LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124645.D
Acq On : 21 Jul 2021 00:53
Operator : JU/CG
Sample : M3089-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAR-N2-(A-D)-(0-12)

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	20	23	27	rBB	10890	12976	6.86%	1.059%
2	5.134	515	518	522	rBB	2913	3015	1.59%	0.246%
3	5.522	579	584	586	rBB	149600	147486	78.02%	12.041%
4	6.522	749	754	757	rBB	144641	153554	81.23%	12.536%
5	6.904	816	819	821	rBB	48175	38460	20.35%	3.140%
6	7.463	909	914	917	rBB	101706	100538	53.19%	8.208%
7	8.086	1016	1020	1023	rBB	72170	56557	29.92%	4.617%
8	8.186	1033	1037	1040	rBB	71919	53182	28.13%	4.342%
9	9.263	1216	1220	1223	rBV	237129	189033	100.00%	15.433%
10	9.945	1332	1336	1339	rBB	71815	57328	30.33%	4.680%
11	10.516	1426	1433	1434	rBV4	1568	3216	1.70%	0.263%
12	10.610	1448	1449	1453	rBV3	2009	2584	1.37%	0.211%
13	10.733	1466	1470	1472	rBV	106789	97072	51.35%	7.925%
14	10.857	1489	1491	1494	rVB3	3589	3416	1.81%	0.279%
15	10.892	1494	1497	1499	rBV4	4565	4415	2.34%	0.360%
16	11.057	1523	1525	1528	rVB4	4226	2529	1.34%	0.206%
17	11.280	1561	1563	1566	rBV4	3268	3874	2.05%	0.316%
18	11.433	1586	1589	1591	rBV	62658	50039	26.47%	4.085%
19	11.821	1653	1655	1658	rVB3	9250	6278	3.32%	0.513%
20	11.951	1675	1677	1680	rVB2	19805	17783	9.41%	1.452%
21	12.263	1728	1730	1732	rVV3	5884	5467	2.89%	0.446%
22	12.310	1736	1738	1741	rBV4	4288	4839	2.56%	0.395%
23	12.645	1793	1795	1798	rVB	7548	5832	3.09%	0.476%
24	12.733	1808	1810	1815	rBV5	7943	10399	5.50%	0.849%
25	13.016	1855	1858	1862	rVB	119497	108616	57.46%	8.868%
26	13.080	1867	1869	1874	rVB4	4423	5890	3.12%	0.481%
27	13.674	1968	1970	1972	rBV3	2572	2376	1.26%	0.194%
28	13.910	2005	2010	2018	rBV5	8079	13945	7.38%	1.138%
29	14.068	2034	2037	2040	rVB	33197	26055	13.78%	2.127%
30	14.374	2084	2089	2091	rBV5	2082	2648	1.40%	0.216%
31	14.927	2179	2183	2186	rBV	4748	4890	2.59%	0.399%
32	14.992	2191	2194	2198	rVB2	2040	2914	1.54%	0.238%
33	15.192	2223	2228	2231	rBV	1973	3328	1.76%	0.272%
34	15.557	2284	2290	2293	rBV2	21443	24337	12.87%	1.987%

Sum of corrected areas: 1224871

Instrument :
BNA_F
ClientSampleId :
PAR-N2-(A-D)-(0-12)

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Instrument :
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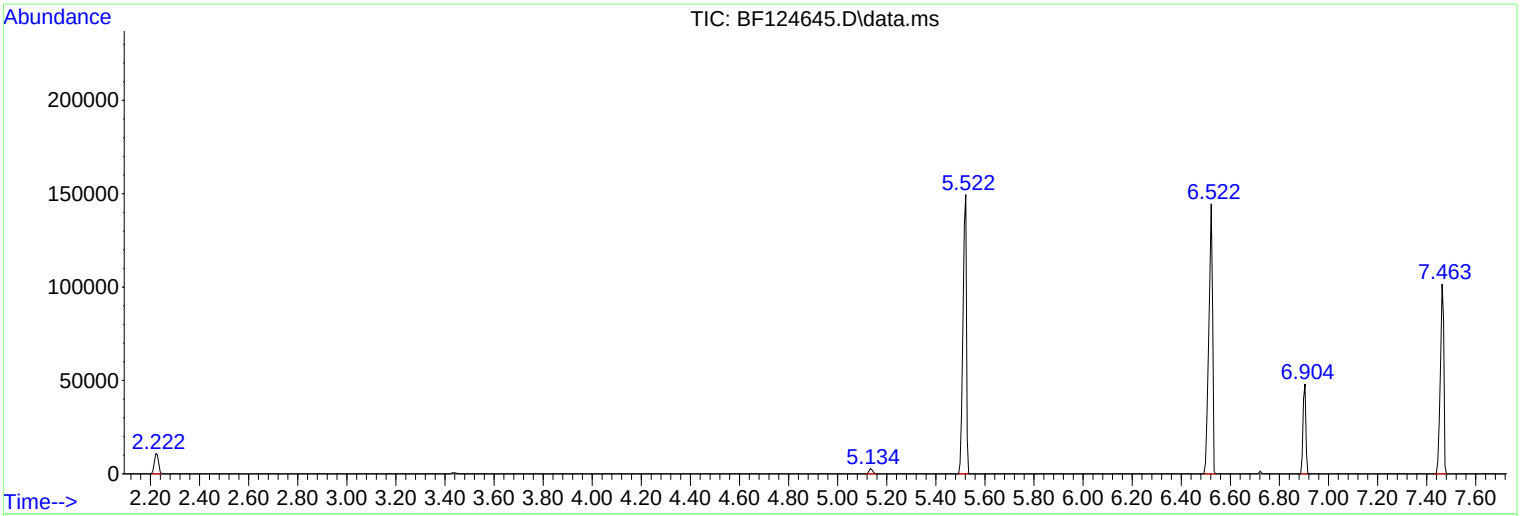
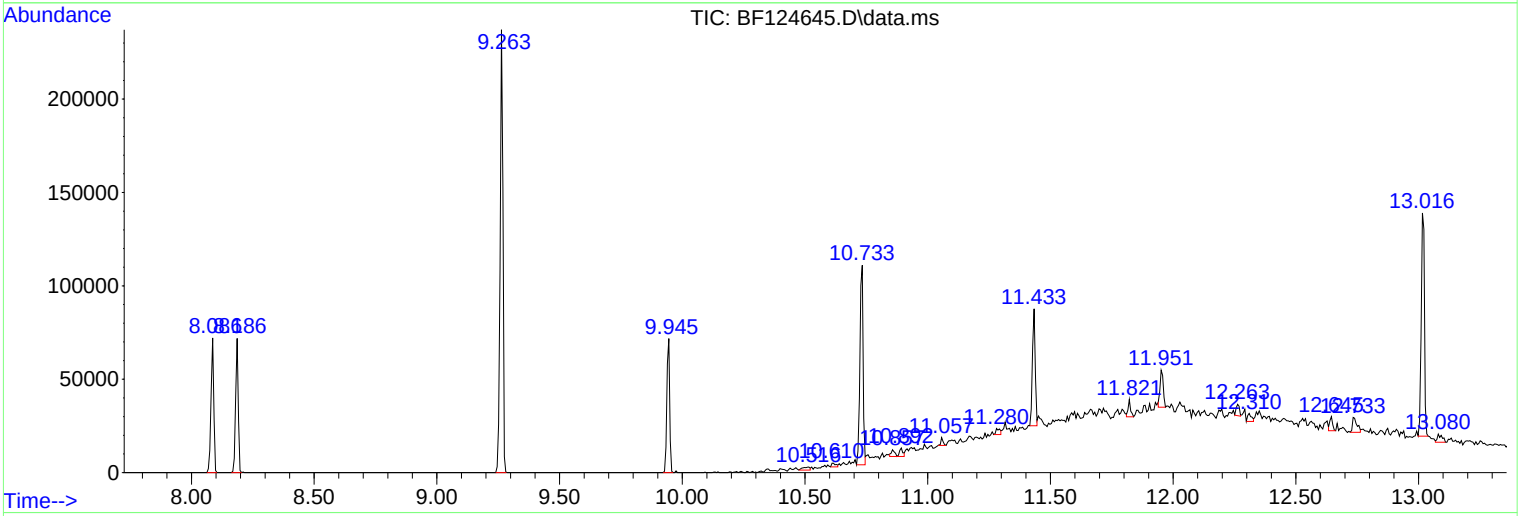
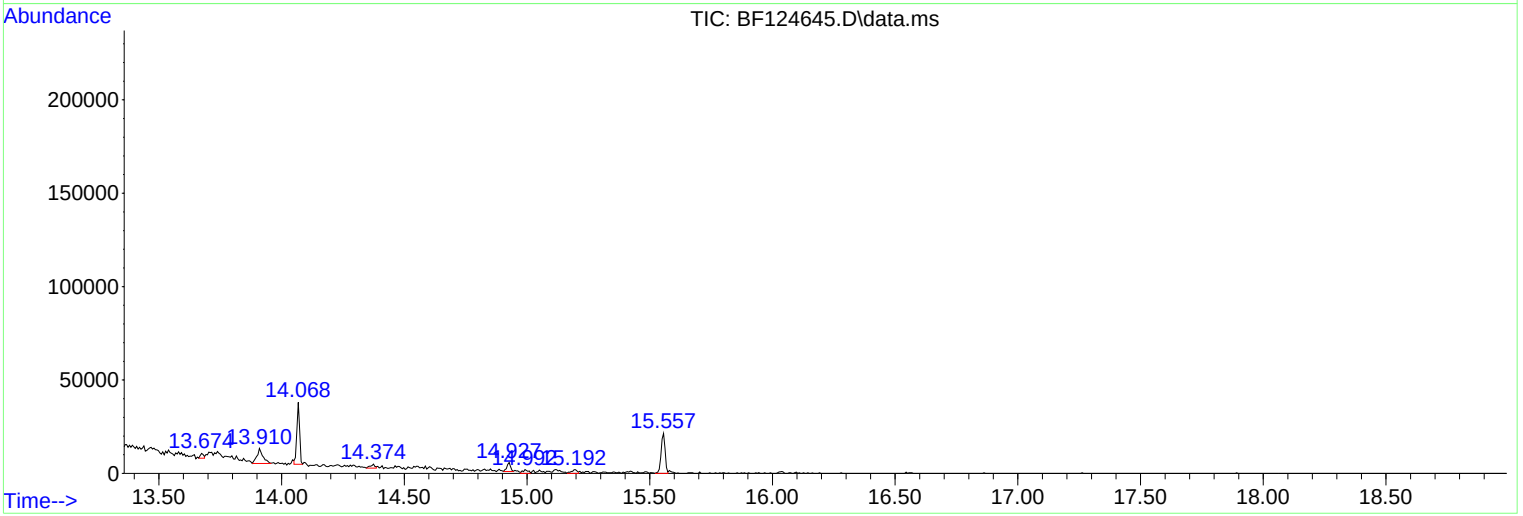
ClientSampleId :
PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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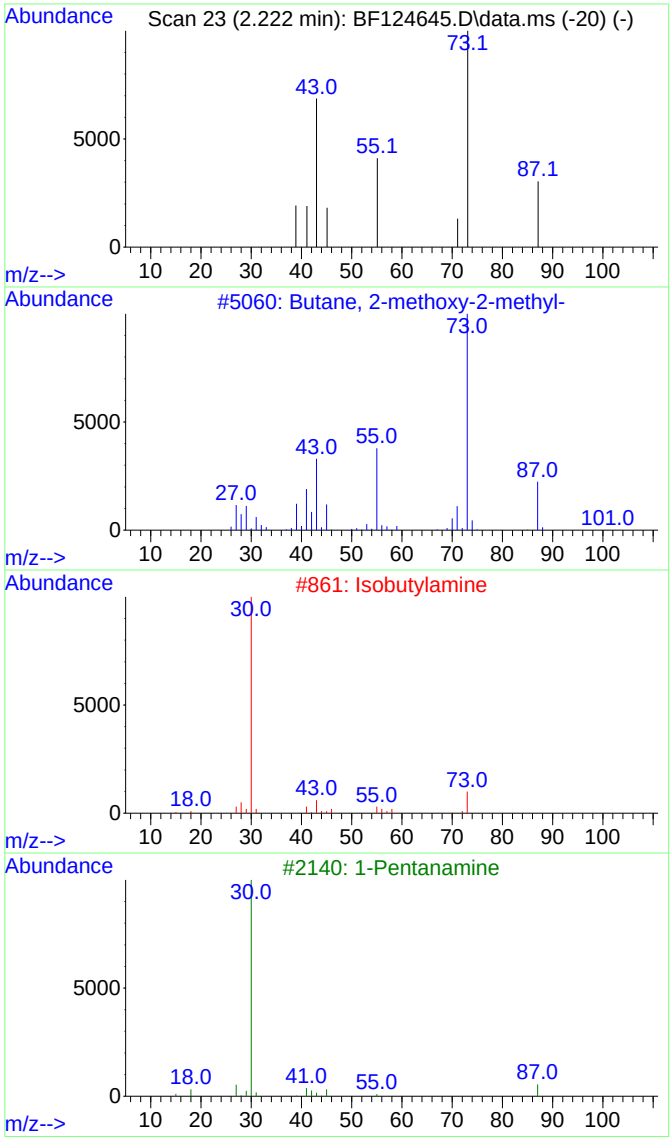
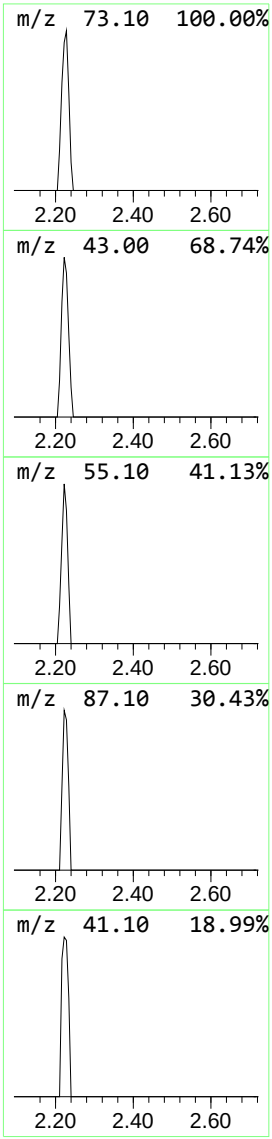
Peak Number 1 unknown2.222 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	6.75 ng	12976	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2	Isobutylamine	73	C4H11N	000078-81-9	4
3	1-Pentanamine	87	C5H13N	000110-58-7	4
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	2





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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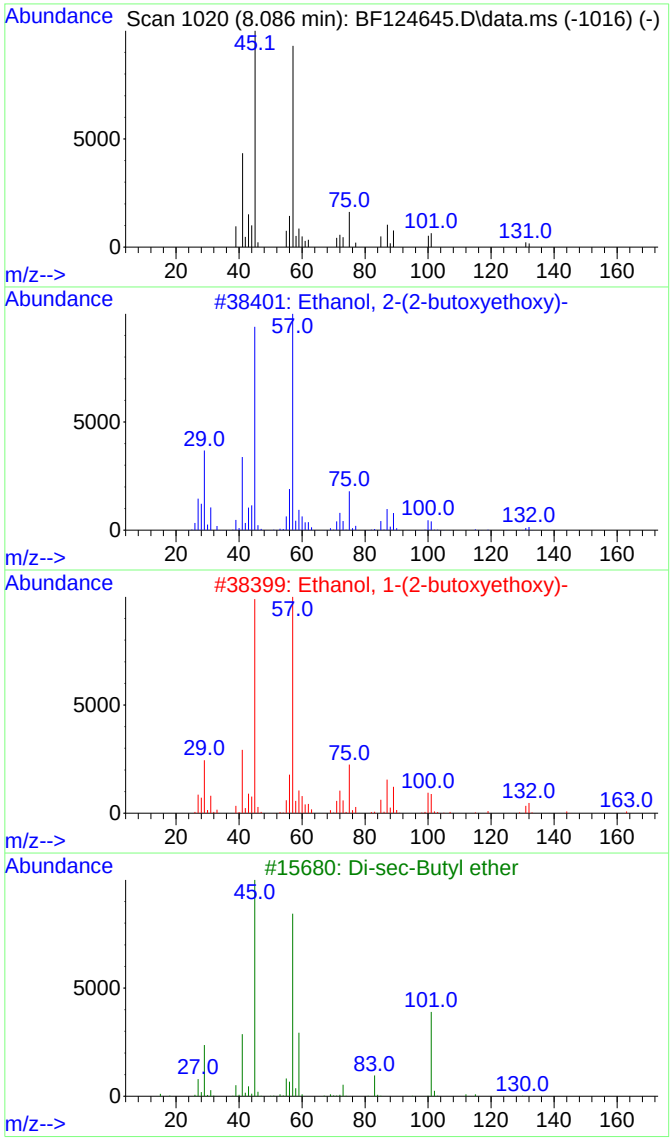
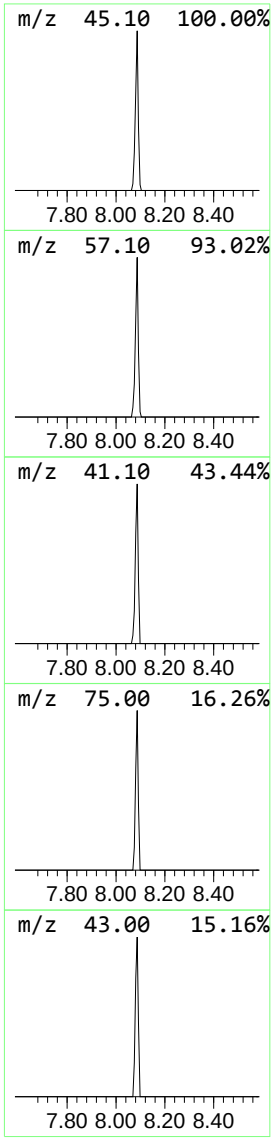
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.086	21.27 ng	56557	Naphthalene-d8	8.186

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	83
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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TIC Integration Parameters: LSCINT.P

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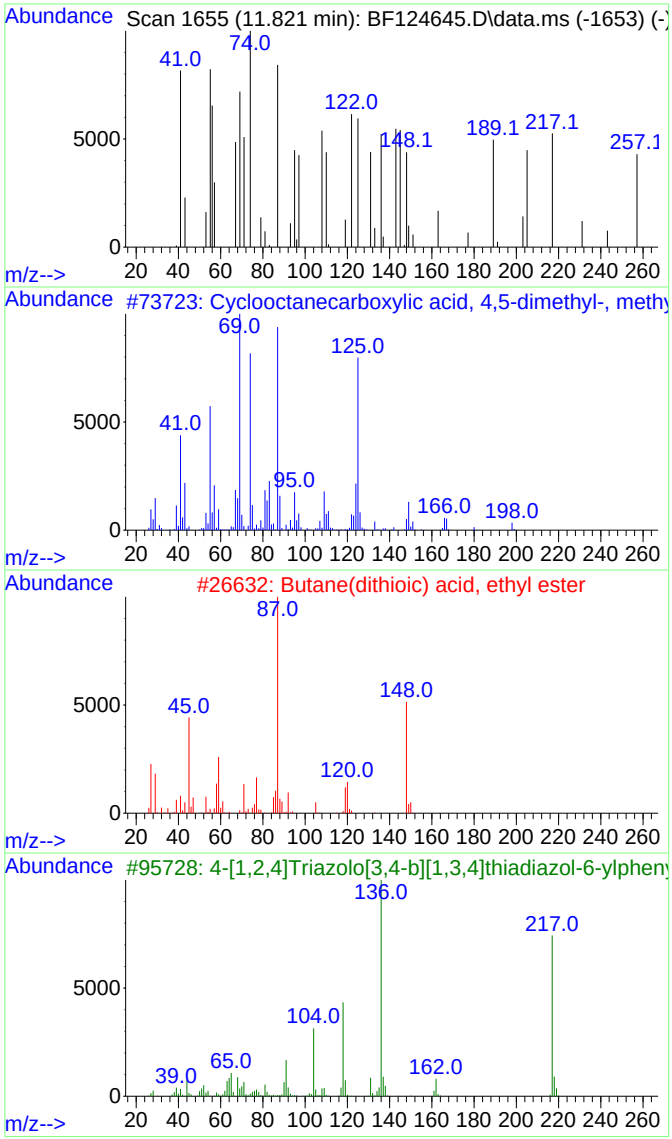
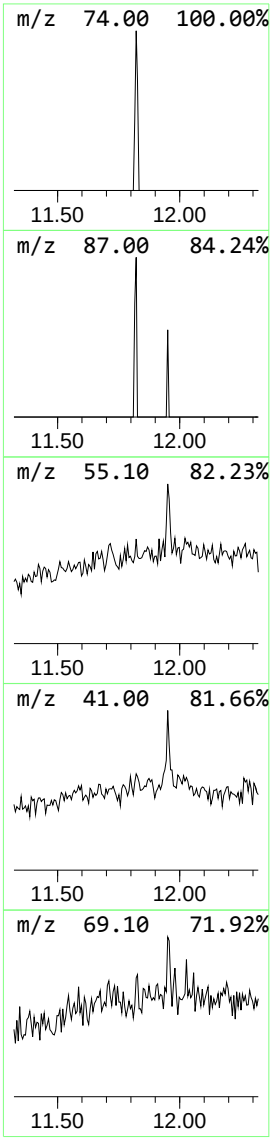
Peak Number 3 unknown11.822 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	2.51 ng	6278	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctanecarboxylic acid, 4,5-...	198	C12H22O2	061141-73-9	10
2	Butane(dithioic) acid, ethyl ester	148	C6H12S2	000924-75-4	9
3	4-[1,2,4]Triazolo[3,4-b][1,3,4]t...	217	C9H7N5S	797767-52-3	9
4	3-methyl-6,7-methylenedioxyisoqu...	217	C11H7NO4	1010371-51-6	9
5	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	9





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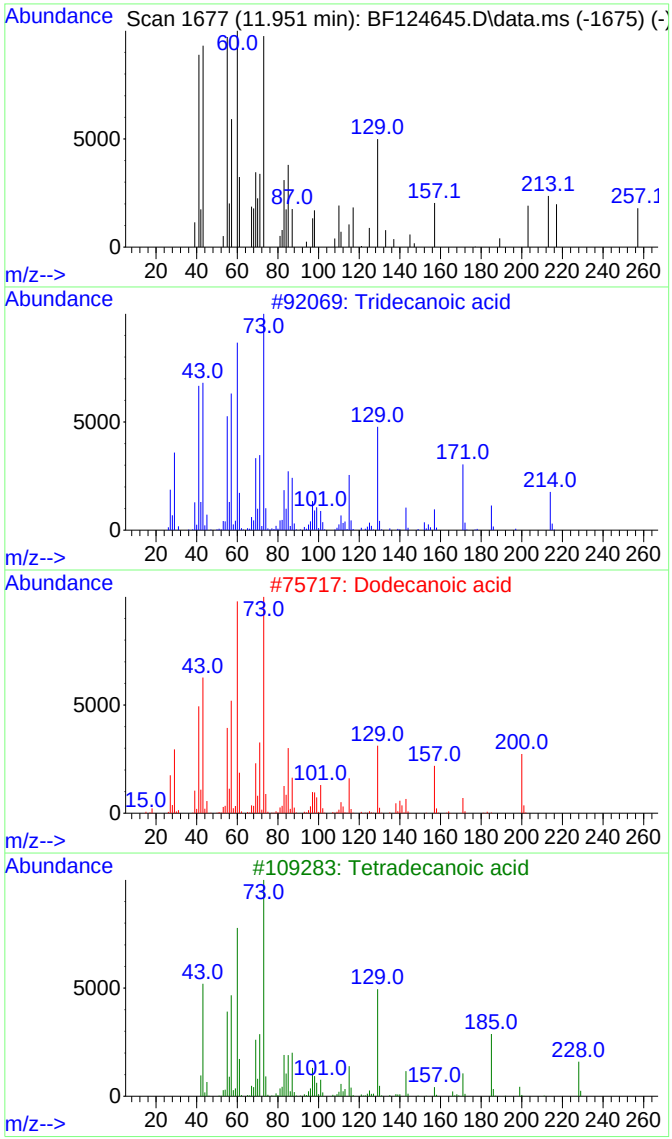
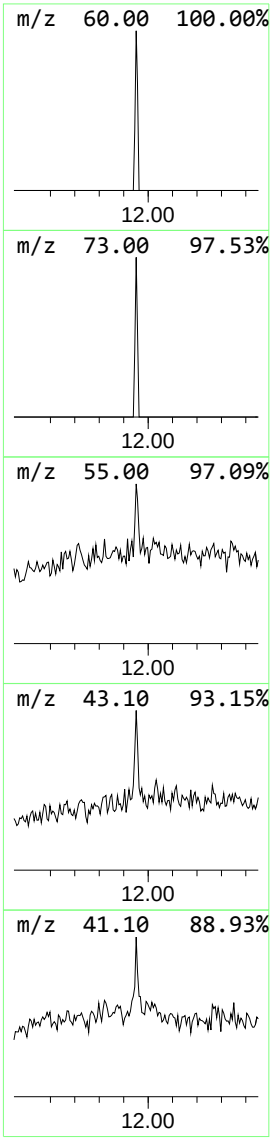
Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	7.11 ng	17783	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	50
2	Dodecanoic acid	200	C12H24O2	000143-07-7	47
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





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Instrument :
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ClientSampleId :
PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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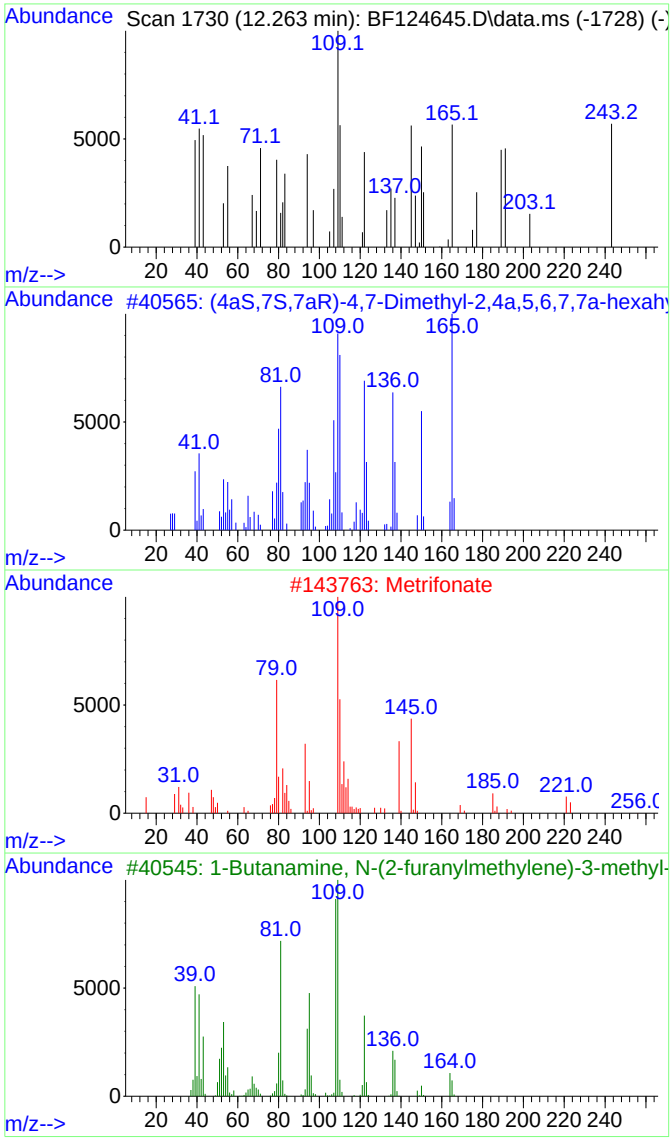
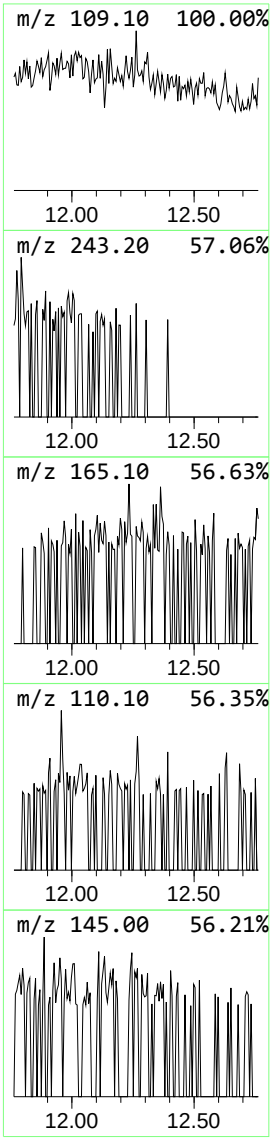
Peak Number 5 unknown12.263 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.263	2.19 ng	5467	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4aS,7S,7aR)-4,7-Dimethyl-2,4a,5...	165	C10H15NO	115421-73-3	38
2	Metrifonate	256	C4H8Cl3O4P	000052-68-6	12
3	1-Butanamine, N-(2-furanylmethyl...	165	C10H15NO	052074-26-7	10
4	2,6-Piperidinedicarbonitrile, N-...	149	C8H11N3	090090-68-9	9
5	2-Amino-4-methylpyrimidine	109	C5H7N3	000108-52-1	9





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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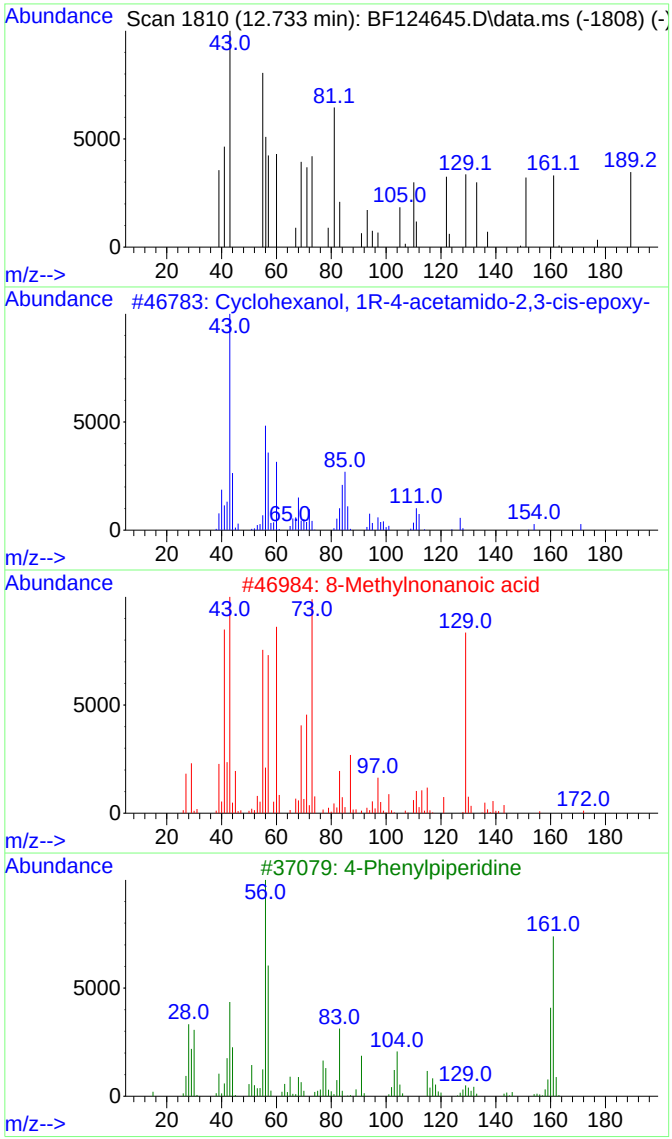
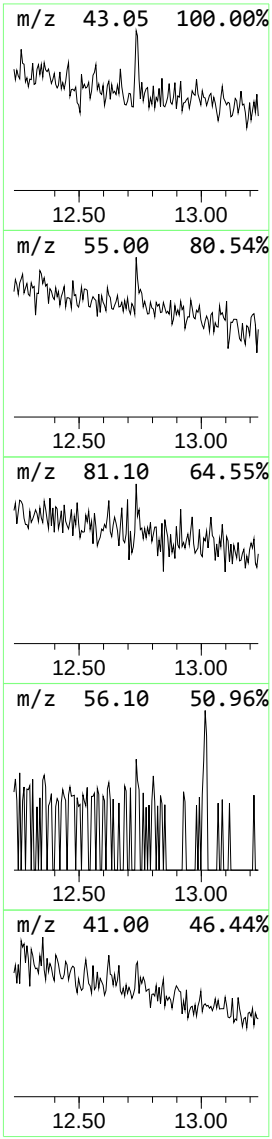
Peak Number 6 unknown12.733 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	4.16 ng	10399	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 1R-4-acetamido-2,3...	171	C8H13NO3	077803-84-0	12
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	10
3	4-Phenylpiperidine	161	C11H15N	000771-99-3	9
4	4-Heptanol, 2,6-dimethyl-, acetate	186	C11H22O2	010250-45-0	9
5	Cyclopentane, 2-ethyl-1,1-dimethyl-	126	C9H18	054549-80-3	9





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TIC Library : C:\Database\NIST20.L
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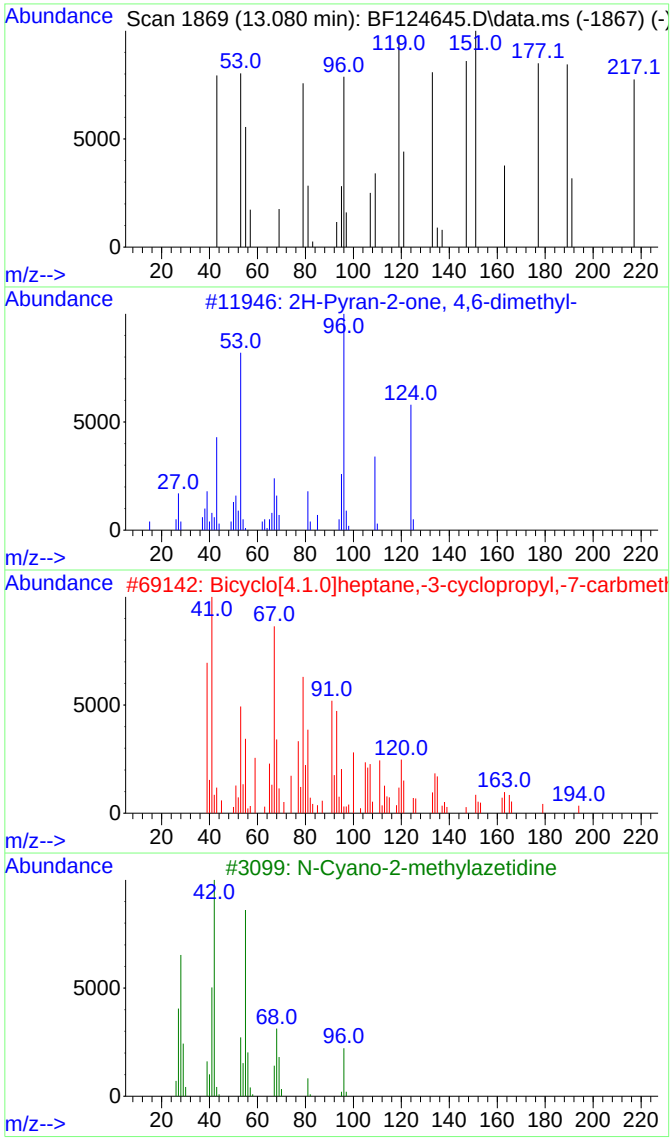
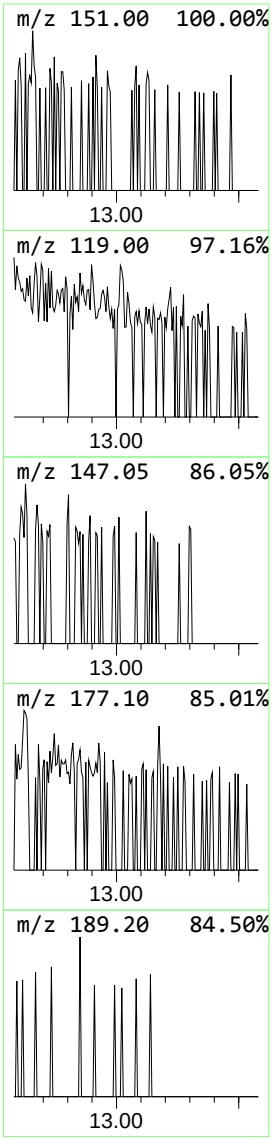
Peak Number 7 unknown13.080 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.080	4.52 ng	5890	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one, 4,6-dimethyl-	124	C7H8O2	000675-09-2	12
2	Bicyclo[4.1.0]heptane,-3-cyclopr...	194	C12H18O2	1000222-97-0	10
3	N-Cyano-2-methylazetidine	96	C5H8N2	042364-46-5	9
4	Bicyclo[3.3.1]non-6-en-2-one oxime	151	C9H13NO	1000186-04-7	9
5	Modephene	204	C15H24	068269-87-4	9





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TIC Library : C:\Database\NIST20.L
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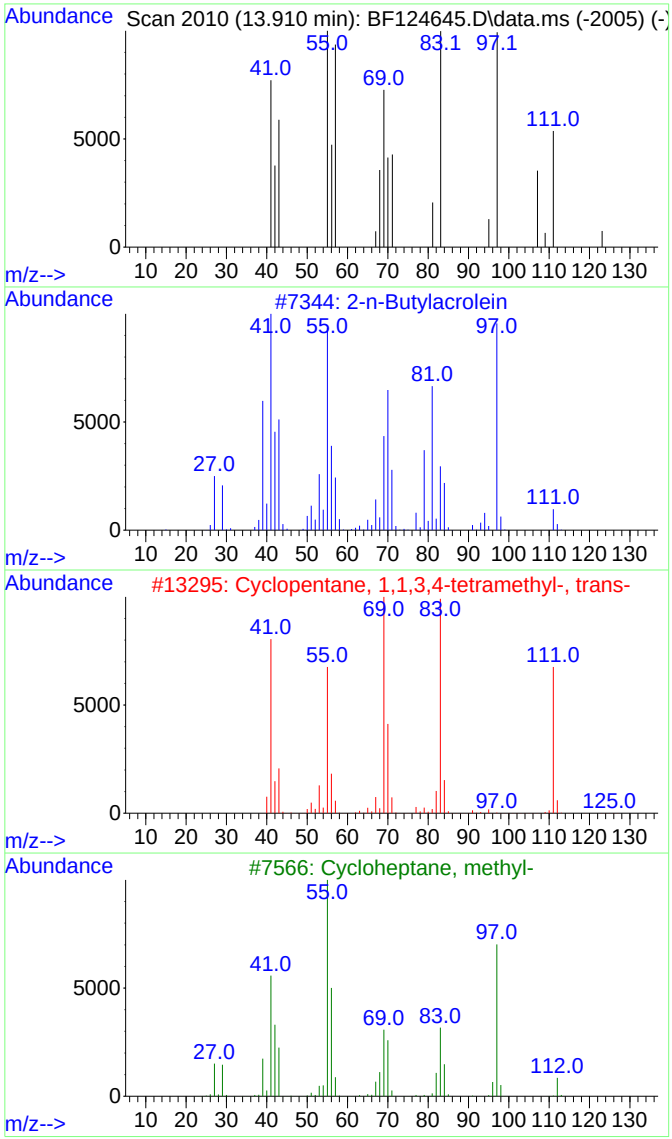
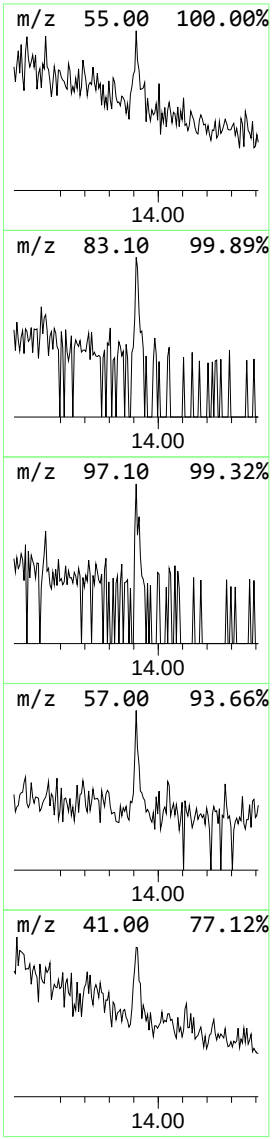
Peak Number 8 unknown13.910 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	10.70 ng	13945	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-n-Butylacrolein	112	C7H12O	001070-66-2	35
2	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	35
3	Cycloheptane, methyl-	112	C8H16	004126-78-7	32
4	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	32
5	2-Heptenal, (E)-	112	C7H12O	018829-55-5	32





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Instrument :
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PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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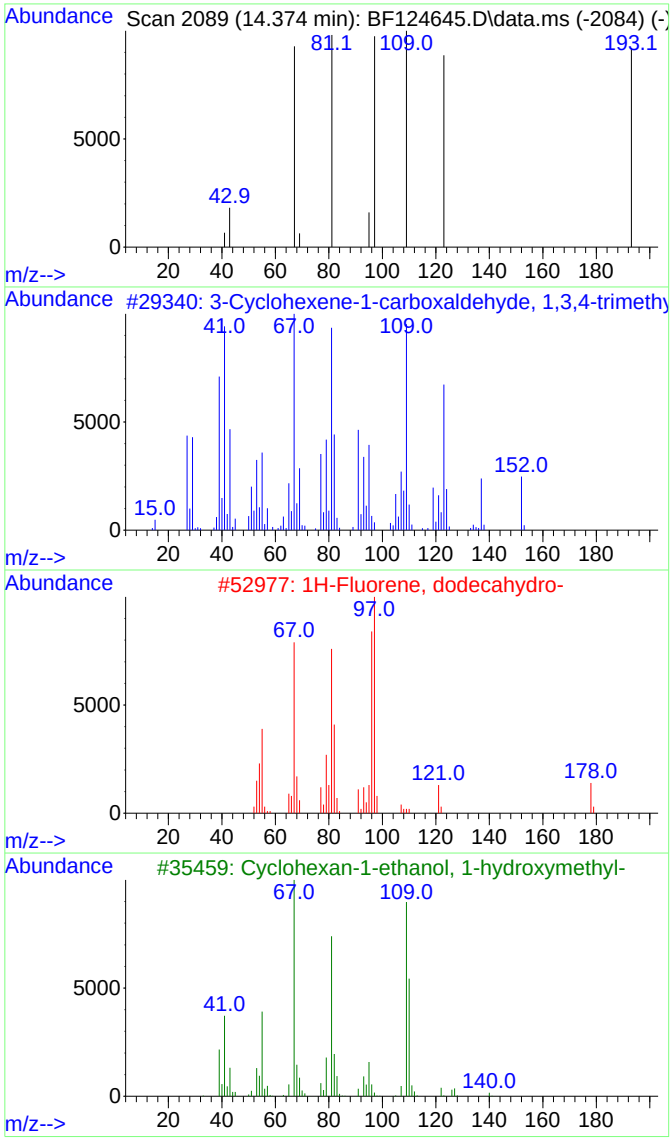
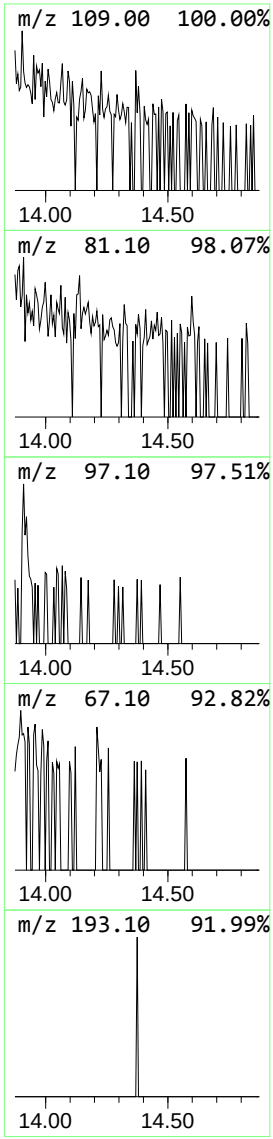
Peak Number 9 unknown14.374 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.374	2.03 ng	2648	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	33
2	1H-Fluorene, dodecahydro-	178	C13H22	005744-03-6	23
3	Cyclohexan-1-ethanol, 1-hydroxym...	158	C9H18O2	003187-28-8	23
4	Propanal, 3-cyclohexylidene-2-me...	152	C10H16O	053155-83-2	23
5	Cyclopentaneacetaldehyde, 2-form...	166	C10H14O2	005951-57-5	9





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Data File : BF124645.D
Acq On : 21 Jul 2021 00:53
Operator : JU/CG
Sample : M3089-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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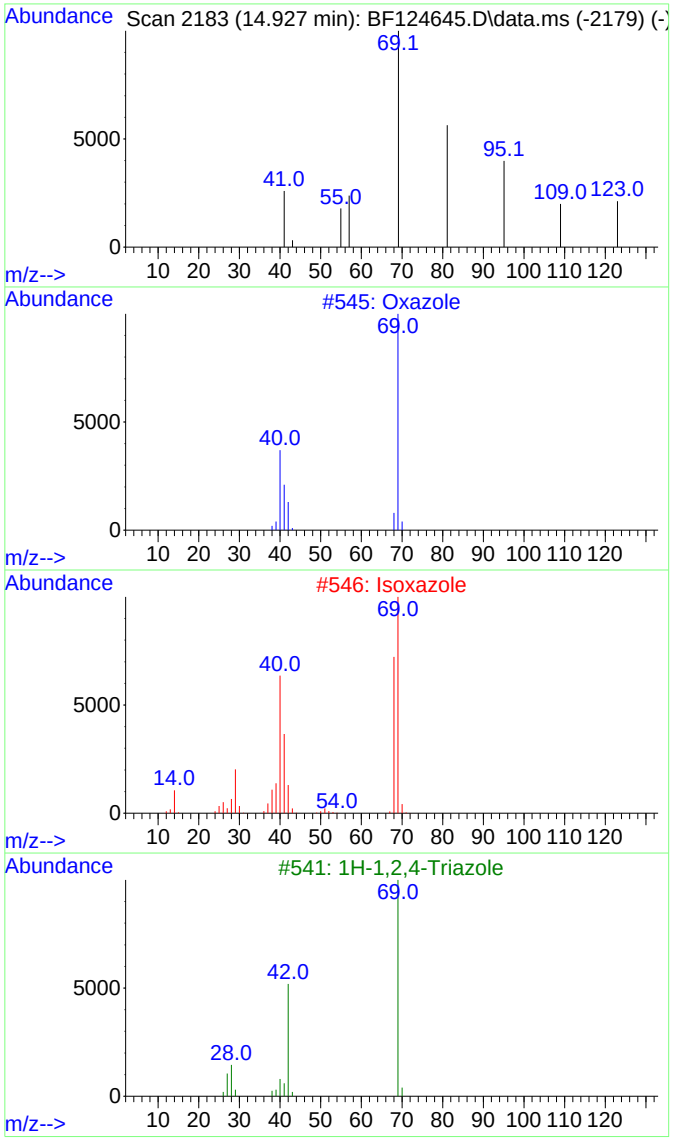
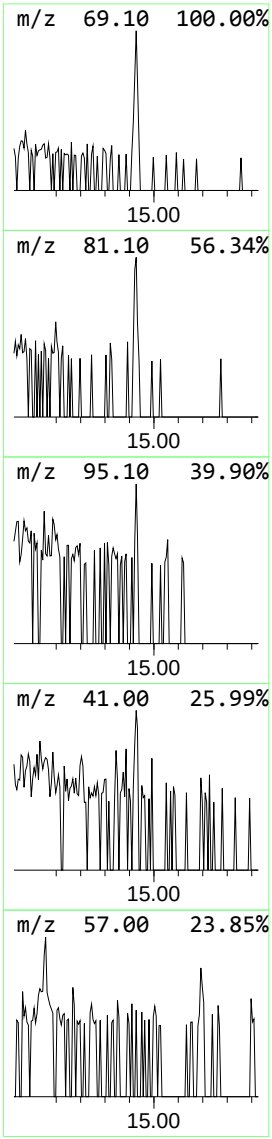
Peak Number 10 unknown14.927 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	4.02 ng	4890	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole	69	C3H3NO	000288-42-6	3
2	Isoxazole	69	C3H3NO	000288-14-2	3
3	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	3
4	2,4-Dodecadienal	180	C12H20O	013162-47-5	2
5	2,4-Dodecadienal, (E,E)-	180	C12H20O	021662-16-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124645.D
Acq On : 21 Jul 2021 00:53
Operator : JU/CG
Sample : M3089-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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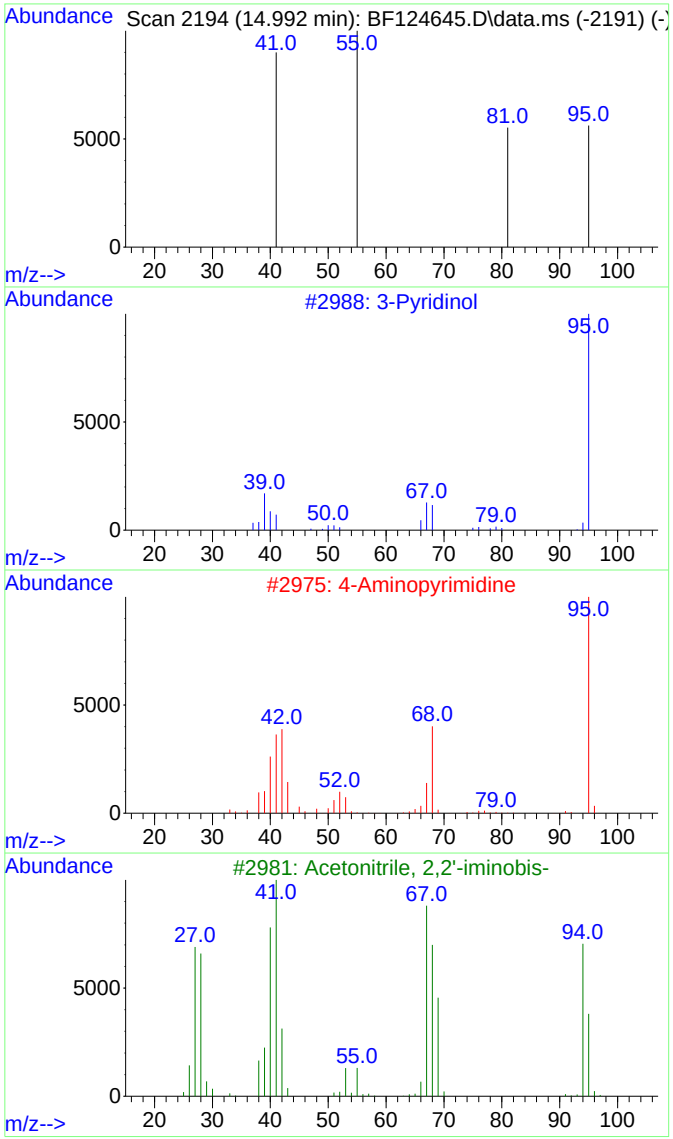
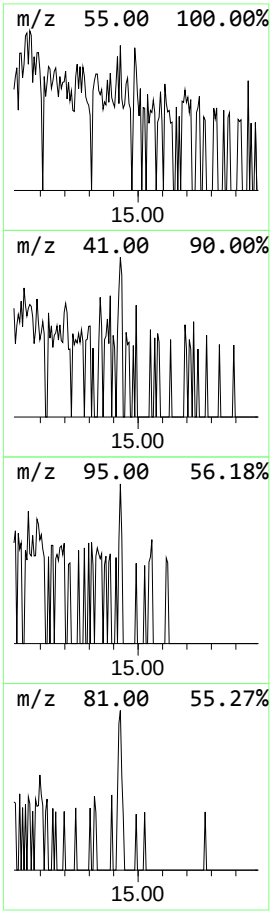
Peak Number 11 unknown14.992 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	2.39 ng	2914	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyridinol	95	C5H5NO	000109-00-2	2
2	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
3	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	2
4	Ethyl isocyanide	55	C3H5N	000624-79-3	1
5	1,5-Heptadiene, 2-methyl-, (Z)-	110	C8H14	041044-64-8	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124645.D
Acq On : 21 Jul 2021 00:53
Operator : JU/CG
Sample : M3089-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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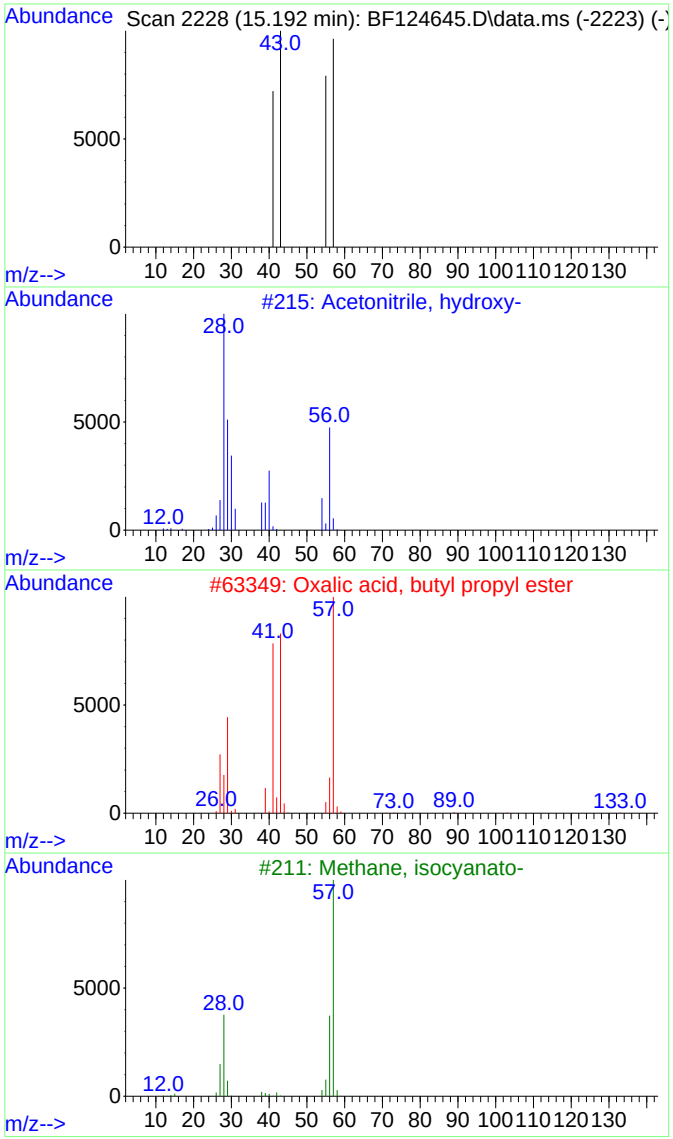
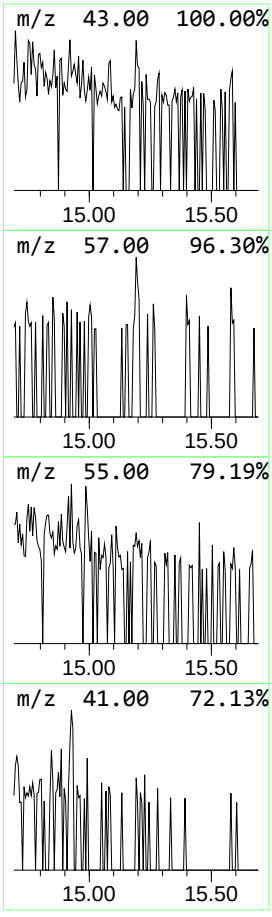
Peak Number 12 unknown15.192 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.73 ng	3328	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
2	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	2
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4	Ethyl isocyanide	55	C3H5N	000624-79-3	1
5	Azetidine	57	C3H7N	000503-29-7	1





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124645.D
Acq On : 21 Jul 2021 00:53
Operator : JU/CG
Sample : M3089-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAR-N2-(A-D)-(0-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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
unknown2.222	2.222	6.8	ng	12976	1	6.904	38460	20.0
Ethanol, 2-(2-b...	8.086	21.3	ng	56557	2	8.186	53182	20.0
unknown11.822	11.822	2.5	ng	6278	4	11.433	50039	20.0
Tridecanoic acid	11.951	7.1	ng	17783	4	11.433	50039	20.0
unknown12.263	12.263	2.2	ng	5467	4	11.433	50039	20.0
unknown12.733	12.733	4.2	ng	10399	4	11.433	50039	20.0
unknown13.080	13.080	4.5	ng	5890	5	14.068	26055	20.0
unknown13.910	13.910	10.7	ng	13945	5	14.068	26055	20.0
unknown14.374	14.374	2.0	ng	2648	5	14.068	26055	20.0
unknown14.927	14.927	4.0	ng	4890	6	15.557	24337	20.0
unknown14.992	14.992	2.4	ng	2914	6	15.557	24337	20.0
unknown15.192	15.192	2.7	ng	3328	6	15.557	24337	20.0