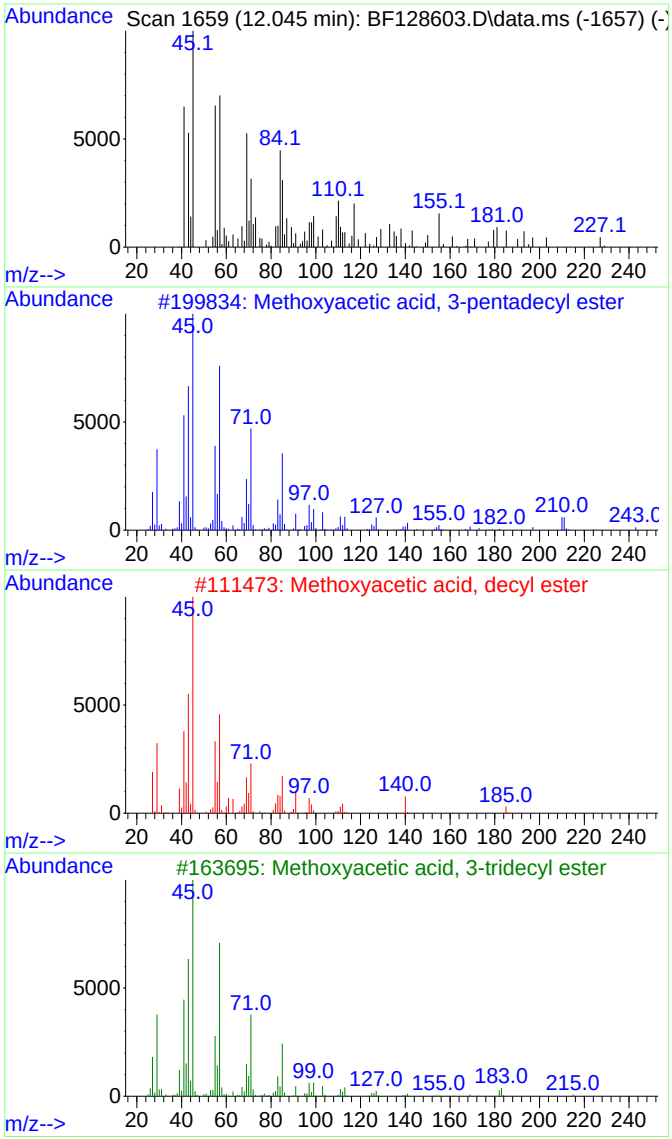
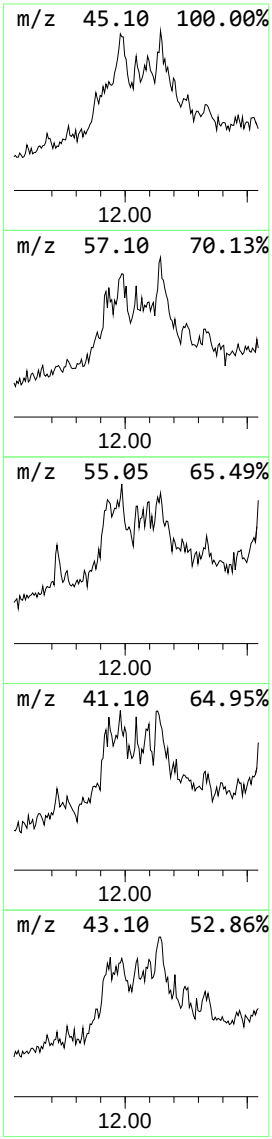
Peak Number 5 unknown12.045 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.045	2.41 ng	83928	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 3-pentadecyl...	300	C18H36O3	1010282-05-2	38
2	Methoxyacetic acid, decyl ester	230	C13H26O3	259141-02-1	35
3	Methoxyacetic acid, 3-tridecyl e...	272	C16H32O3	1000282-04-6	35
4	Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	35
5	Methoxyacetic acid, dodecyl ester	258	C15H30O3	1000281-81-9	35





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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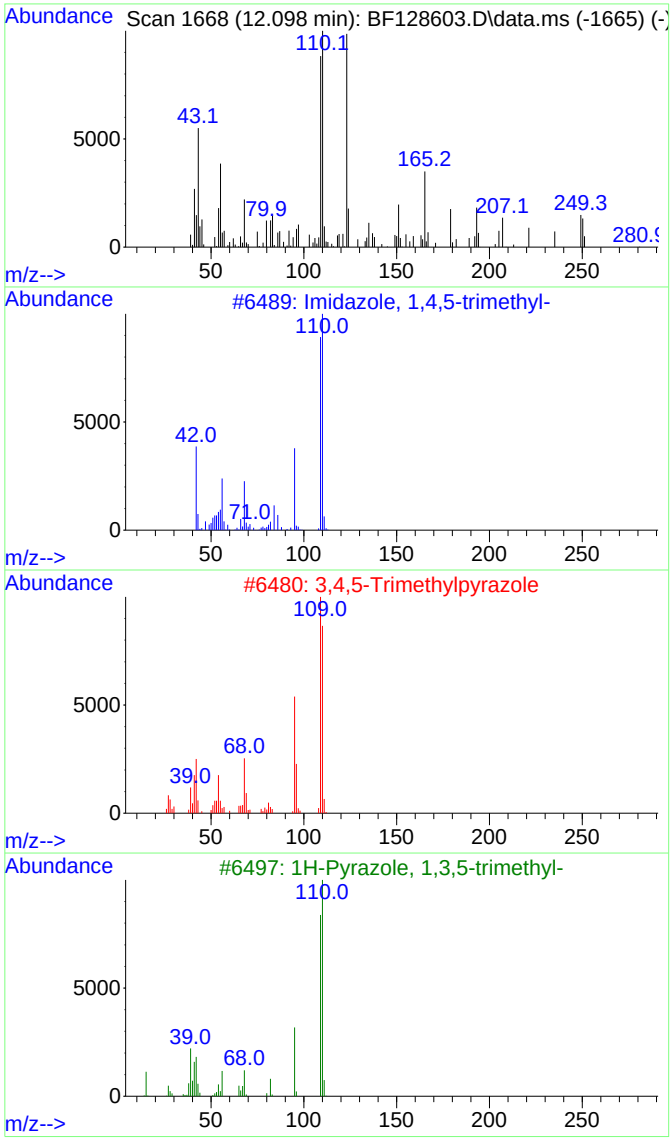
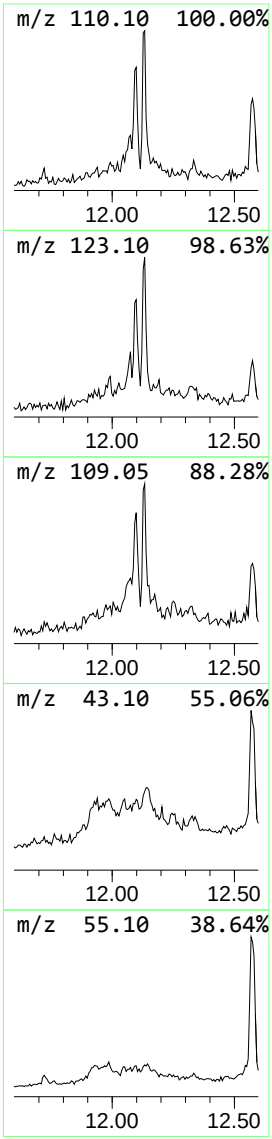
Peak Number 6 unknown12.098 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	2.84 ng	99123	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazole, 1,4,5-trimethyl-	110	C6H10N2	020185-22-2	43
2	3,4,5-Trimethylpyrazole	110	C6H10N2	005519-42-6	43
3	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	38
4	4-Pyrimidinamine, 6-methyl-	109	C5H7N3	003435-28-7	18
5	Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	18





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
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TIC Library : C:\Database\NIST20.L
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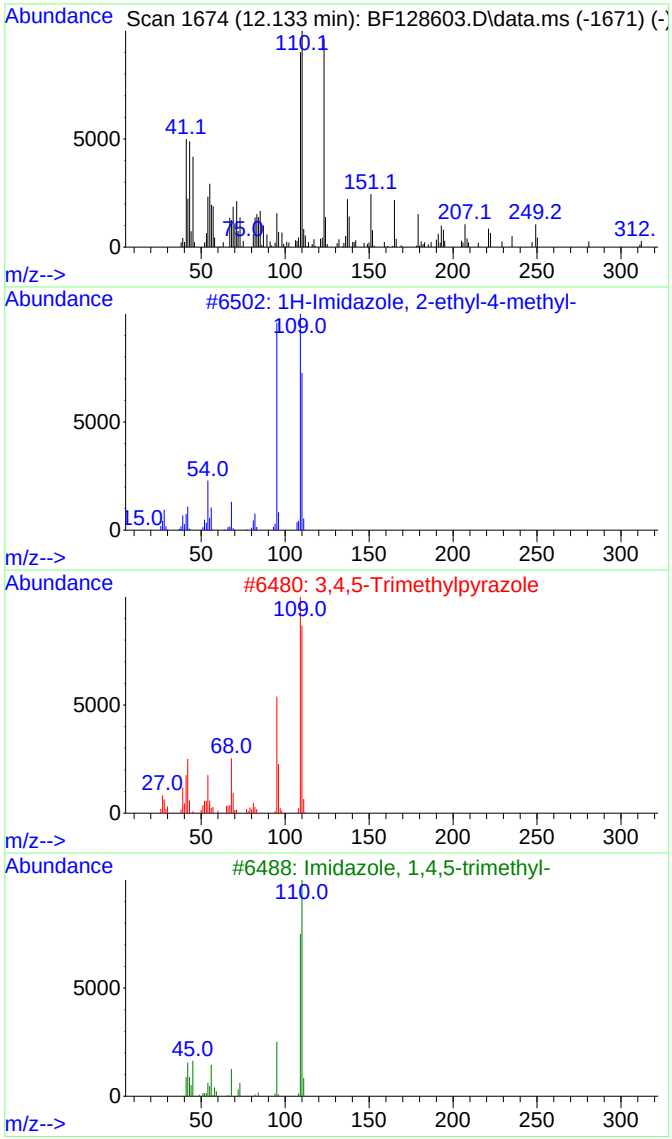
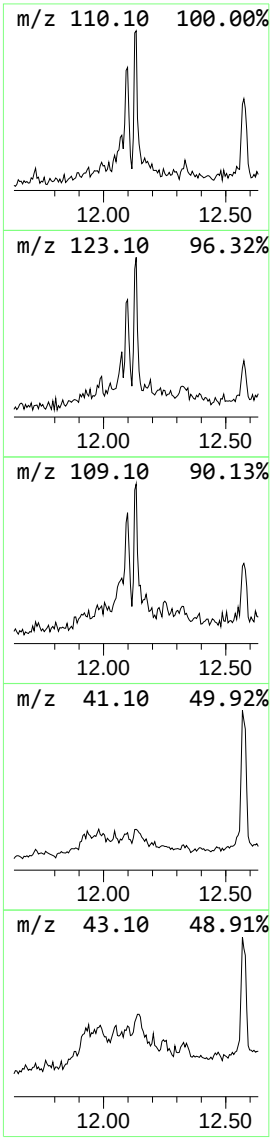
Peak Number 7 unknown12.133 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.133	5.45 ng	189975	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	41
2	3,4,5-Trimethylpyrazole	110	C6H10N2	005519-42-6	38
3	Imidazole, 1,4,5-trimethyl-	110	C6H10N2	020185-22-2	38
4	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	38
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	25





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TIC Library : C:\Database\NIST20.L
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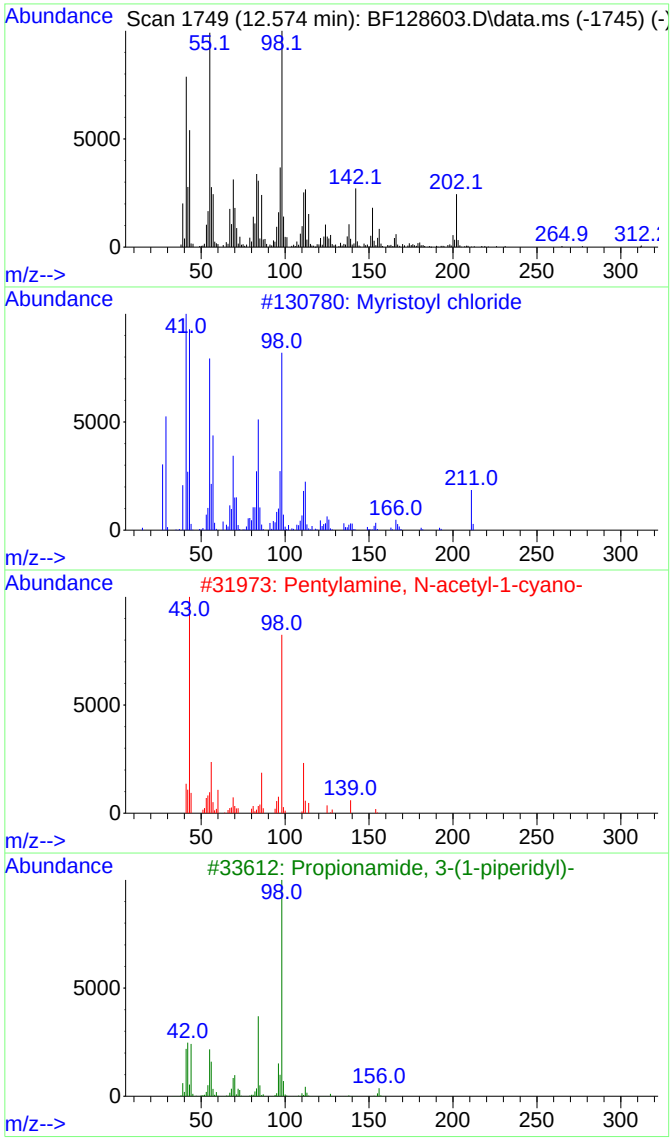
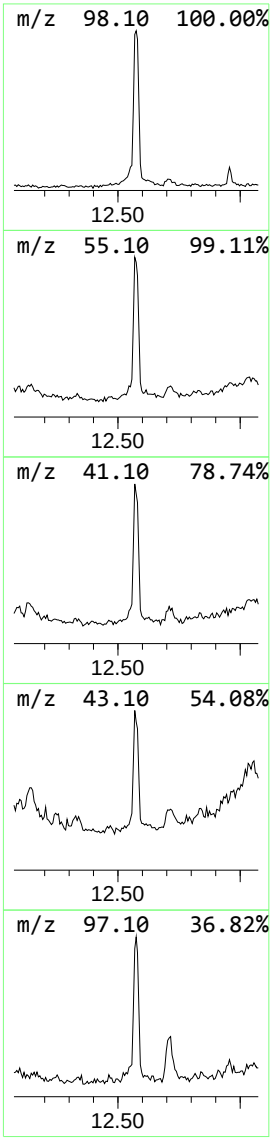
Peak Number 8 unknown12.574 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	19.07 ng	665193	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristoyl chloride	246	C14H27ClO	000112-64-1	47
2	Pentylamine, N-acetyl-1-cyano-	154	C8H14N2O	027395-08-0	38
3	Propionamide, 3-(1-piperidyl)-	156	C8H16N2O	004269-30-1	35
4	3-Undecylthiophene	238	C15H26S	129607-86-9	35
5	3-Decylthiophene	224	C14H24S	065016-55-9	35





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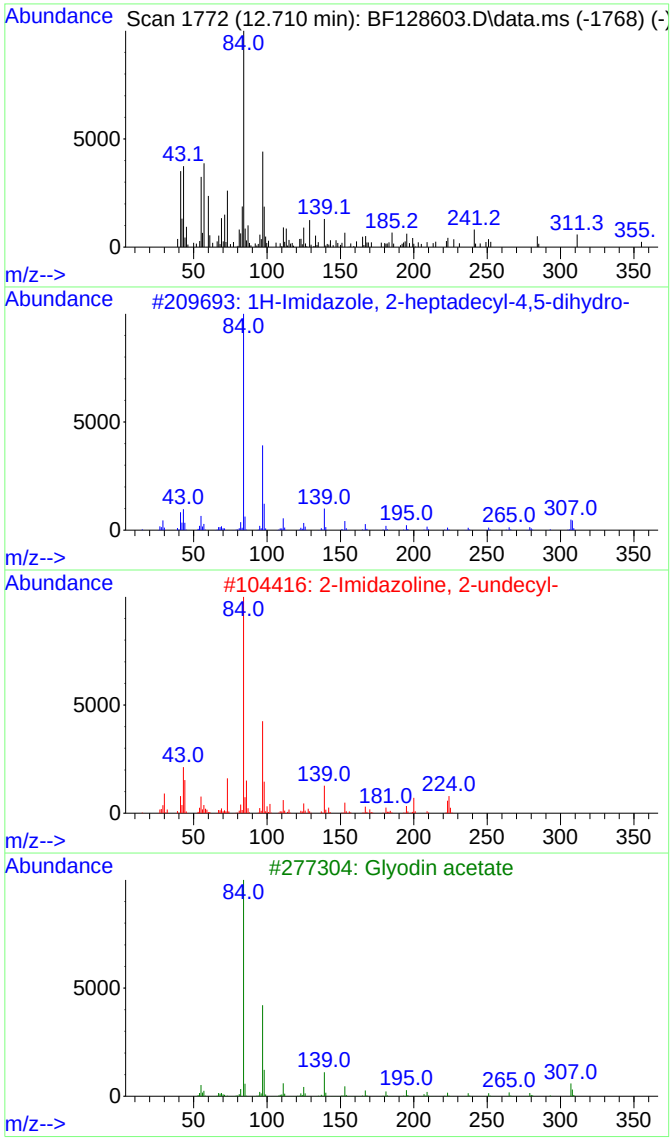
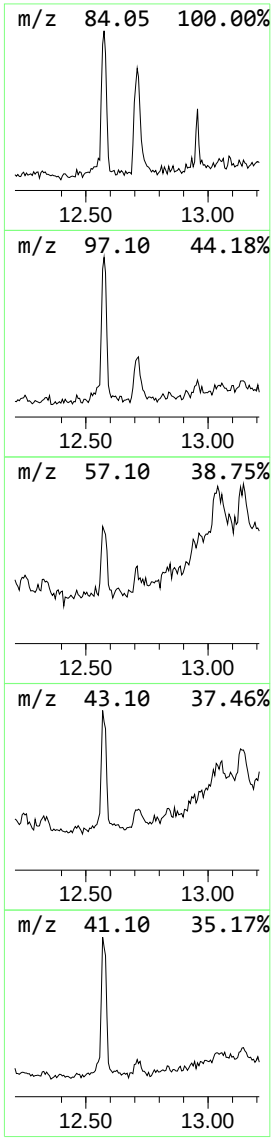
****
Peak Number 9 1H-Imidazole, 2-heptadecyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	5.29 ng	154629	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole, 2-heptadecyl-4,5-d...	308	C20H40N2	000105-28-2	53
2	2-Imidazoline, 2-undecyl-	224	C14H28N2	010443-61-5	53
3	Glyodin acetate	368	C22H44N2O2	000556-22-9	53
4	Rolicyprine	244	C14H16N2O2	002829-19-8	35
5	4-Methylproline	129	C6H11NO2	1000131-14-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128603.D
Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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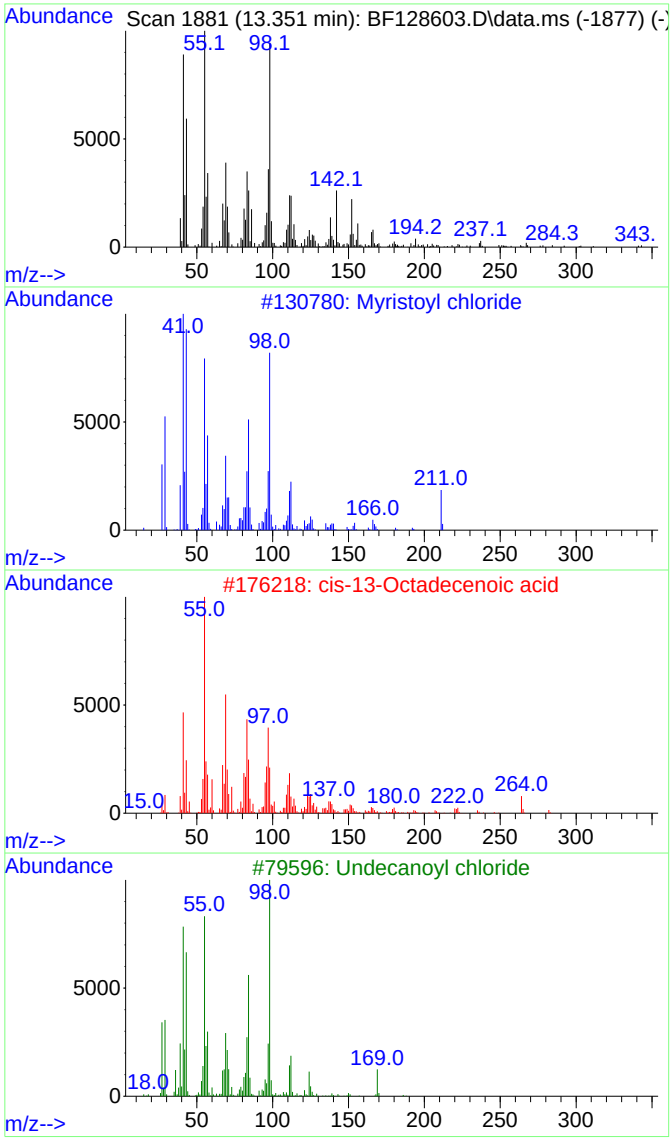
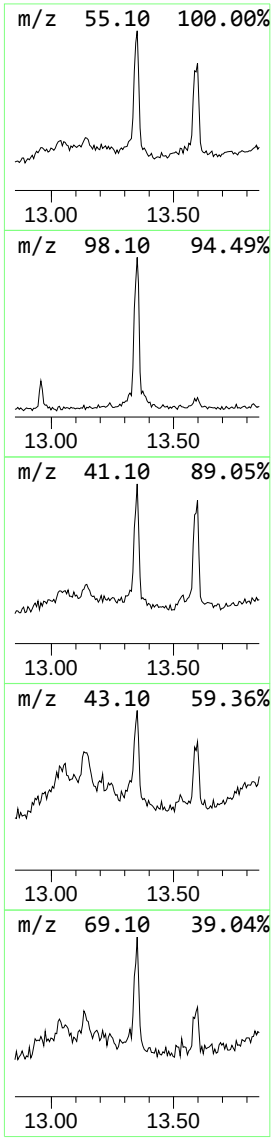
Peak Number 10 unknown13.351 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	13.16 ng	384407	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristoyl chloride	246	C14H27ClO	000112-64-1	47
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	46
3	Undecanoyl chloride	204	C11H21ClO	017746-05-3	43
4	3-Furanmethanol	98	C5H6O2	004412-91-3	38
5	2-(1-Methyl-3-butenyl)cyclohexanone	166	C11H18O	1000424-67-7	38





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Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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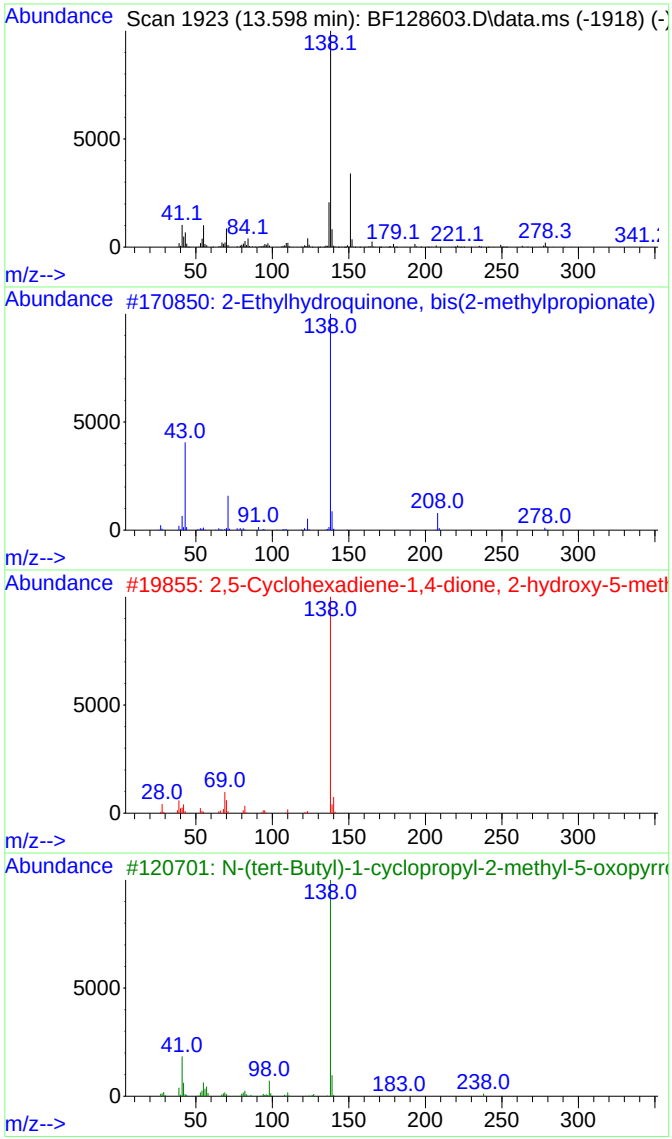
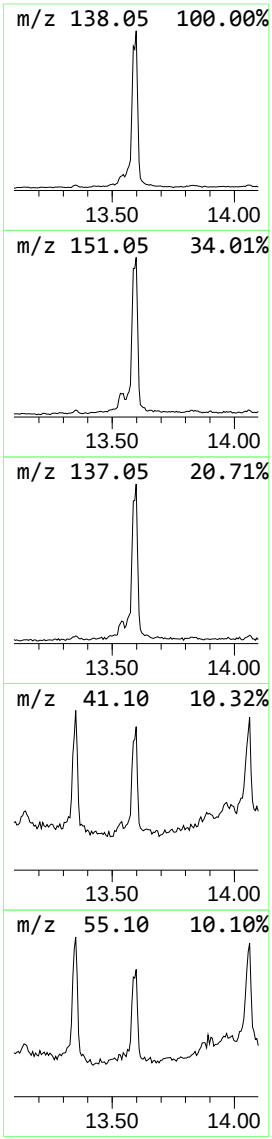
Peak Number 11 unknown13.598 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.598	31.14 ng	909823	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhydroquinone, bis(2-methy...	278	C16H22O4	1000463-14-5	47
2	2,5-Cyclohexadiene-1,4-dione, 2-...	138	C7H6O3	000615-91-8	46
3	N-(tert-Butyl)-1-cyclopropyl-2-m...	238	C13H22N2O2	1000458-30-5	43
4	2-Ethyl-3-methoxypyrazine	138	C7H10N2O	025680-58-4	42
5	(5R,8R,8aS)-8-Methyl-5-((Z)-non-...	263	C18H33N	1000367-14-0	40





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Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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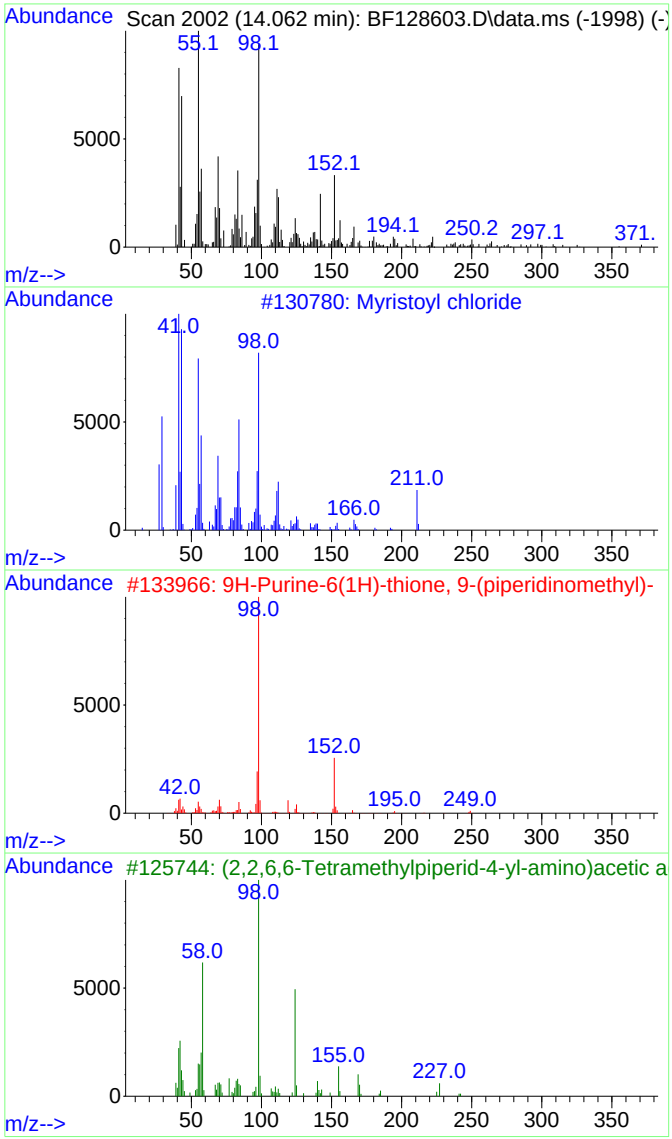
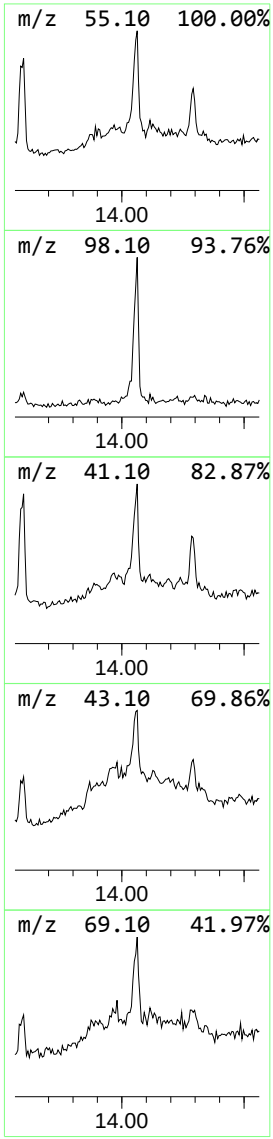
Peak Number 12 Myristoyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	13.40 ng	391351	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristoyl chloride	246	C14H27ClO	000112-64-1	52
2	9H-Purine-6(1H)-thione, 9-(piper...	249	C11H15N5S	014133-14-3	43
3	(2,2,6,6-Tetramethylpiperid-4-yl...	242	C13H26N2O2	071866-09-6	38
4	Cyclohexene, 1-(1,1-dimethyletho...	154	C10H18O	031053-82-4	38
5	Furan, 2,5-dihydro-3,4-dimethyl-	98	C6H10O	053720-72-2	30





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Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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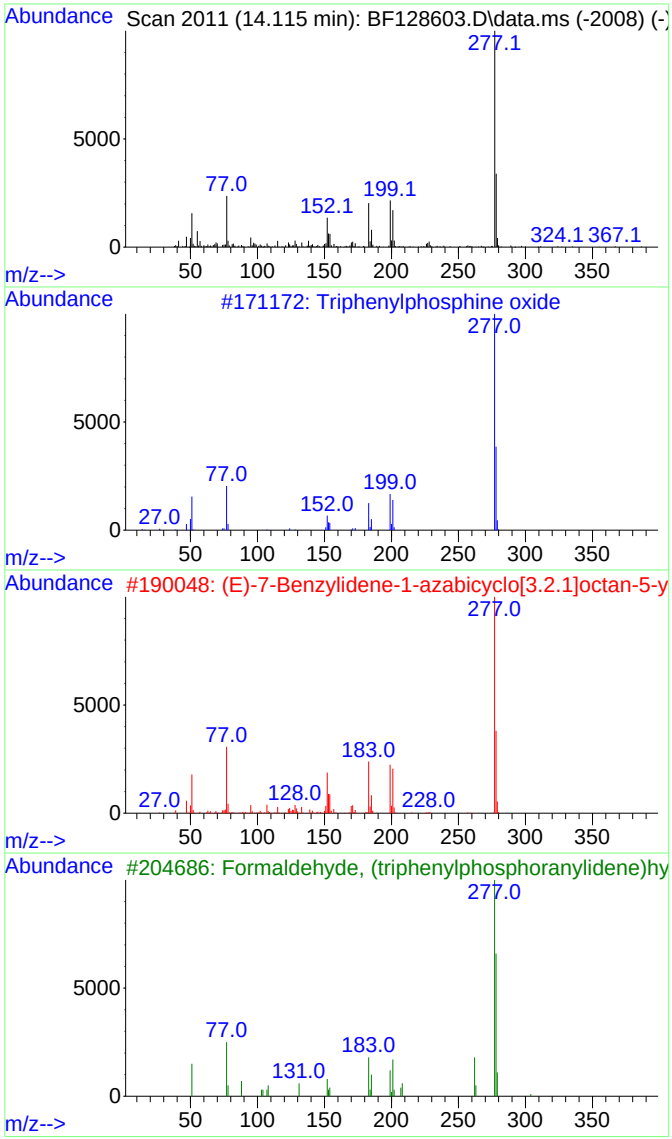
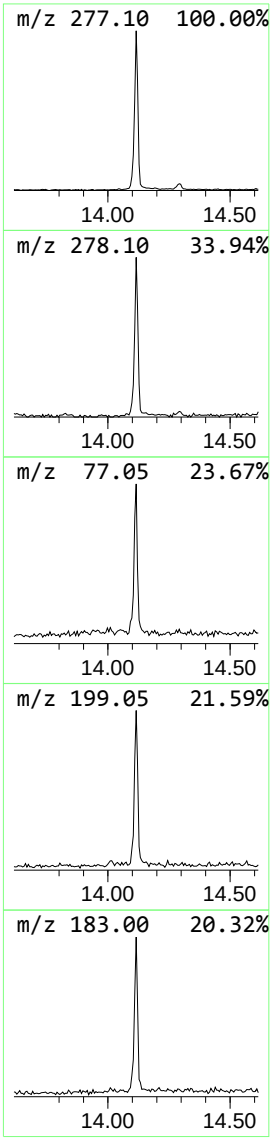
Peak Number 13 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.115	10.50 ng	306619	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
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Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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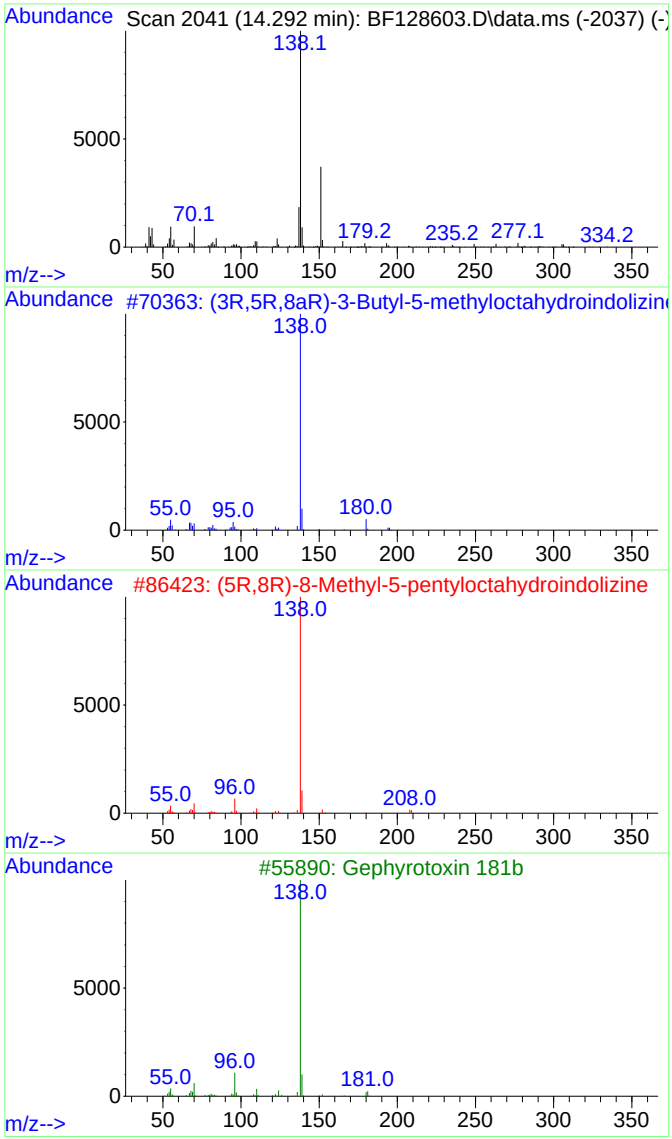
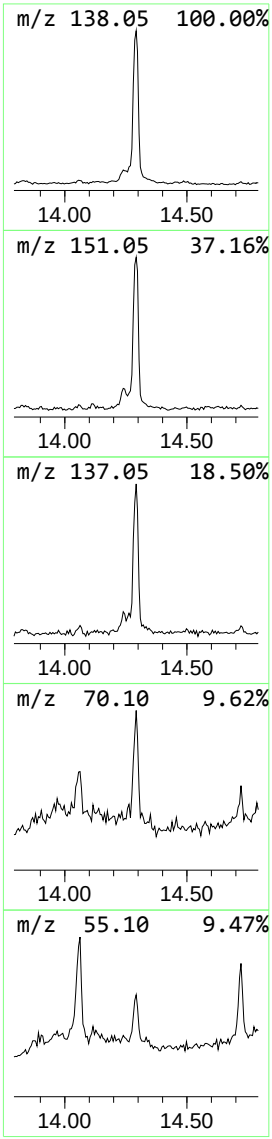
Peak Number 14 (3R,5R,8aR)-3-Butyl-5-methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.292	13.75 ng	401728	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3R,5R,8aR)-3-Butyl-5-methylocta...	195	C13H25N	053447-41-9	52
2	(5R,8R)-8-Methyl-5-pentyloctahyd...	209	C14H27N	117959-79-2	50
3	Gephyrotoxin 181b	181	C12H23N	120030-08-2	50
4	N-(tert-Butyl)-1-cyclopropyl-2-m...	238	C13H22N2O2	1000458-30-5	50
5	2,5-Cyclohexadiene-1,4-dione, 2-...	138	C7H6O3	000615-91-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128603.D
Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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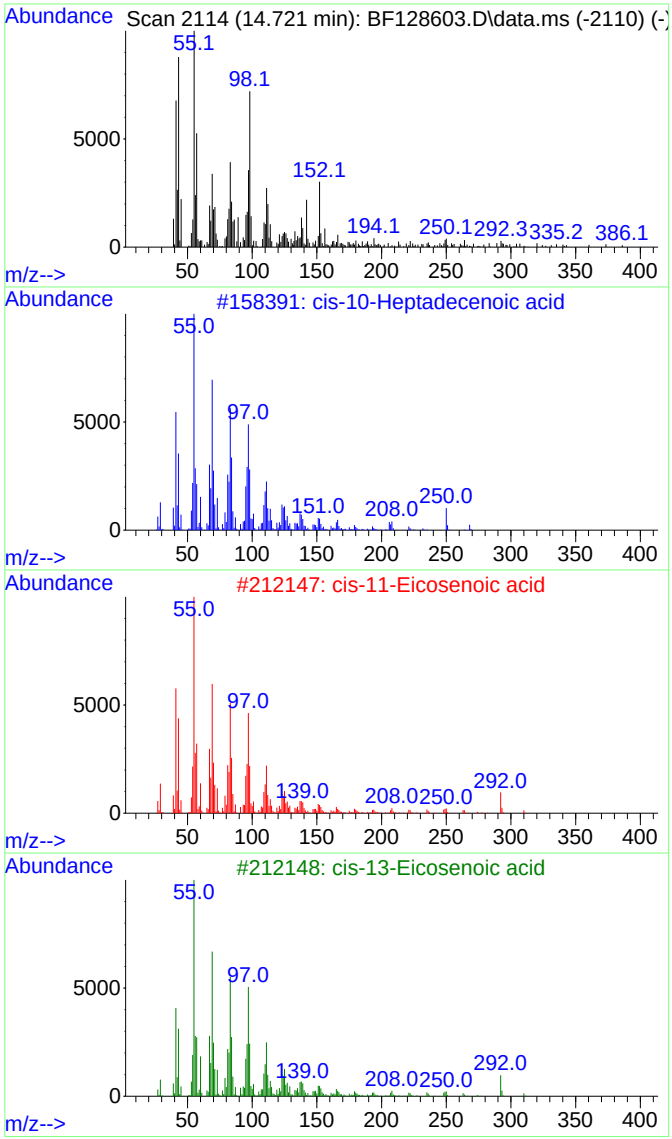
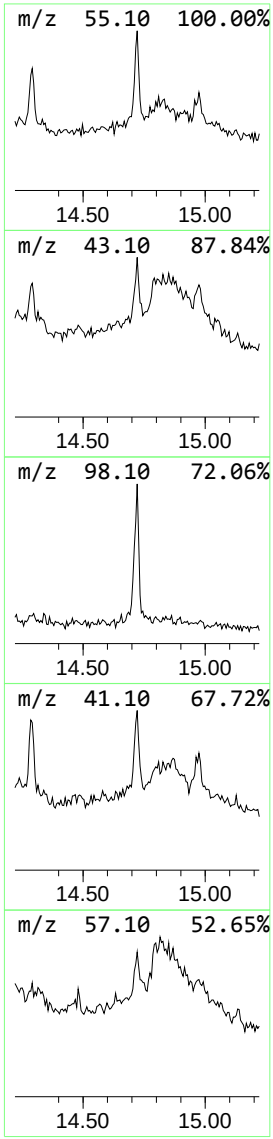
Peak Number 15 cis-10-Heptadecenoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	10.07 ng	294165	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-10-Heptadecenoic acid	268	C17H32O2	029743-97-3	70
2	cis-11-Eicosenoic acid	310	C20H38O2	005561-99-9	66
3	cis-13-Eicosenoic acid	310	C20H38O2	017735-94-3	64
4	cis-10-Nonadecenoic acid	296	C19H36O2	073033-09-7	62
5	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
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Acq On : 31 May 2022 19:28
Operator : CG\JU
Sample : N3109-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BB-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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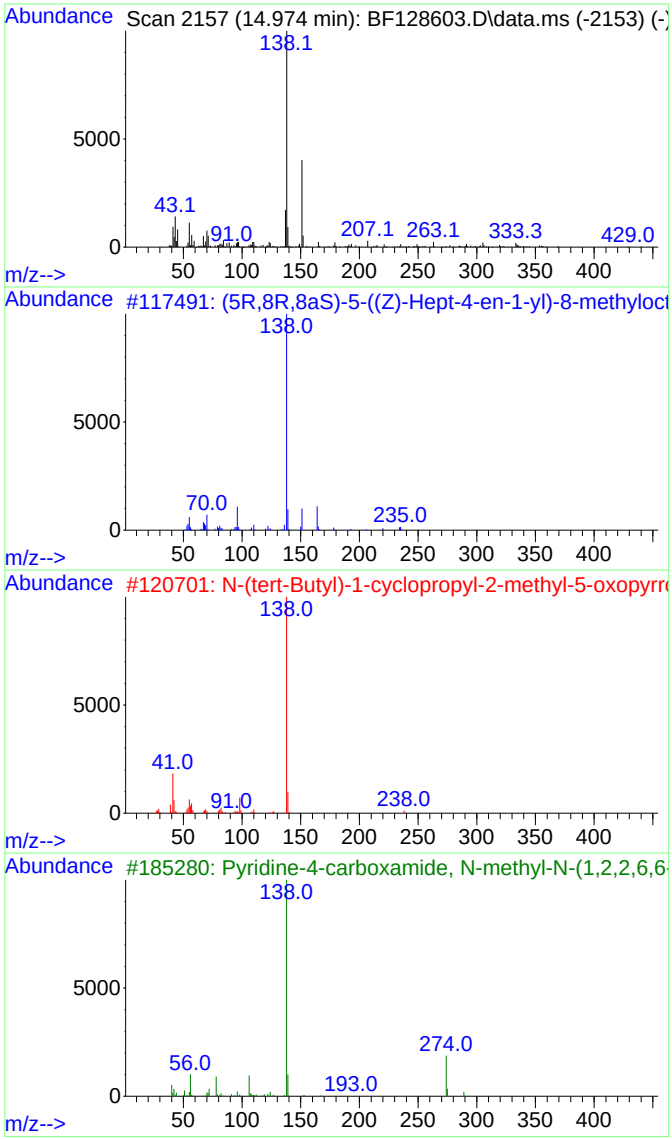
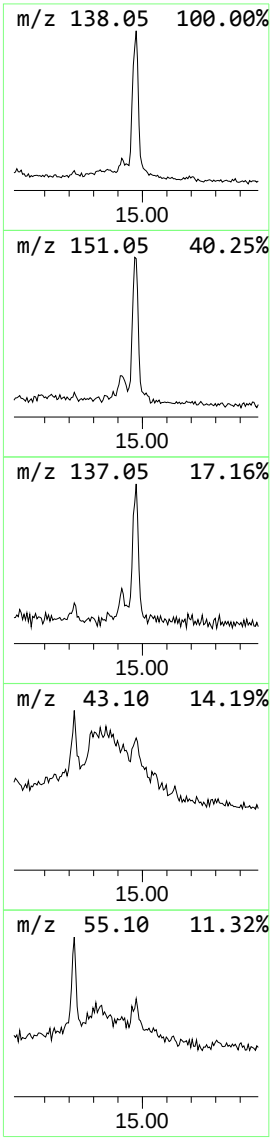
Peak Number 16 unknown14.974 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	16.91 ng	393291	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(5R,8R,8aS)-5-((Z)-Hept-4-en-1-y...	235	C16H29N	109175-47-5	47
2	N-(tert-Butyl)-1-cyclopropyl-2-m...	238	C13H22N2O2	1000458-30-5	43
3	Pyridine-4-carboxamide, N-methyl...	289	C17H27N3O	1000261-12-9	43
4	Gephyrotoxin 195b'	195	C13H25N	1000116-01-4	43
5	l-Alanine, N-(2-furoyl)-, octade...	435	C26H45NO4	1000314-29-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128603.D
Acq On : 31 May 2022 19:28
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ClientSampleId :
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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
unknown10.780	10.780	2.9	ng	100181	4	11.368	697634	20.0
unknown11.016	11.016	3.5	ng	122778	4	11.368	697634	20.0
unknown11.933	11.933	4.1	ng	143189	4	11.368	697634	20.0
unknown11.986	11.986	5.1	ng	177091	4	11.368	697634	20.0
unknown12.045	12.045	2.4	ng	83928	4	11.368	697634	20.0
unknown12.098	12.098	2.8	ng	99123	4	11.368	697634	20.0
unknown12.133	12.133	5.5	ng	189975	4	11.368	697634	20.0
unknown12.574	12.574	19.1	ng	665193	4	11.368	697634	20.0
1H-Imidazole, 2...	12.710	5.3	ng	154629	5	14.009	584308	20.0
unknown13.351	13.351	13.2	ng	384407	5	14.009	584308	20.0
unknown13.598	13.598	31.1	ng	909823	5	14.009	584308	20.0
Myristoyl chloride	14.063	13.4	ng	391351	5	14.009	584308	20.0
Triphenylphosph...	14.115	10.5	ng	306619	5	14.009	584308	20.0
(3R,5R,8aR)-3-B...	14.292	13.8	ng	401728	5	14.009	584308	20.0
cis-10-Heptadec...	14.721	10.1	ng	294165	5	14.009	584308	20.0
unknown14.974	14.974	16.9	ng	393291	6	15.486	465205	20.0