LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125013.D
Acq On : 9 Aug 2021 21:34
Operator : JU/CG
Sample : M3298-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1940

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	564	567	571	rVB	32220	27394	6.43%	2.152%
2	6.445	738	741	745	rBB	37945	31462	7.38%	2.472%
3	6.816	801	804	807	rBV	42629	35671	8.37%	2.802%
4	7.228	867	874	880	rBV5	27151	40748	9.56%	3.201%
5	7.387	896	901	904	rVB	112889	98712	23.16%	7.755%
6	7.692	950	953	956	rBV	29685	31156	7.31%	2.448%
7	7.739	959	961	963	rBV	31228	33267	7.81%	2.613%
8	8.045	1011	1013	1017	rBV4	34517	33817	7.93%	2.657%
9	8.104	1017	1023	1027	rBV2	75318	106705	25.04%	8.383%
10	8.157	1029	1032	1034	rVV	30758	27490	6.45%	2.160%
11	8.187	1034	1037	1039	rBV2	22311	24847	5.83%	1.952%
12	8.339	1059	1063	1065	rBV2	33652	39454	9.26%	3.099%
13	8.398	1065	1073	1075	rBV6	56452	125960	29.55%	9.895%
14	14.763	2150	2155	2158	rVB	378555	426223	100.00%	33.484%
15	15.304	2244	2247	2250	rBV4	20178	24981	5.86%	1.962%
16	15.463	2270	2274	2280	rVB3	38438	56964	13.36%	4.475%
17	15.592	2294	2296	2301	rVB6	24509	27115	6.36%	2.130%
18	16.133	2384	2388	2398	rVB5	23213	49718	11.66%	3.906%
19	16.557	2454	2460	2467	rVB6	17008	31234	7.33%	2.454%

Sum of corrected areas: 1272918

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
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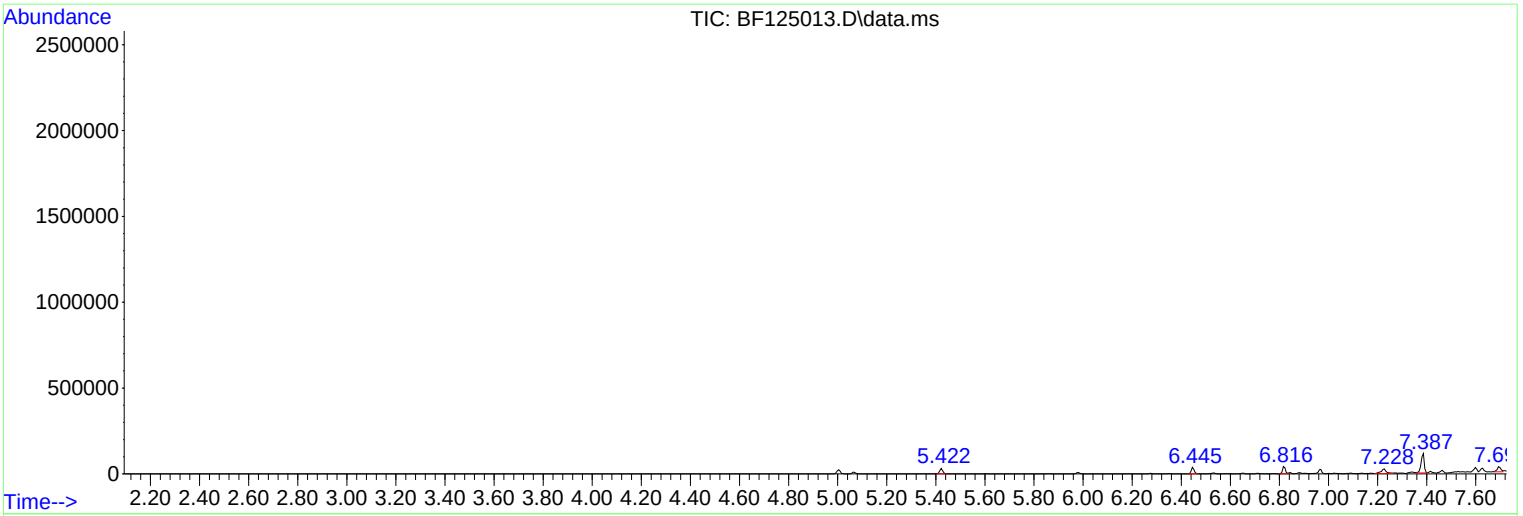
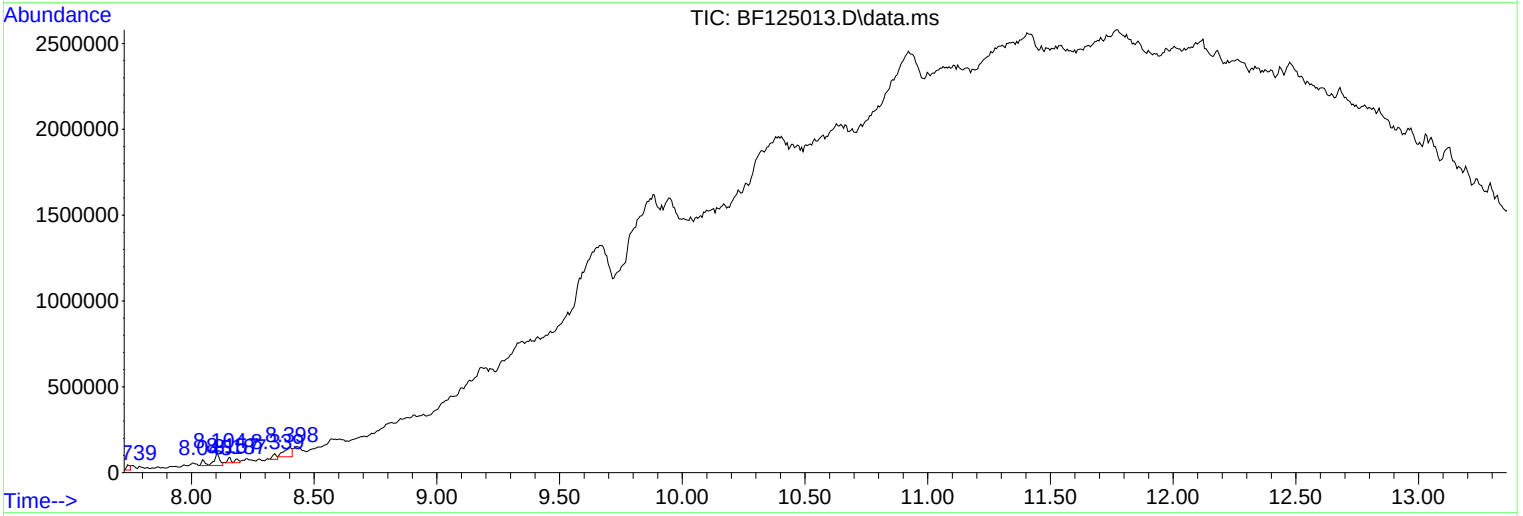
Misc :
ALS Vial : 10 Sample Multiplier: 1

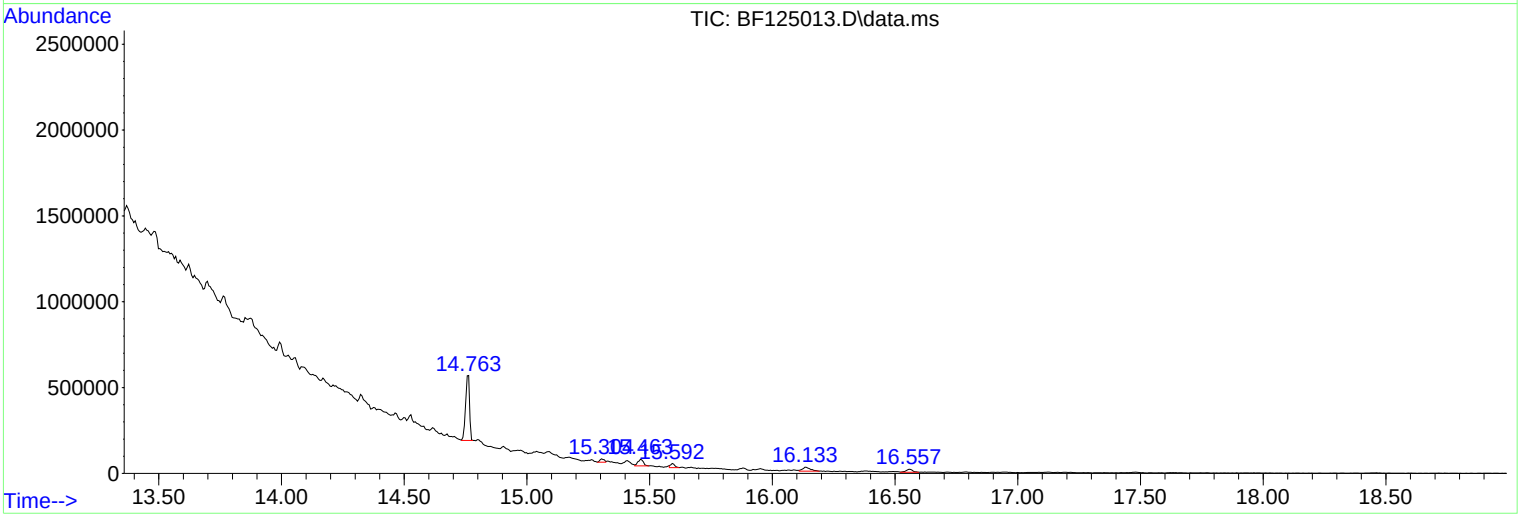
Instrument :
BNA_F
ClientSampleId :
1940

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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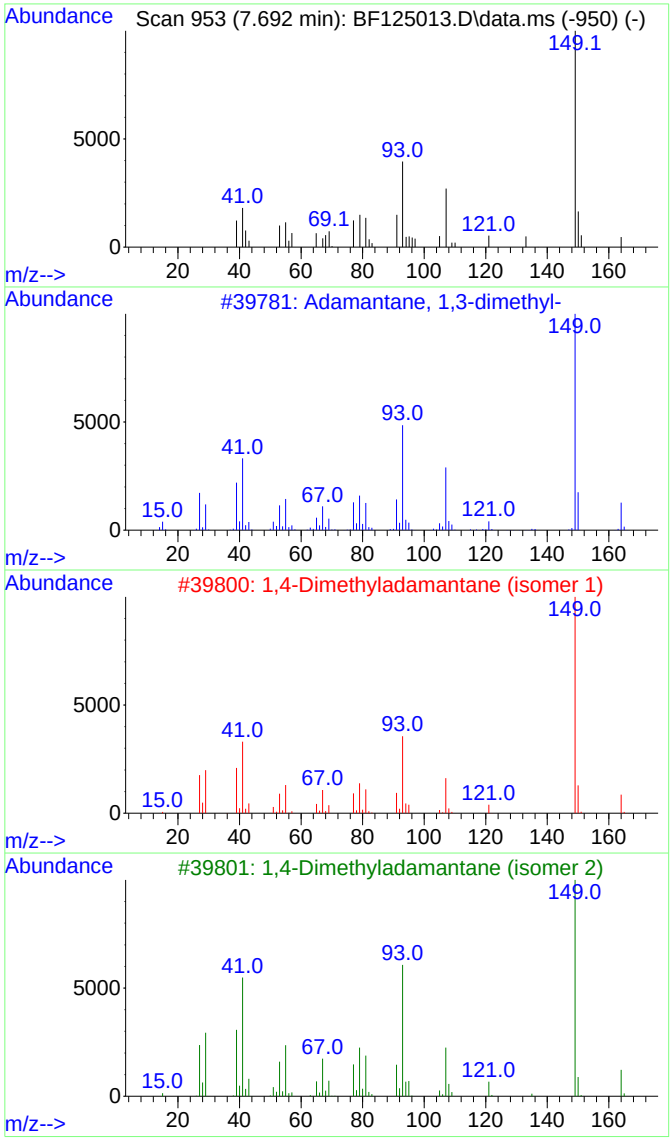
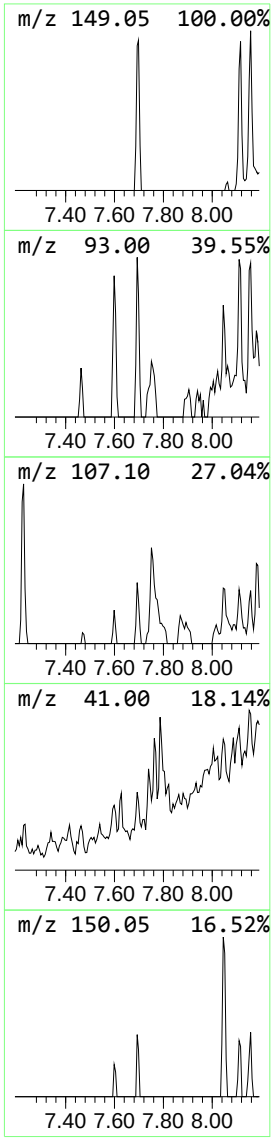
Peak Number 1 Adamantane, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.692	5.84 ng	31156	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	80
2	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	72
3	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	64
4	Added stereo to name	164	C12H20	024145-88-8	56
5	Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	53





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Misc :
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Instrument : BNA_F
ClientSampleId : 1940

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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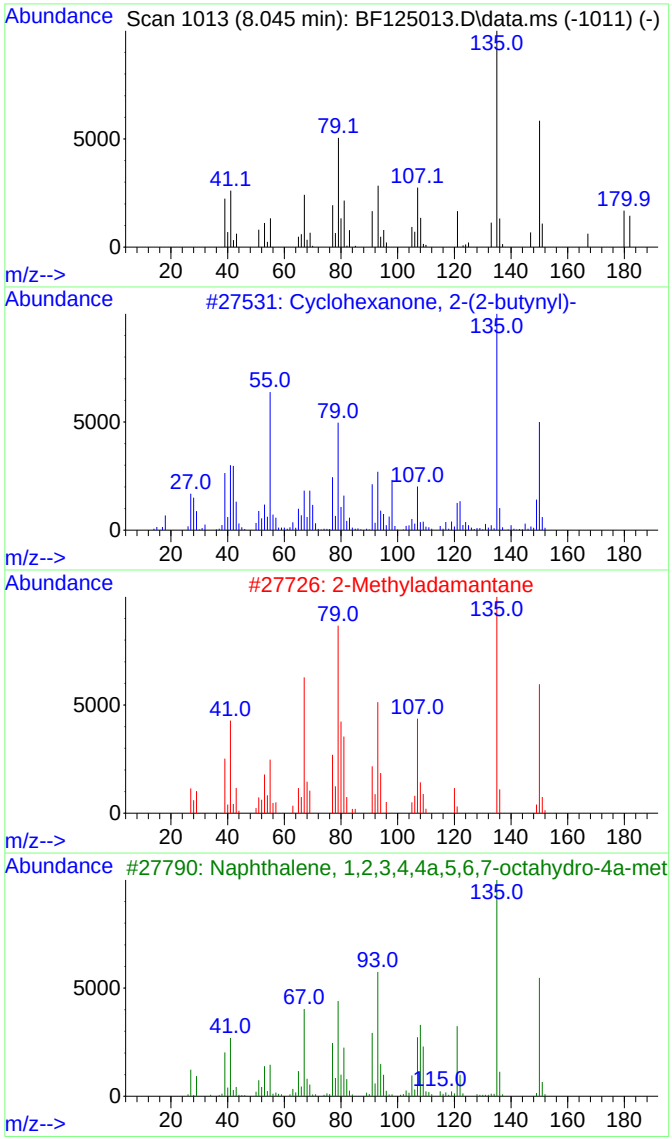
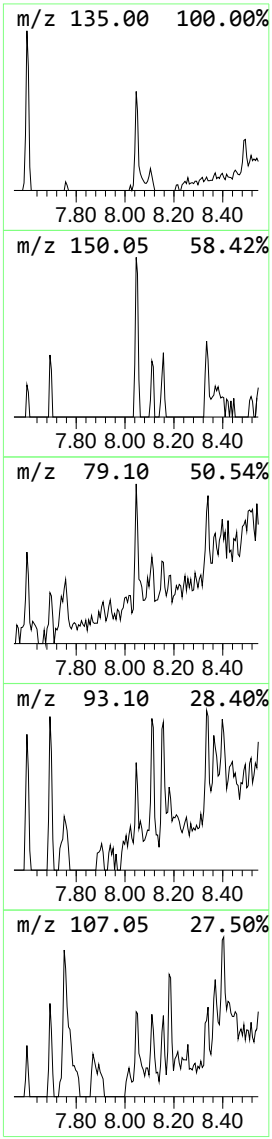
Peak Number 2 Cyclohexanone, 2-(2-butynyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.045	6.34 ng	33817	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2-(2-butynyl)-	150	C10H14O	054166-48-2	87
2	2-Methyladamantane	150	C11H18	000700-56-1	74
3	Naphthalene, 1,2,3,4,4a,5,6,7-oc...	150	C11H18	013943-77-6	72
4	3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	72
5	p-Cymen-7-ol	150	C10H14O	000536-60-7	64





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Operator : JU/CG
Sample : M3298-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1940

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
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TIC Library : C:\Database\NIST20.L
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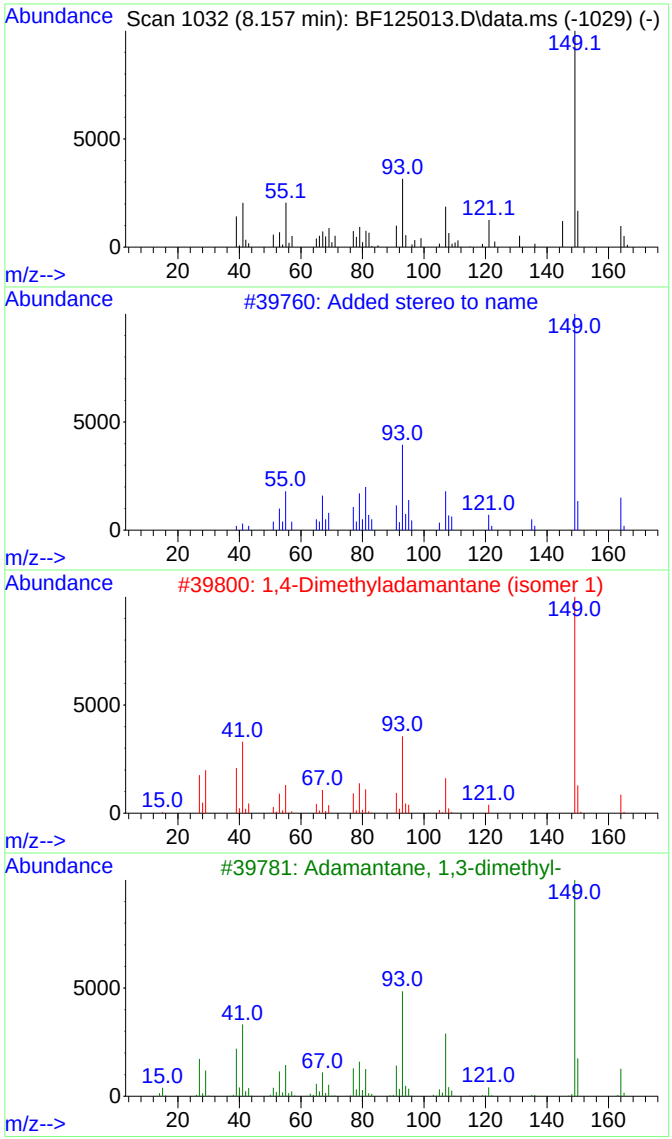
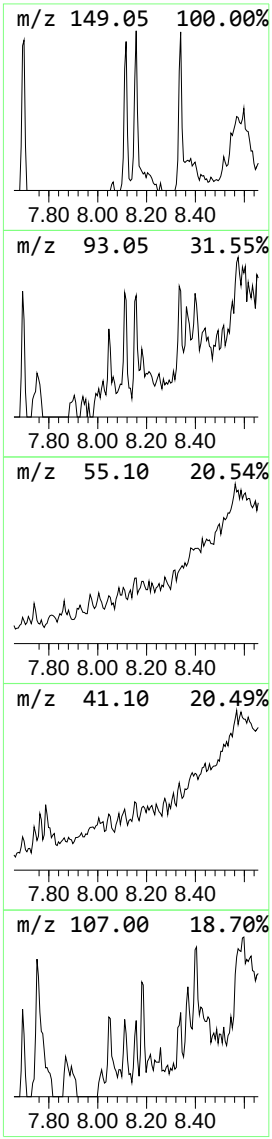
****
Peak Number 3 1,4-Dimethyladamantane (iso... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.157	5.15 ng	27490	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name	164	C12H20	024145-88-8	83
2	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	81
3	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	81
4	Added stereo to name	164	C12H20	024145-89-9	80
5	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	64





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1940

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
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TIC Library : C:\Database\NIST20.L
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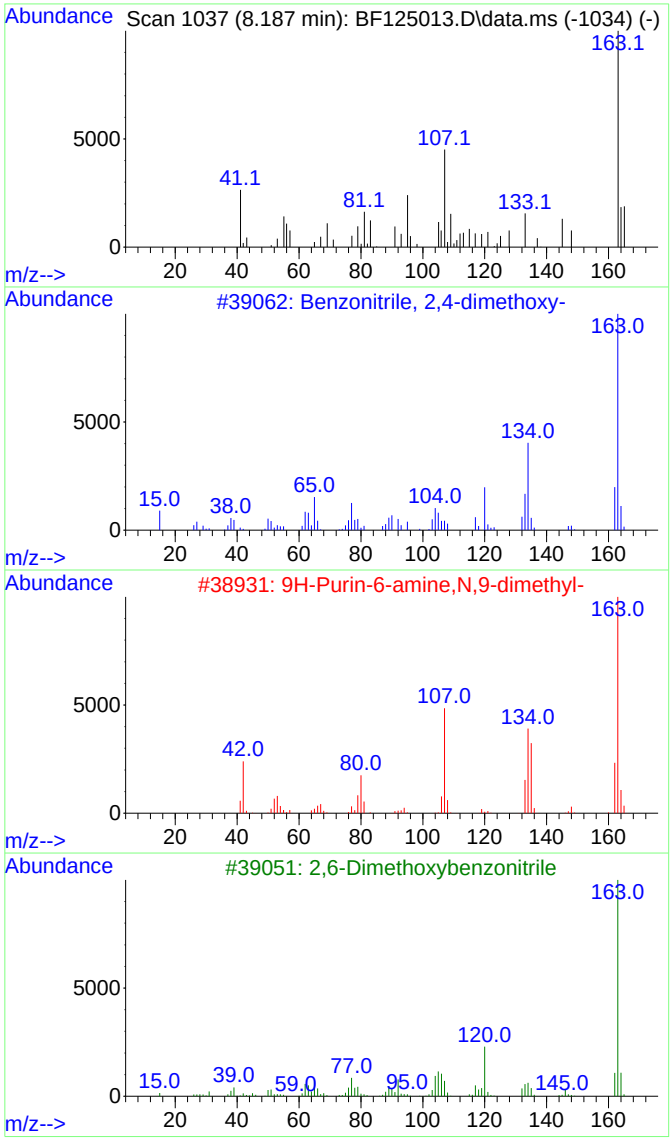
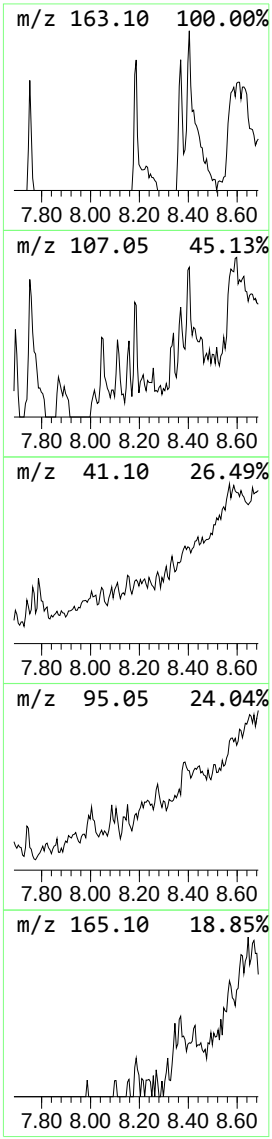
Peak Number 4 unknown8.187 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.187	4.66 ng	24847	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	37
2	9H-Purin-6-amine,N,9-dimethyl-	163	C7H9N5	002009-52-1	36
3	2,6-Dimethoxybenzonitrile	163	C9H9NO2	016932-49-3	35
4	Benzofurazan, 5-(dimethylamino)-	163	C8H9N3O	006124-22-7	35
5	Tricyclo[3.3.1.1(3,7)-]decane, 1...	242	C12H19Br	000941-37-7	33





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Operator : JU/CG
Sample : M3298-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1940

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
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TIC Library : C:\Database\NIST20.L
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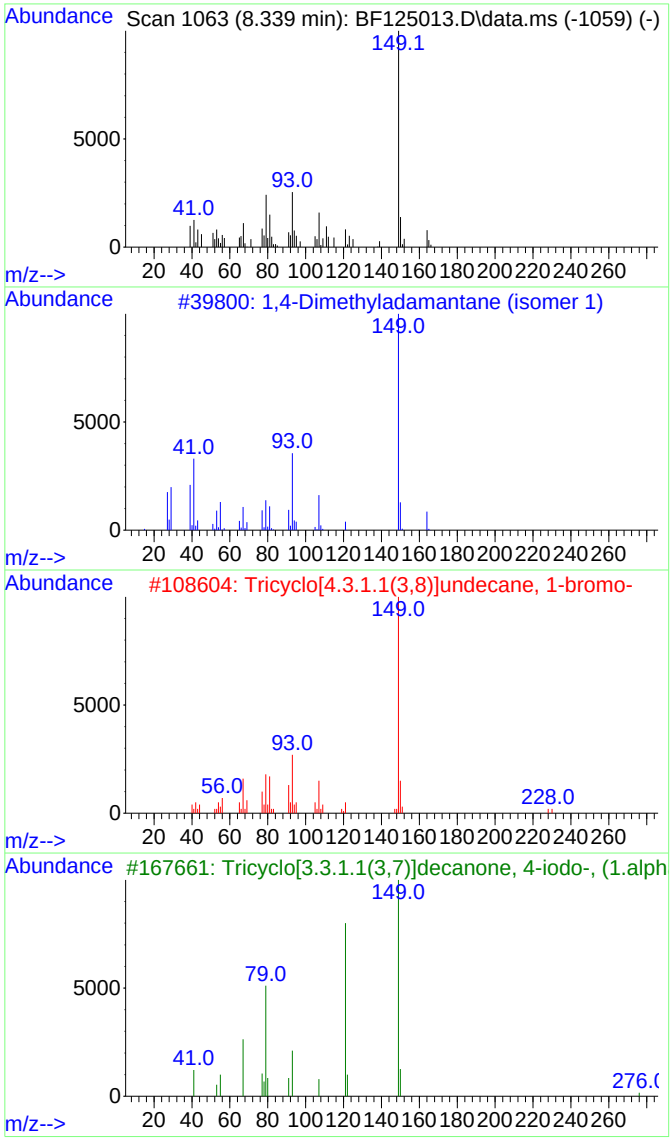
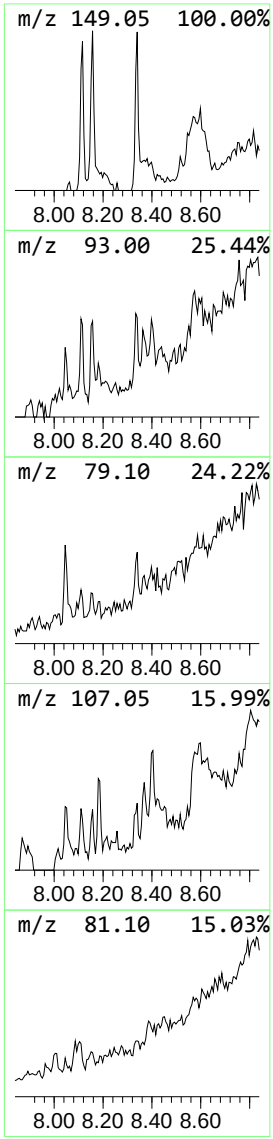
****
Peak Number 5 Tricyclo[4.3.1.1(3,8)]undec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.339	7.39 ng	39454	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	74
2	Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	59
3	Tricyclo[3.3.1.1(3,7)]decanone, ...	276	C10H13IO	056781-85-2	53
4	Tricyclo[3.3.1.1(3,7)]decanone, ...	276	C10H13IO	056781-86-3	50
5	Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	45





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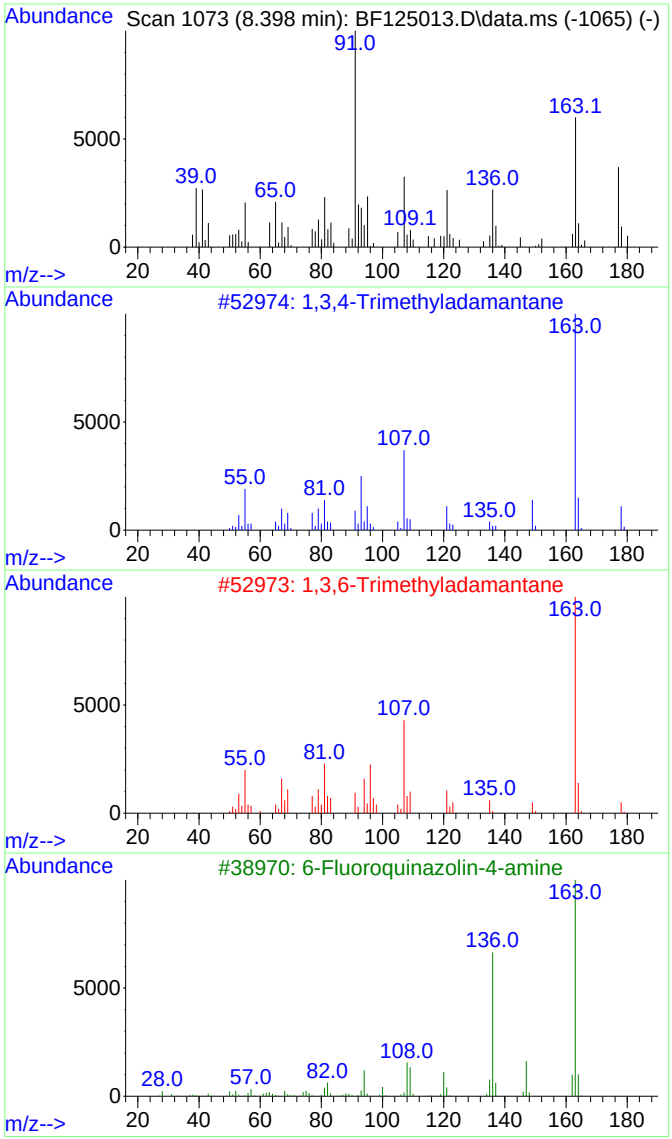
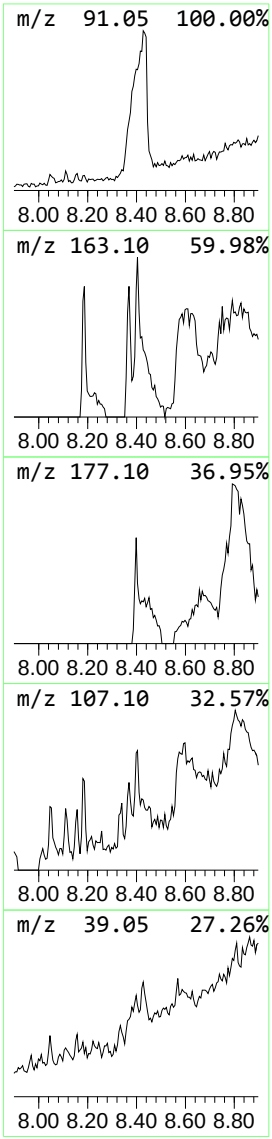
Peak Number 6 unknown8.398 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.398	23.61 ng	125960	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	41
2	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	35
3	6-Fluoroquinazolin-4-amine	163	C8H6FN3	1190320-08-1	27
4	2-Propanone, 1-(3,5,5-trimethyl-...	178	C12H18O	016695-72-0	25
5	l-Tyrophanamide	180	C9H12N2O2	1000131-25-3	22





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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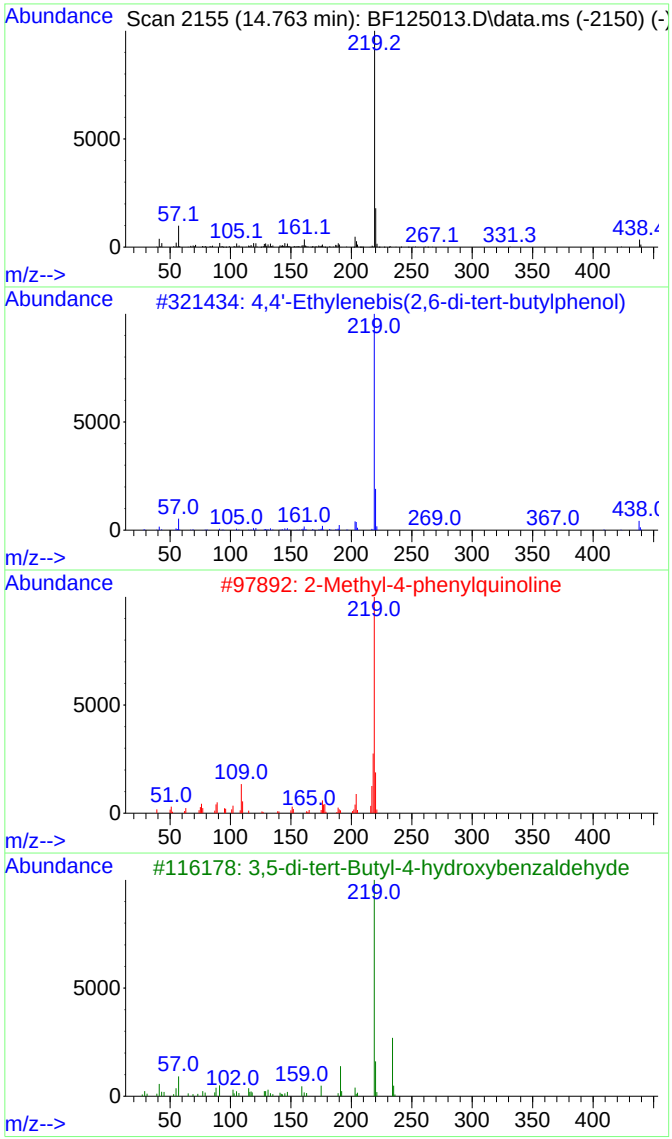
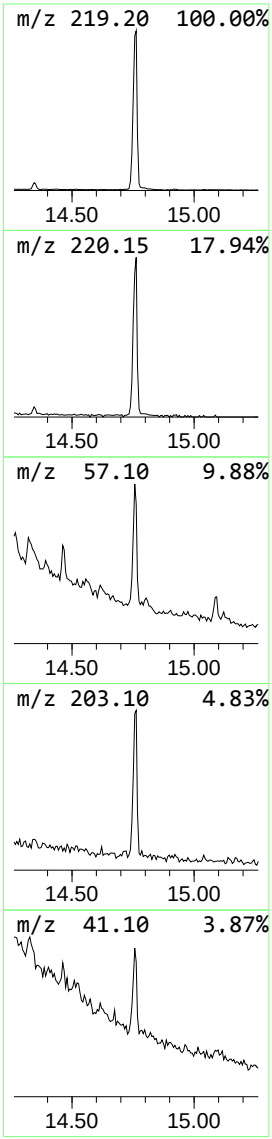
****
Peak Number 7 4,4'-Ethylenebis(2,6-di-ter... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	149.65 ng	426223	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Ethylenebis(2,6-di-tert-but...	438	C30H46O2	001516-94-5	90
2	2-Methyl-4-phenylquinoline	219	C16H13N	001721-92-2	64
3	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	56
4	Quinoline, 2-(3-tolyl)-	219	C16H13N	024641-30-3	53
5	1-Naphthalenamine, N-phenyl-	219	C16H13N	000090-30-2	53





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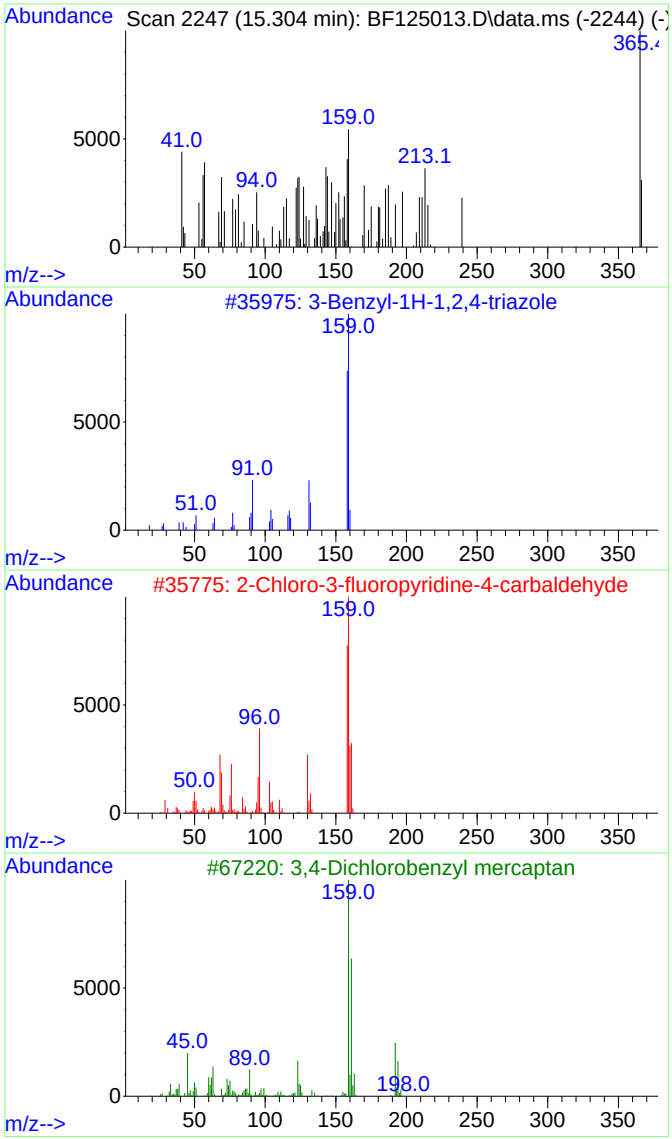
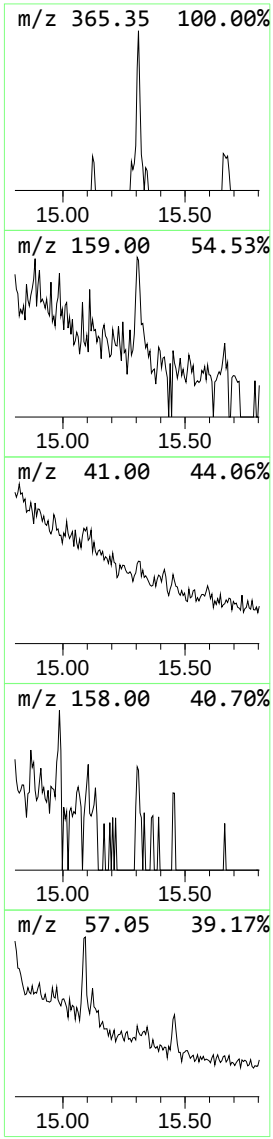
Peak Number 8 unknown15.304 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	8.77 ng	24981	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Benzyl-1H-1,2,4-triazole	159	C9H9N3	021117-34-0	10
2	2-Chloro-3-fluoropyridine-4-carb...	159	C6H3ClFNO	329794-28-7	9
3	3,4-Dichlorobenzyl mercaptan	192	C7H6Cl2S	059293-67-3	9
4	4-(Methylamino)quinazoline	159	C9H9N3	007154-47-4	9
5	2-Methoxy-5-nitrophenol, heptafl...	365	C11H6F7NO5	1000375-94-1	9





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TIC Library : C:\Database\NIST20.L
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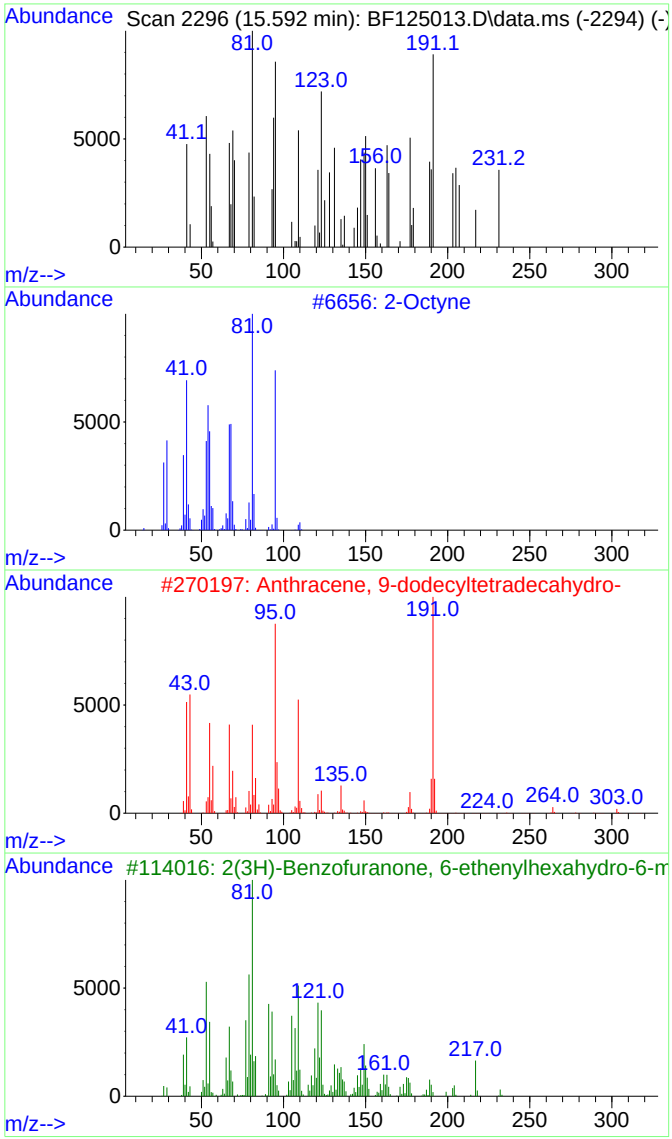
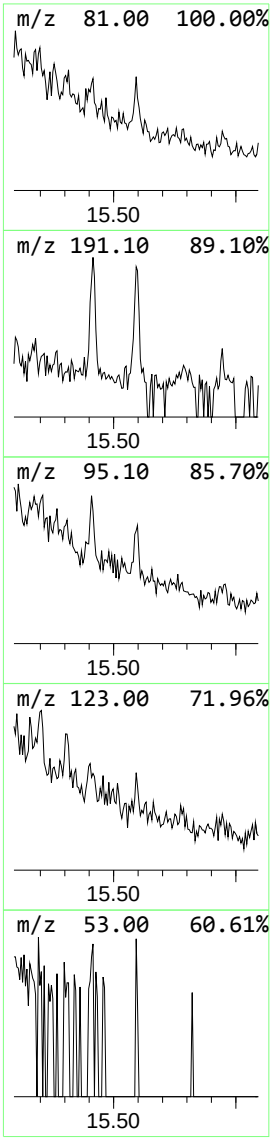
Peak Number 9 unknown15.592 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.592	9.52 ng	27115	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octyne	110	C8H14	002809-67-8	30
2	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	14
3	2(3H)-Benzofuranone, 6-ethenylhe...	232	C15H20O2	028290-35-9	12
4	2-Cyclohexen-1-one, 4-ethyl-4-me...	138	C9H14O	017429-32-2	12
5	2,6a-Methano-6aH-indeno[4,5-b]ox...	150	C10H14O	016489-32-0	11





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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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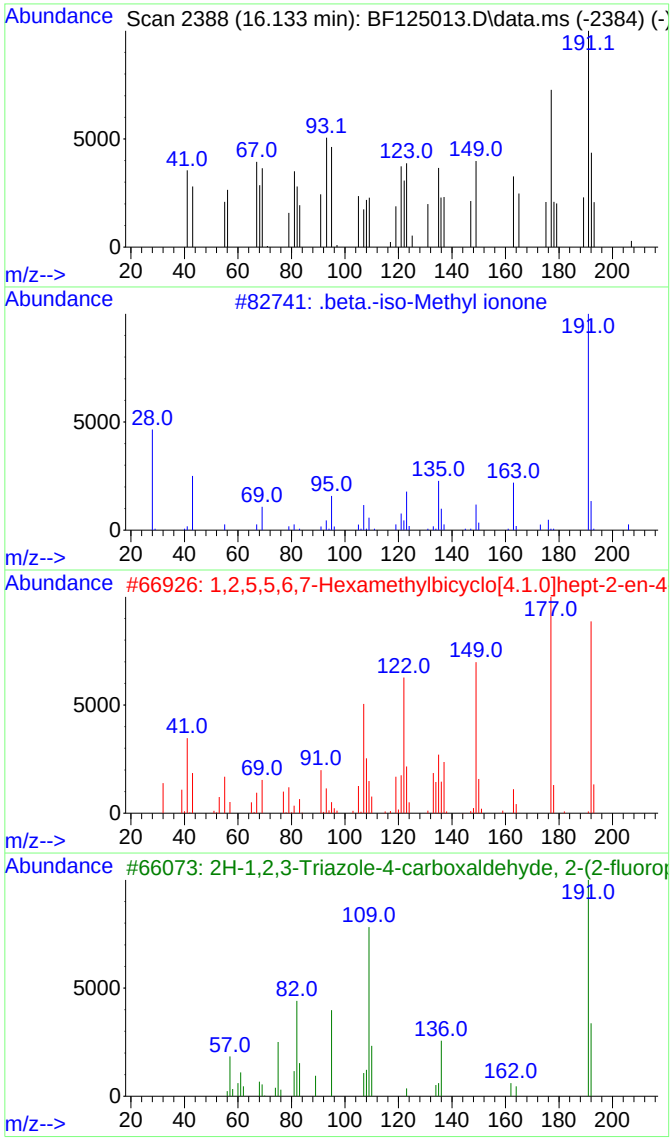
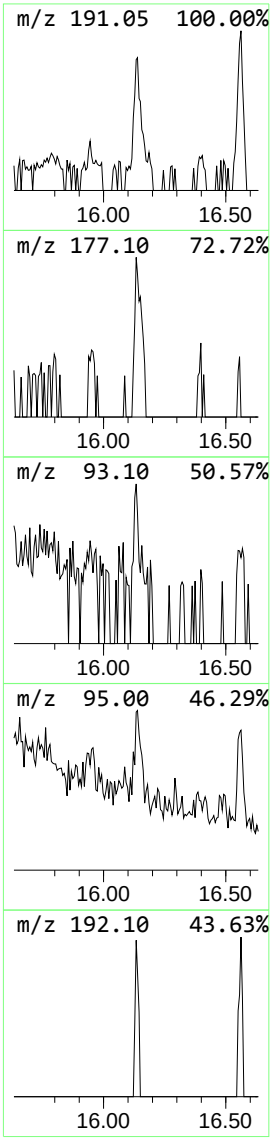
Peak Number 10 unknown16.133 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.133	17.46 ng	49718	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	23
2	1,2,5,5,6,7-Hexamethylbicyclo[4....	192	C13H20O	1000110-52-5	22
3	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	16
4	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	12
5	(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125013.D
Acq On : 9 Aug 2021 21:34
Operator : JU/CG
Sample : M3298-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1940

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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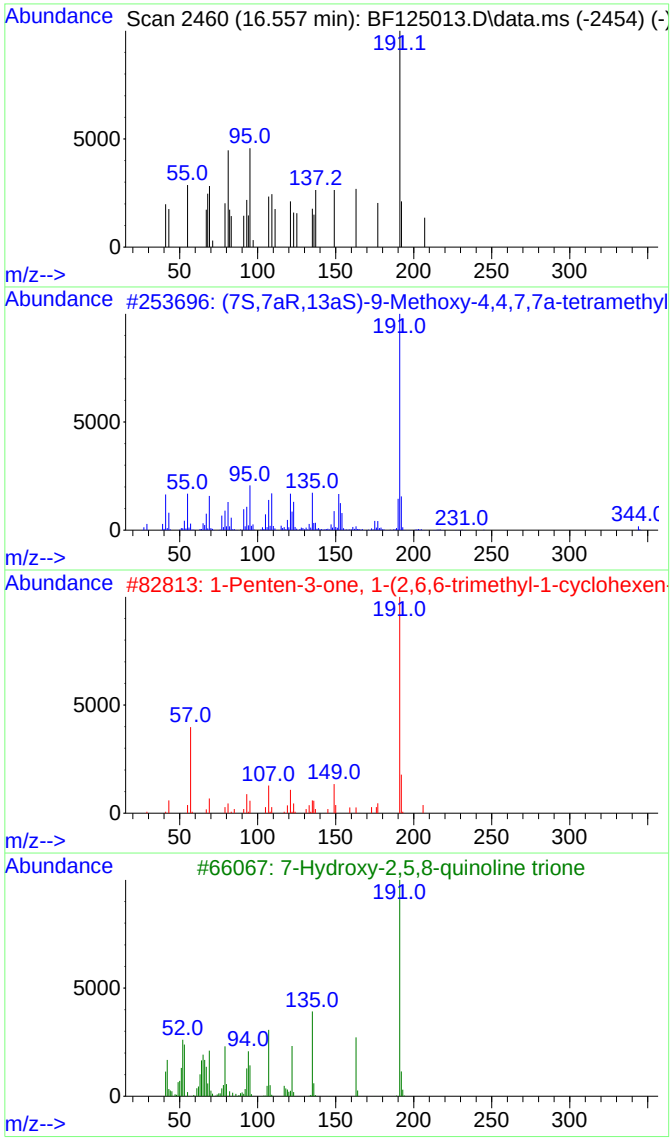
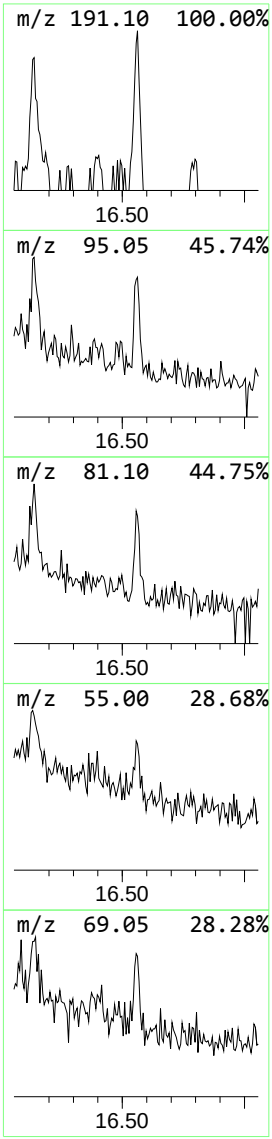
Peak Number 11 unknown16.557 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	10.97 ng	31234	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	43
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
3	7-Hydroxy-2,5,8-quinoline trione	191	C9H5NO4	015544-54-4	38
4	thiazolo[5,4-b]pyridin-2-amine, ...	191	C9H9N3S	1000400-23-3	35
5	3,6-Methano-1,2,3,4,4a,5,6,8a-oc...	191	C12H17NO	1000188-01-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125013.D
Acq On : 9 Aug 2021 21:34
Operator : JU/CG
Sample : M3298-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1940

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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
Adamantane, 1,3...	7.692	5.8	ng	31156	2	8.104	106705	20.0
Cyclohexanone, ...	8.045	6.3	ng	33817	2	8.104	106705	20.0
1,4-Dimethylada...	8.157	5.2	ng	27490	2	8.104	106705	20.0
unknown8.187	8.187	4.7	ng	24847	2	8.104	106705	20.0
Tricyclo[4.3.1....	8.339	7.4	ng	39454	2	8.104	106705	20.0
unknown8.398	8.398	23.6	ng	125960	2	8.104	106705	20.0
4,4'-Ethylenebi...	14.763	149.7	ng	426223	6	15.468	56964	20.0
unknown15.304	15.304	8.8	ng	24981	6	15.468	56964	20.0
unknown15.592	15.592	9.5	ng	27115	6	15.468	56964	20.0
unknown16.133	16.133	17.5	ng	49718	6	15.468	56964	20.0
unknown16.557	16.557	11.0	ng	31234	6	15.468	56964	20.0