LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124987.D
Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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: BF124987.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.439	567	570	574	rBB	64316	50661	30.98%	5.101%
2	6.457	740	743	746	rBB	73453	53121	32.49%	5.349%
3	6.828	803	806	809	rBB	44851	33468	20.47%	3.370%
4	7.386	898	901	904	rBB	37870	32244	19.72%	3.247%
5	8.110	1021	1024	1027	rBB	58254	44917	27.47%	4.523%
6	9.186	1201	1207	1210	rVB	65414	49993	30.57%	5.034%
7	9.574	1270	1273	1277	rBV3	8288	12344	7.55%	1.243%
8	9.616	1277	1280	1285	rBV4	16831	19366	11.84%	1.950%
9	9.733	1297	1300	1302	rBV2	9040	9136	5.59%	0.920%
10	9.774	1304	1307	1310	rVB3	14367	15629	9.56%	1.574%
11	9.869	1315	1323	1325	rBV	83324	87589	53.56%	8.819%
12	9.904	1325	1329	1331	rBV3	10896	13092	8.01%	1.318%
13	10.039	1348	1352	1353	rBV4	11790	16605	10.15%	1.672%
14	10.121	1364	1366	1368	rBV2	17866	16157	9.88%	1.627%
15	10.186	1374	1377	1378	rBV3	17445	19153	11.71%	1.928%
16	10.210	1378	1381	1383	rVV4	15787	20986	12.83%	2.113%
17	10.274	1389	1392	1395	rBV3	41033	42454	25.96%	4.275%
18	10.663	1455	1458	1462	rBV4	41776	67791	41.46%	6.826%
19	10.798	1478	1481	1484	rBV	121777	118076	72.21%	11.889%
20	11.274	1559	1562	1565	rVB	161456	163523	100.00%	16.465%
21	14.004	2023	2026	2029	rVB	49575	48808	29.85%	4.914%
22	14.898	2175	2178	2181	rVB3	9841	10052	6.15%	1.012%
23	15.121	2213	2216	2222	rVB5	9128	12770	7.81%	1.286%
24	15.456	2268	2273	2276	rBV	23547	27017	16.52%	2.720%
25	15.662	2305	2308	2314	rVB5	5531	8205	5.02%	0.826%

Sum of corrected areas: 993157

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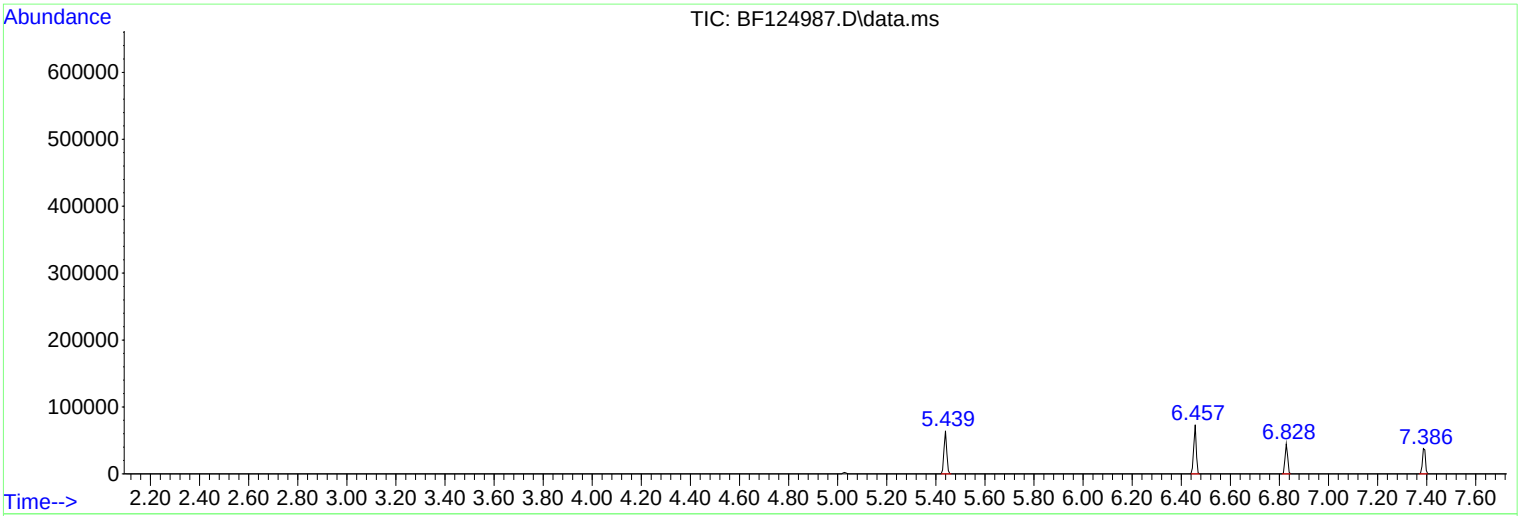
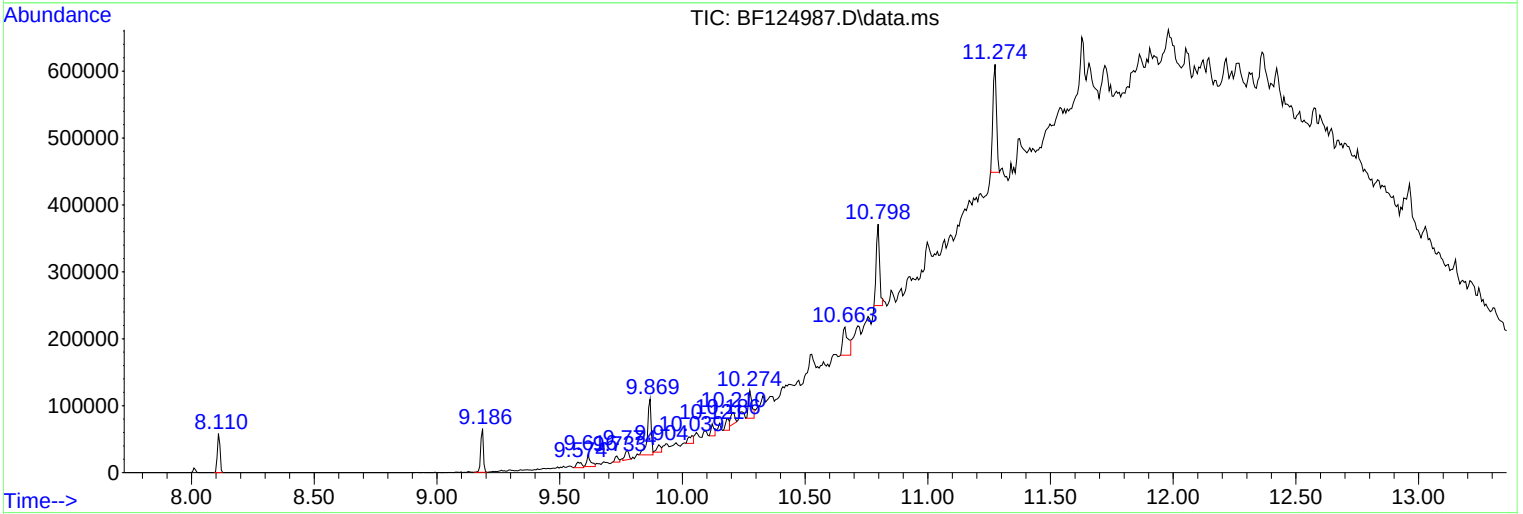
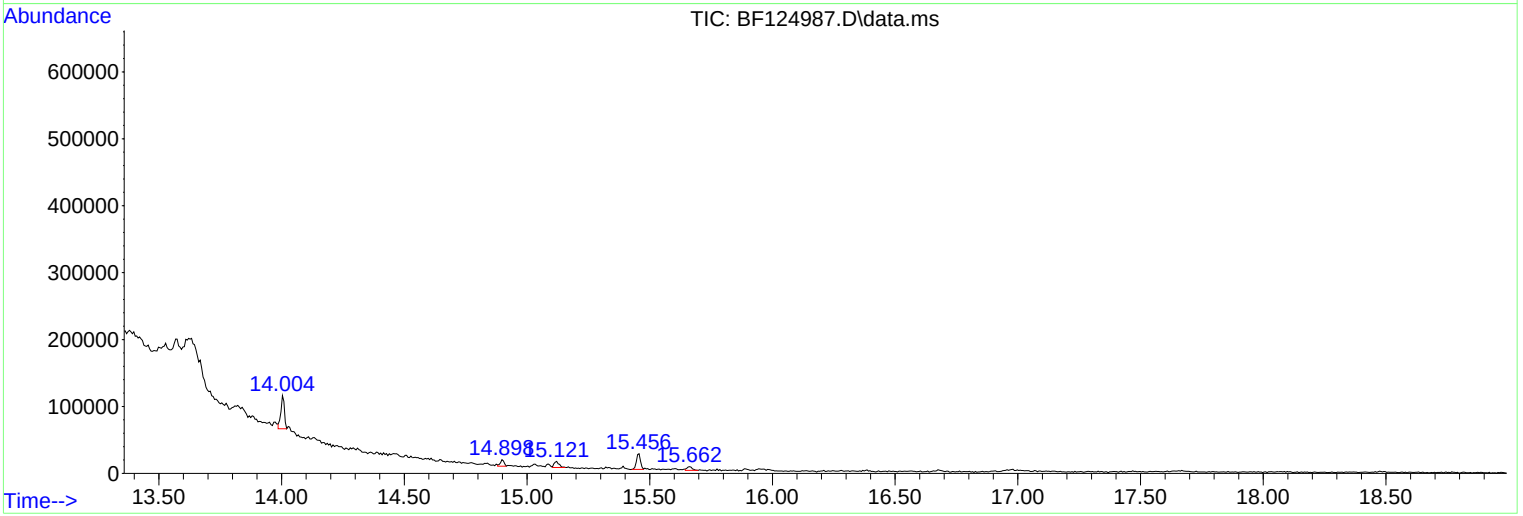
Instrument :
BNA_F
ClientSampleId :
2071

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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TIC Library : C:\Database\NIST20.L
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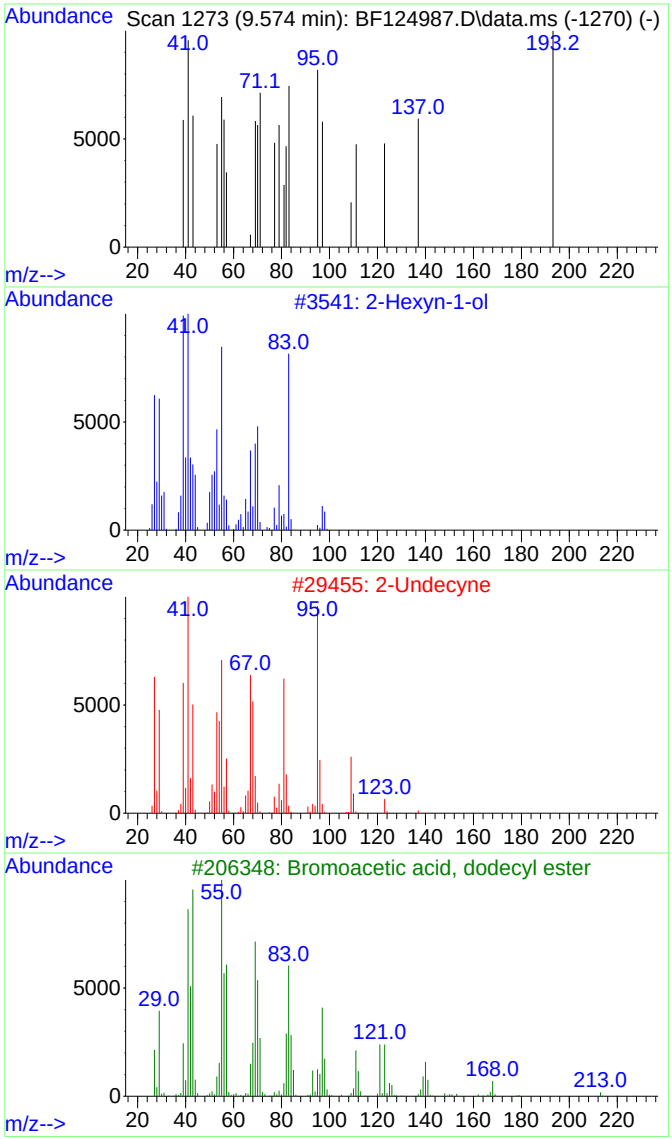
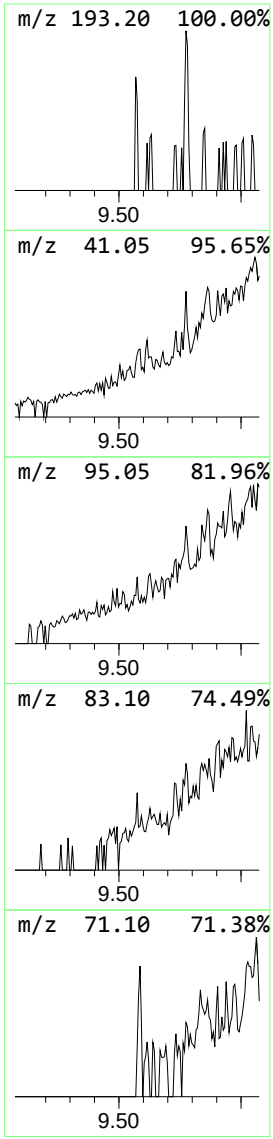
Peak Number 1 unknown9.574 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.574	2.82 ng	12344	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyn-1-ol	98	C6H10O	000764-60-3	27
2	2-Undecyne	152	C11H20	060212-29-5	27
3	Bromoacetic acid, dodecyl ester	306	C14H27BrO2	003674-07-5	14
4	Formic acid, dodecyl ester	214	C13H26O2	028303-42-6	14
5	Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	054889-87-1	14





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Data File : BF124987.D
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Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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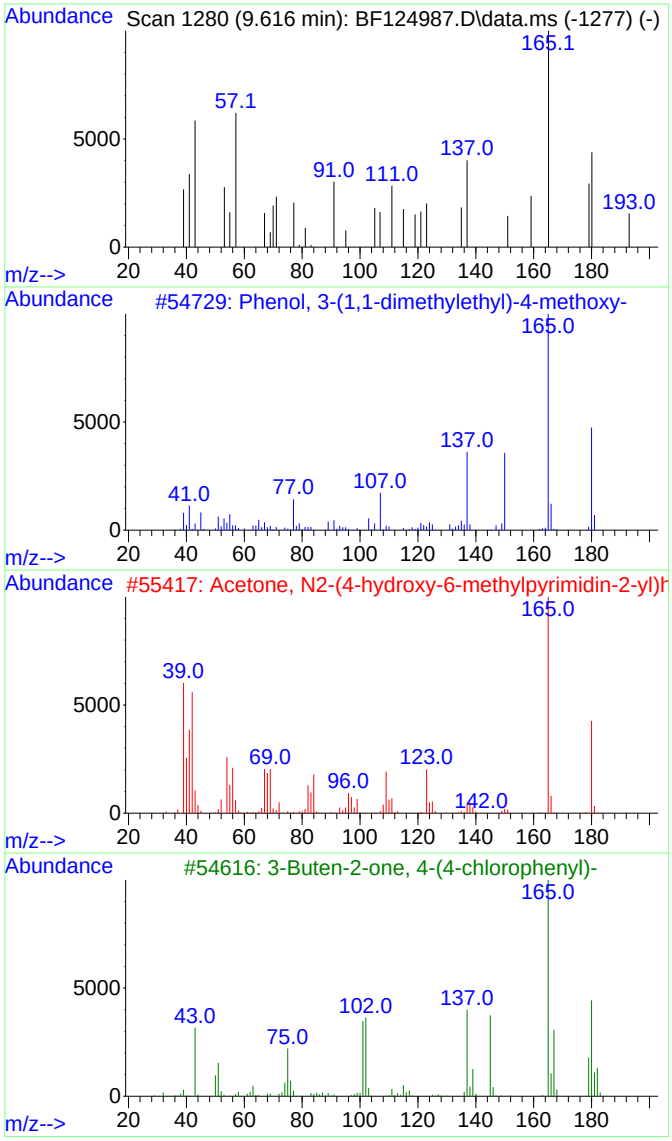
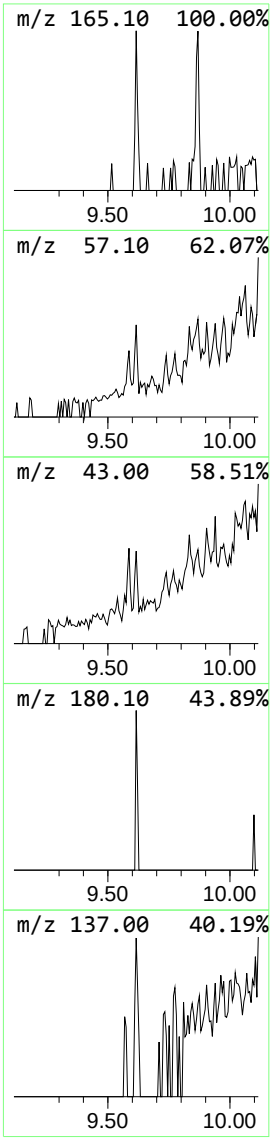
Peak Number 2 unknown9.616 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	4.42 ng	19366	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	47
2	Acetone, N2-(4-hydroxy-6-methylp...	180	C8H12N4O	066680-04-4	38
3	3-Buten-2-one, 4-(4-chlorophenyl)-	180	C10H9ClO	003160-40-5	38
4	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	38
5	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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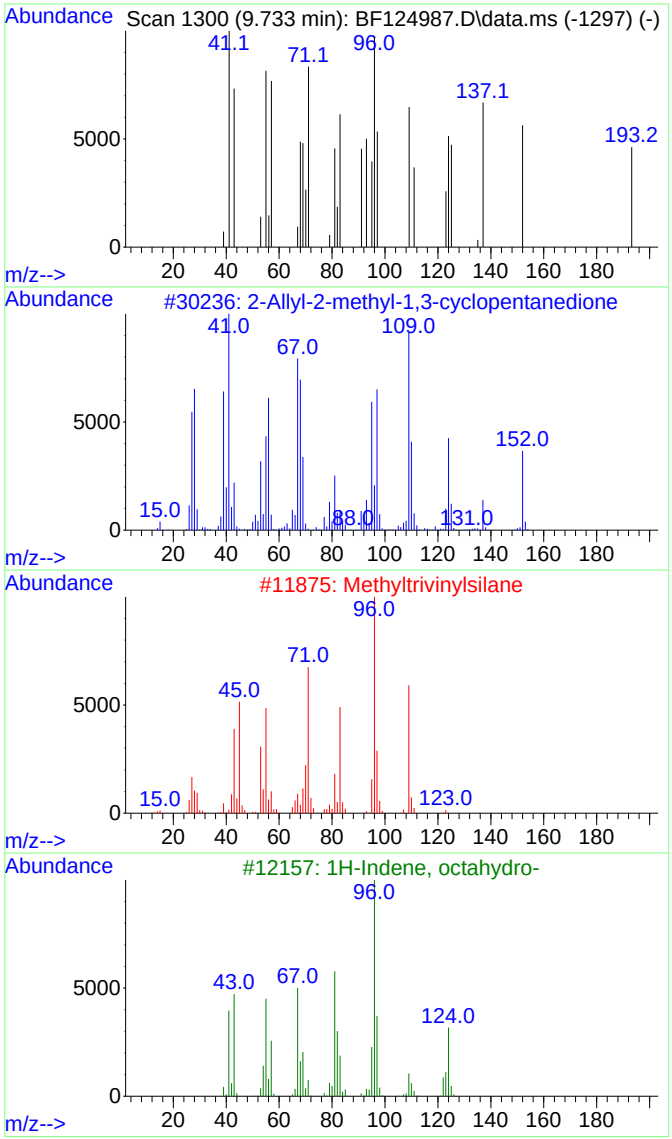
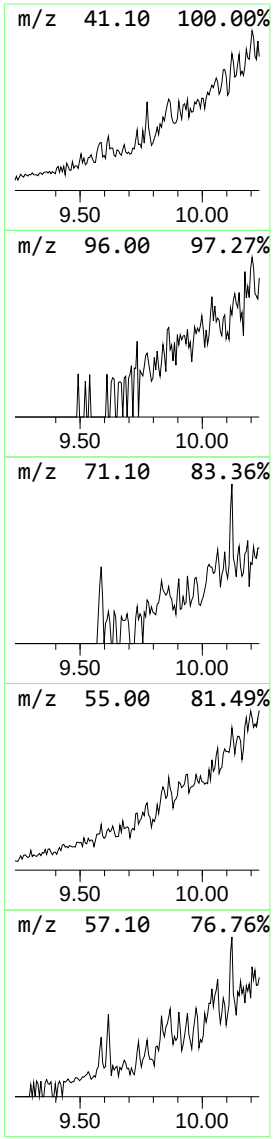
Peak Number 3 unknown9.733 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	2.09 ng	9136	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Allyl-2-methyl-1,3-cyclopentan...	152	C9H12O2	026828-48-8	35
2	Methyltrivinylsilane	124	C7H12Si	018244-95-6	25
3	1H-Indene, octahydro-	124	C9H16	000496-10-6	22
4	3-(methylselanyl)propanal	152	C4H8OSe	1000366-05-4	22
5	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124987.D
Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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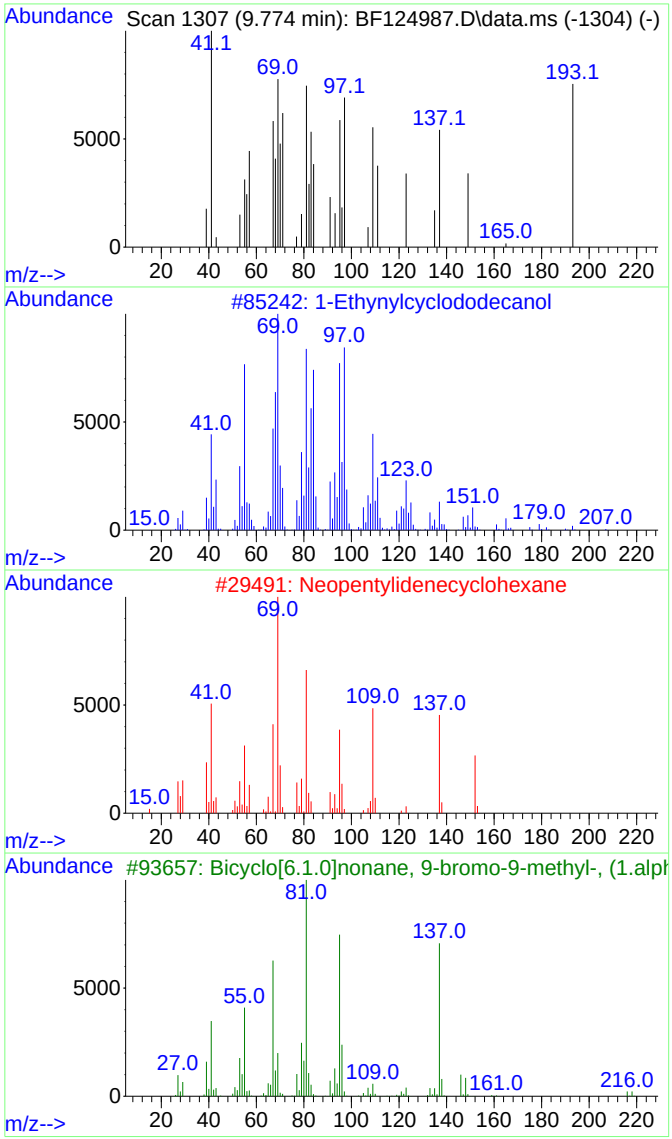
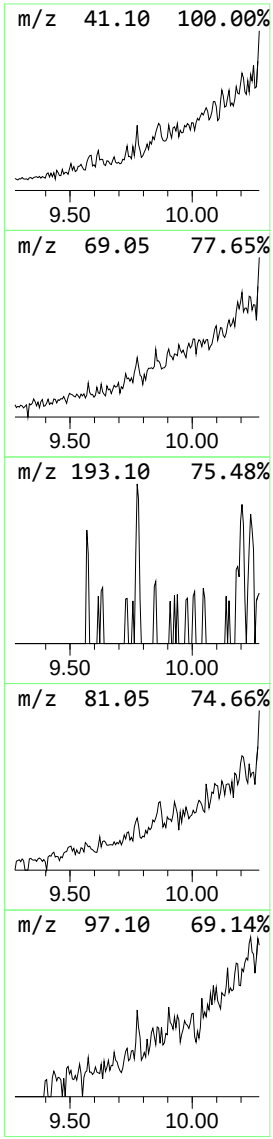
Peak Number 4 unknown9.774 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.774	3.57 ng	15629	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	43
2	Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
3	Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	22
4	cis,trans-2-Ethylbicyclo[4.4.0]d...	166	C12H22	066660-38-6	22
5	5-Dodecyne	166	C12H22	019780-12-2	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124987.D
Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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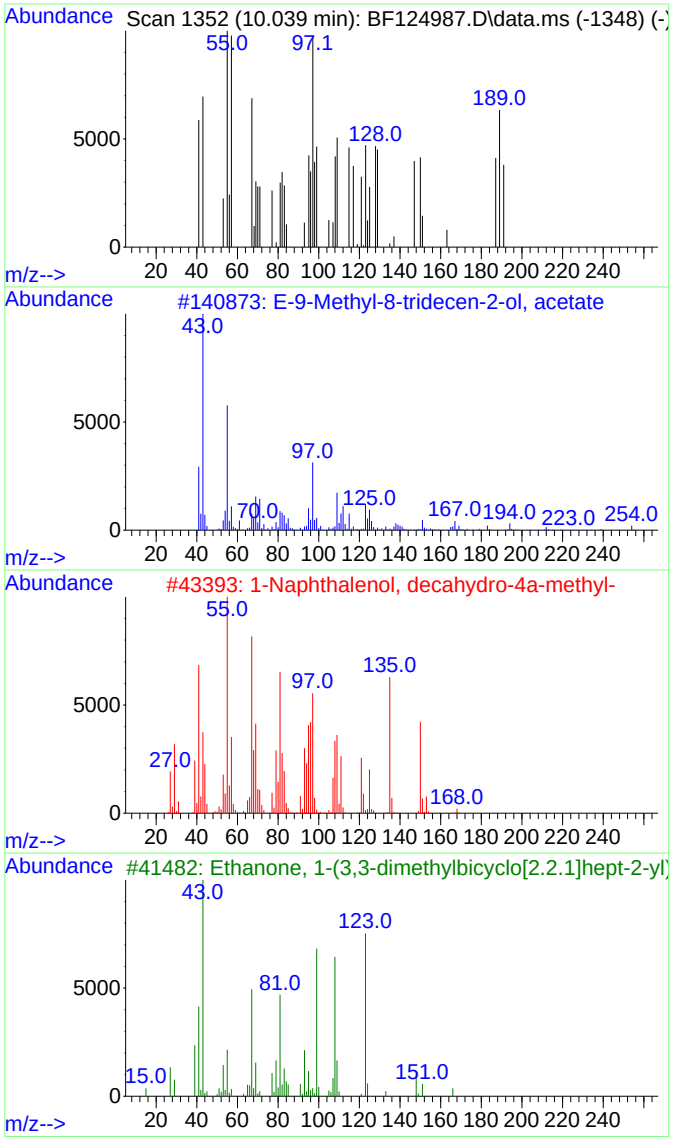
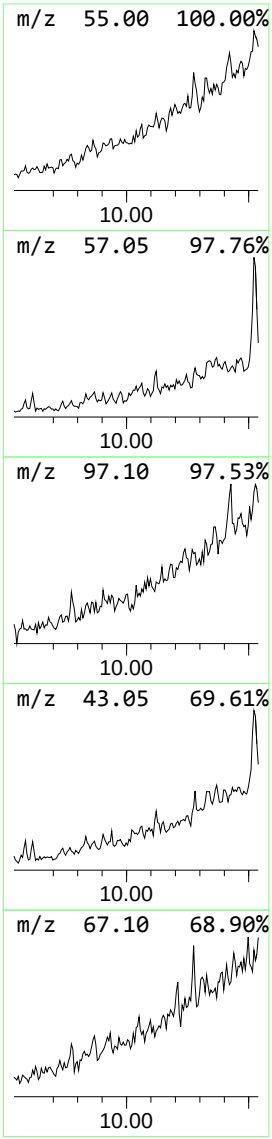
Peak Number 5 unknown10.039 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.039	3.79 ng	16605	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-9-Methyl-8-tridecen-2-ol, acetate	254	C16H30O2	1000131-35-6	12
2	1-Naphthalenol, decahydro-4a-met...	168	C11H20O	054972-52-0	10
3	Ethanone, 1-(3,3-dimethylbicyclo...	166	C11H18O	015780-34-4	10
4	2-Phenyl-1,3-thiazole-4-carbalde...	189	C10H7NOS	020949-81-9	9
5	4-Hydroxy-.beta.-thujone	168	C10H16O2	273406-45-4	9





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Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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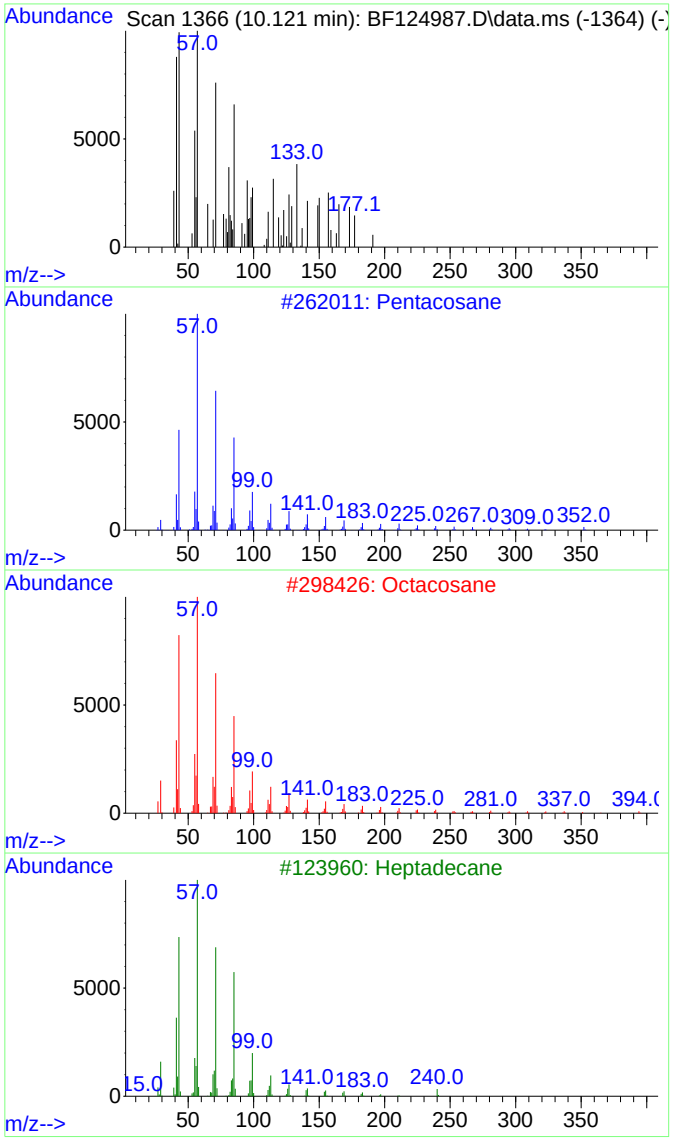
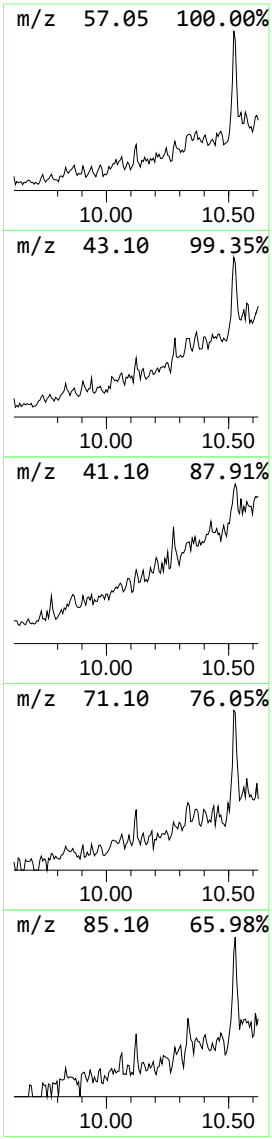
Peak Number 6 unknown10.121 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.121	3.69 ng	16157	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	38
2	Octacosane	394	C28H58	000630-02-4	38
3	Heptadecane	240	C17H36	000629-78-7	38
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	38
5	Hexacosane	366	C26H54	000630-01-3	38





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Data File : BF124987.D
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Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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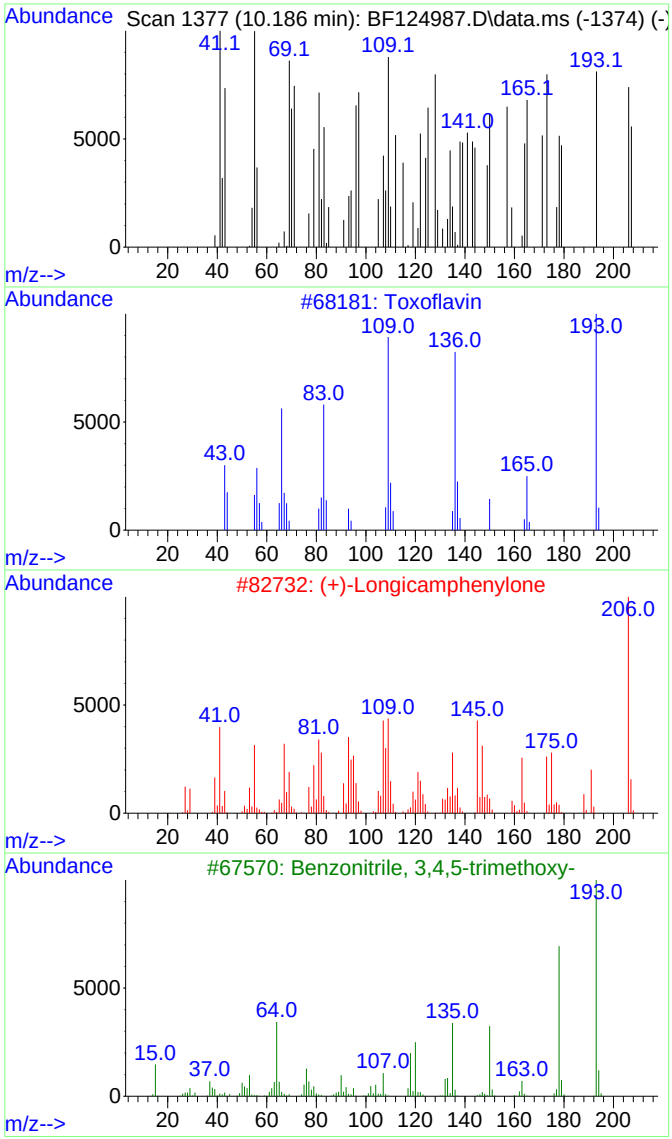
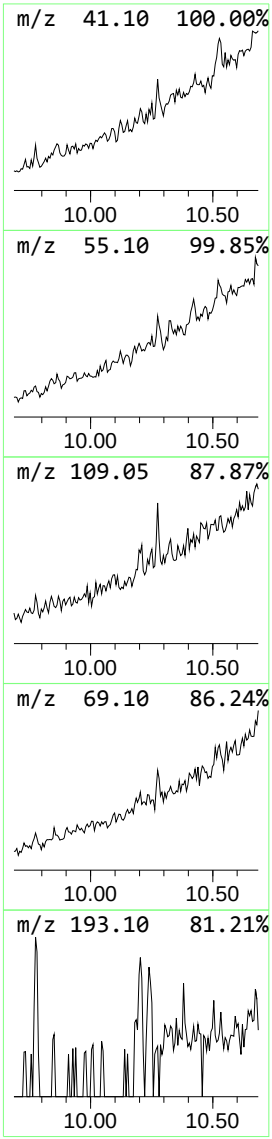
Peak Number 7 unknown10.186 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	4.37 ng	19153	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toxoflavin	193	C7H7N5O2	000084-82-2	14
2	(+)-Longicamphenylone	206	C14H22O	1000161-37-1	10
3	Benzonitrile, 3,4,5-trimethoxy-	193	C10H11NO3	001885-35-4	10
4	1,2-Oxazino[2,3-b]isoquinoline, ...	193	C12H19NO	1000196-68-0	10
5	Pent-2-en-2-ol, 4-(2-mercaptophe...	207	C11H13NOS	028788-72-9	10





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

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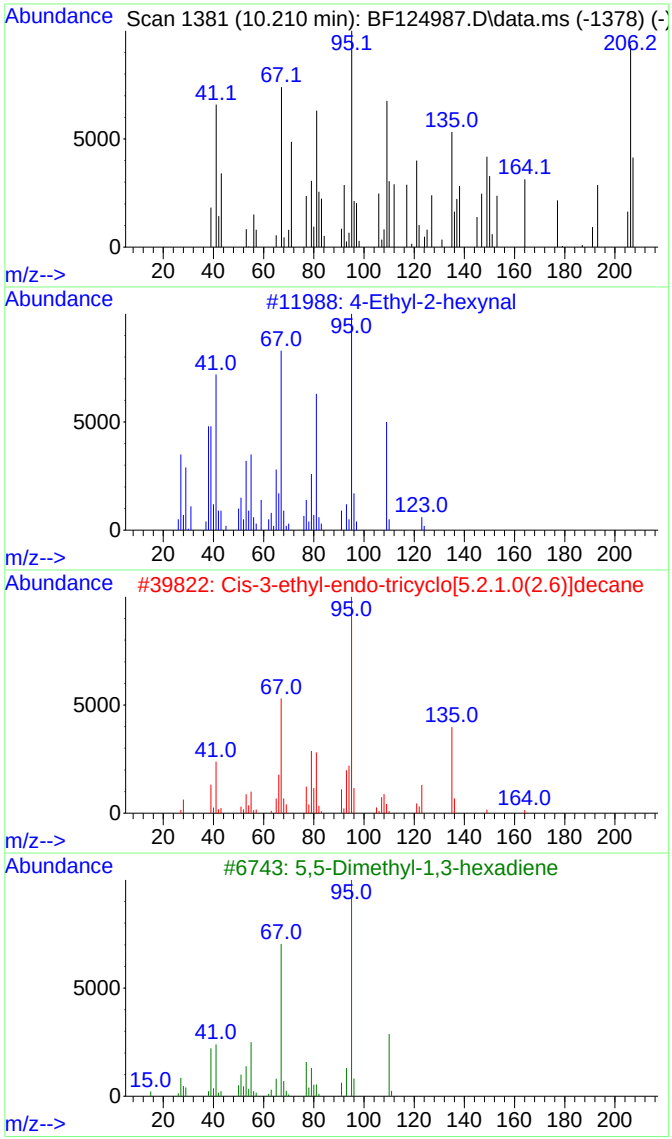
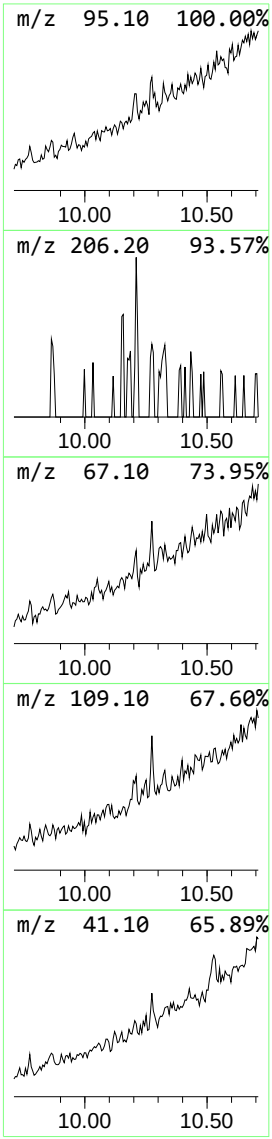
Peak Number 8 unknown10.210 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.210	4.79 ng	20986	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	27
2	Cis-3-ethyl-endo-tricyclo[5.2.1....	164	C12H20	1010215-29-1	25
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	22
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	22
5	Santolina epoxide	152	C10H16O	060485-45-2	22





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Operator : JU/CG
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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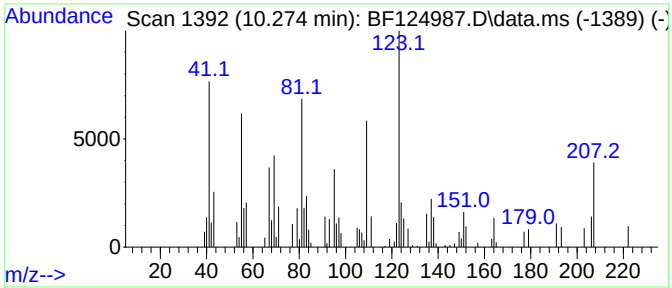
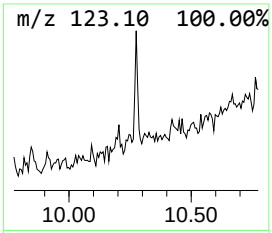
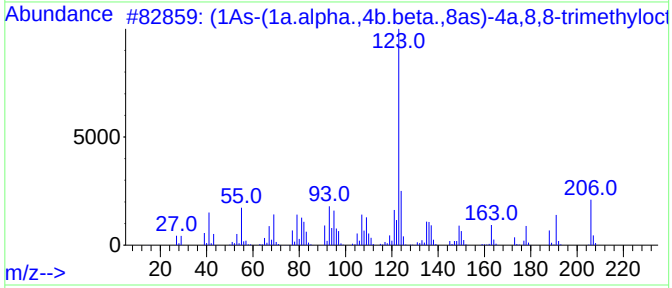
Peak Number 9 unknown10.274 Concentration Rank 3

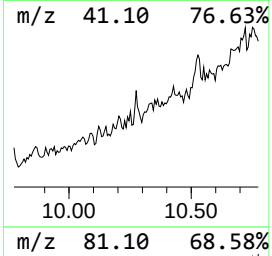
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.274	9.69 ng	42454	Acenaphthene-d10	9.869

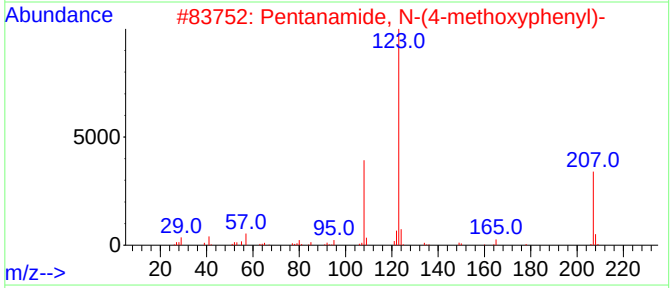
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1As-(1a.alpha.,4b.beta.,8as)-4a...	206	C14H22O	082262-79-1	46
2	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
3	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	35
4	5-Isopropyl-2H-pyrazole-3-carbal...	138	C7H10N2O	1000410-48-4	30
5	di-t-Butylacetylene	138	C10H18	017530-24-4	30

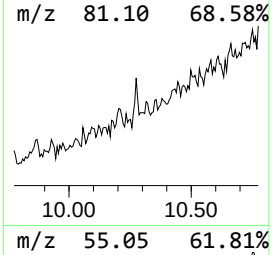


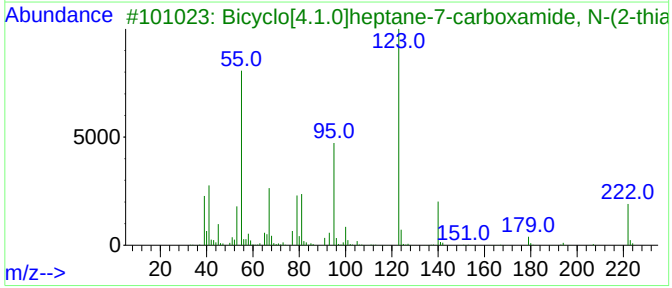


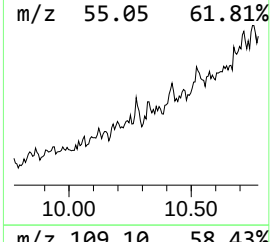


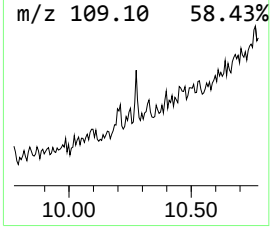












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Data File : BF124987.D
Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

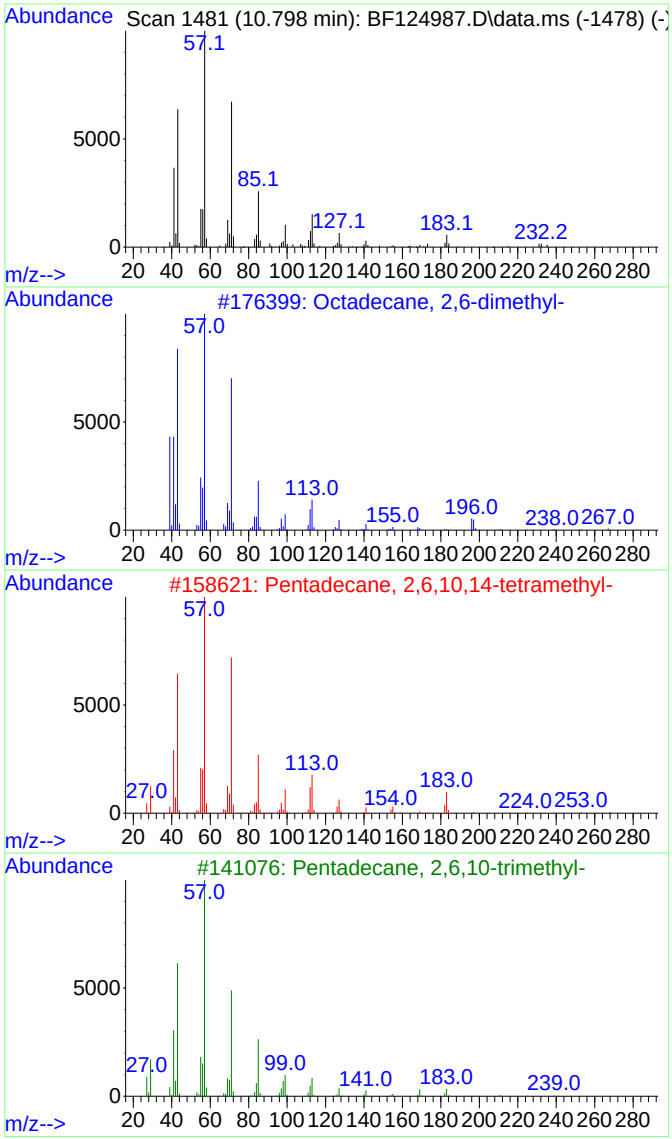
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

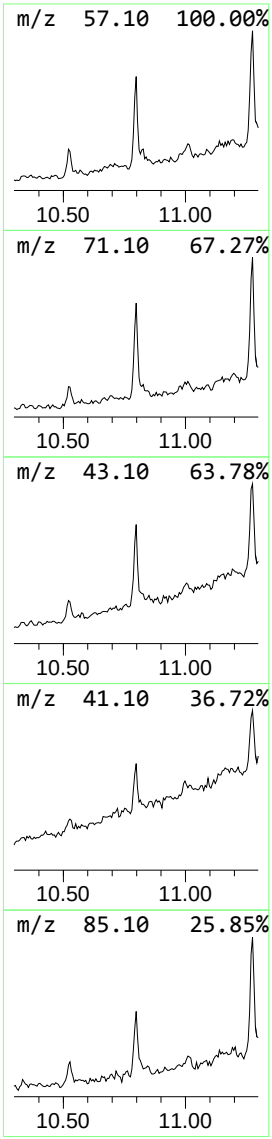
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Octadecane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	14.44 ng	118076	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	86
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	78
4	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	64
5	5,5-Dibutylnonane	240	C17H36	006008-17-9	64





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Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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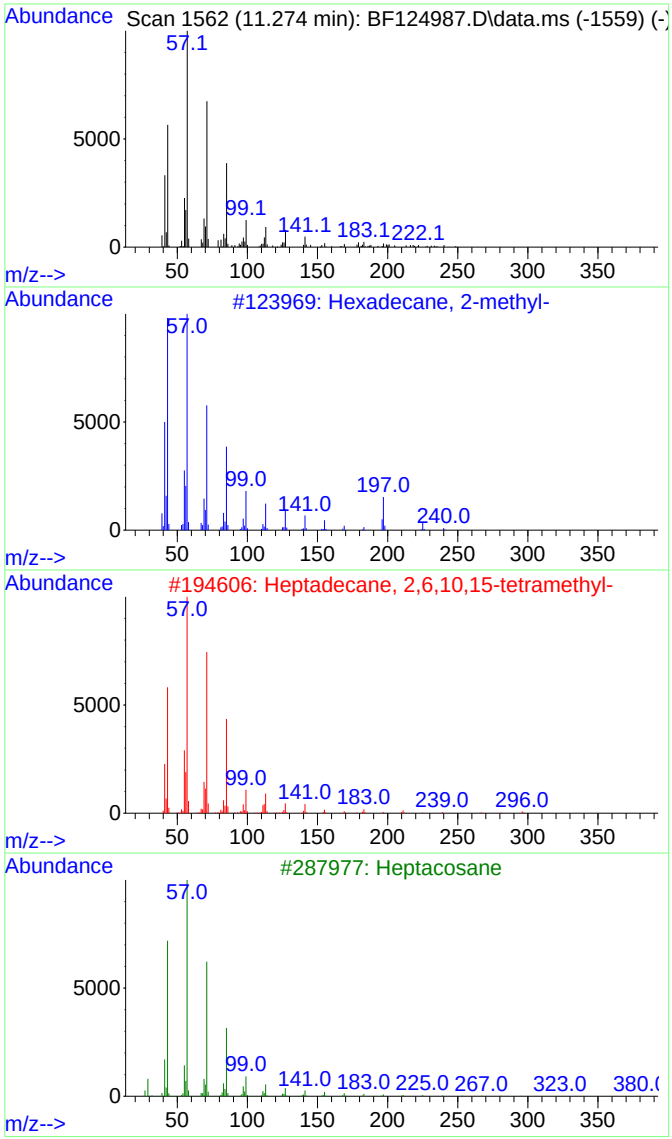
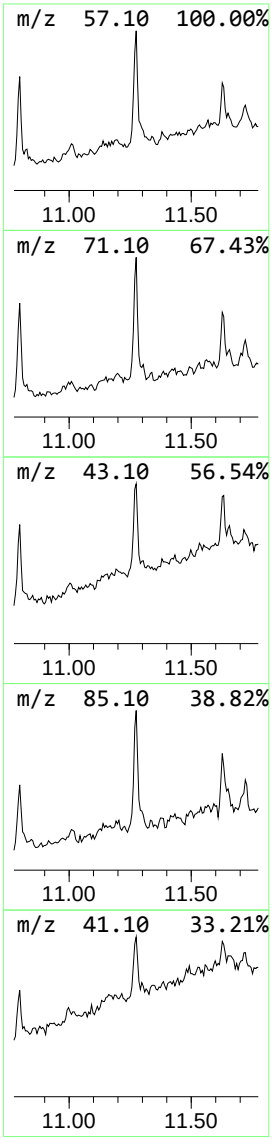
Peak Number 11 Hexadecane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.274	20.00 ng	163523	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86





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Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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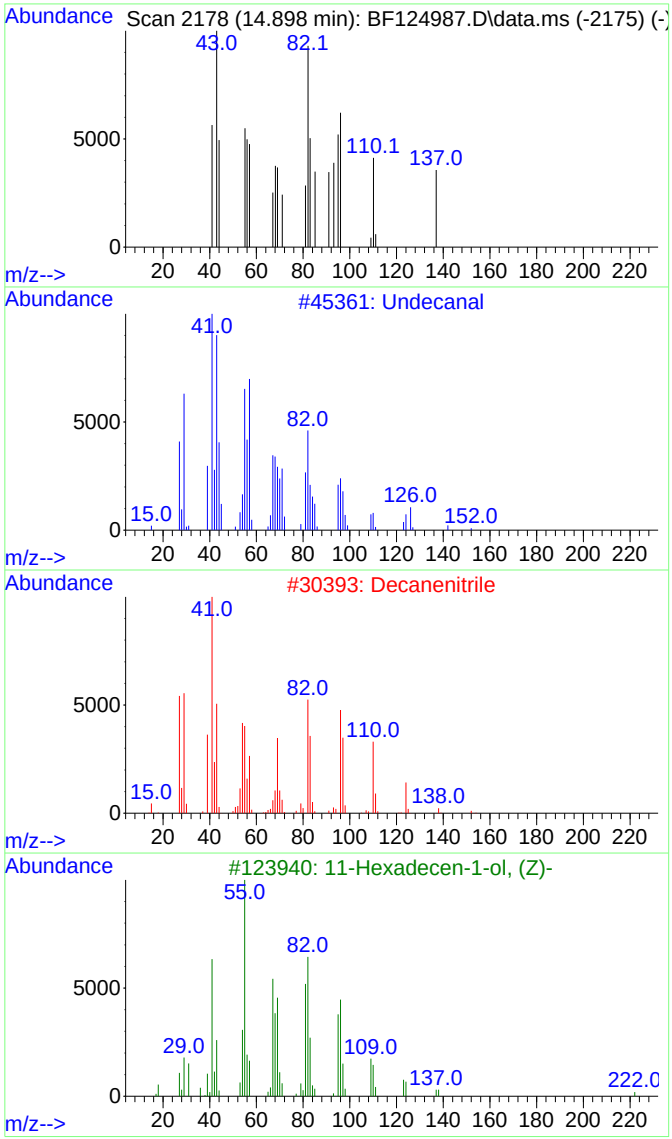
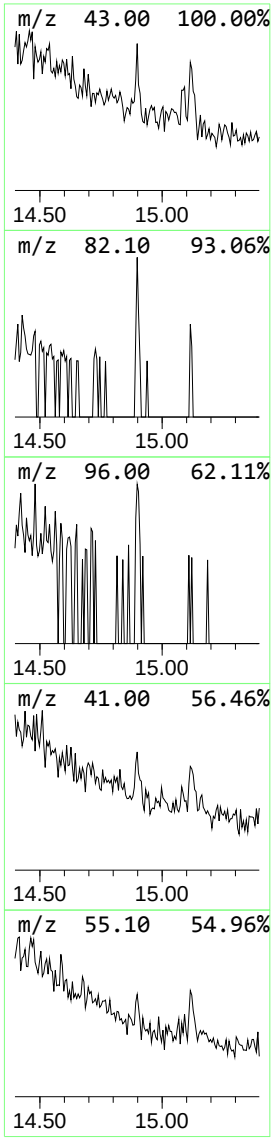
Peak Number 12 unknown14.898 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	7.44 ng	10052	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanal	170	C11H22O	000112-44-7	40
2	Decanenitrile	153	C10H19N	001975-78-6	38
3	11-Hexadecen-1-ol, (Z)-	240	C16H32O	056683-54-6	37
4	2-Propenoic acid, undec-10-enyl ...	224	C14H24O2	020763-72-8	32
5	Bicyclo[5.2.0]nonane, 1,7-dimeth...	152	C11H20	020130-83-0	32





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Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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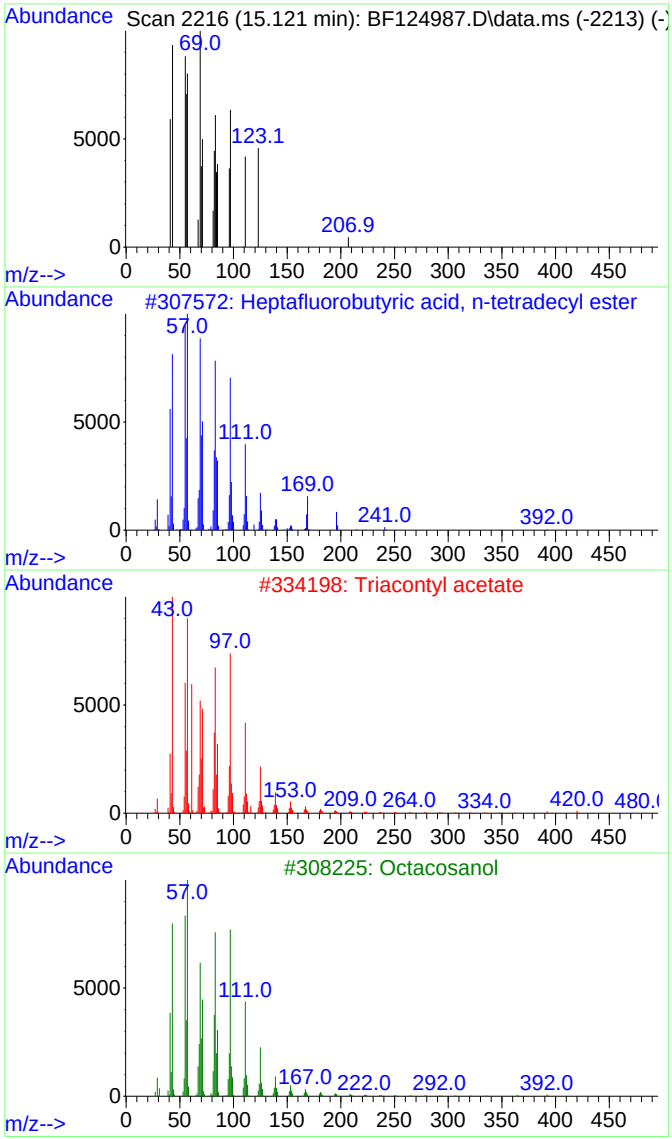
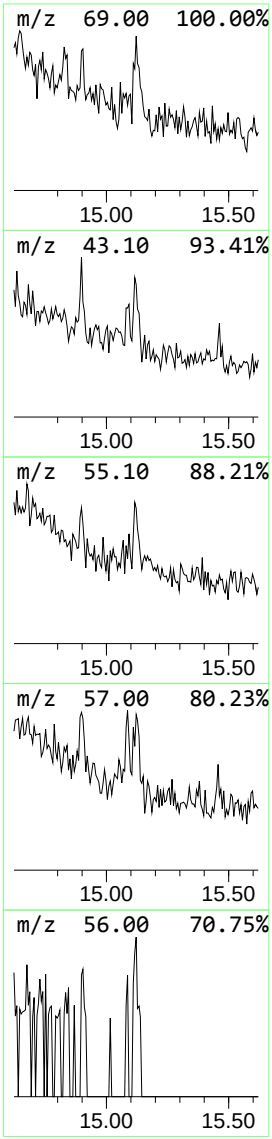
Peak Number 13 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	9.45 ng	12770	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	64
2	Triacontyl acetate	480	C32H64O2	041755-58-2	50
3	Octacosanol	410	C28H58O	000557-61-9	47
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	47
5	Butyl tetradecyl ether	270	C18H38O	1000406-40-4	47





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Data File : BF124987.D
Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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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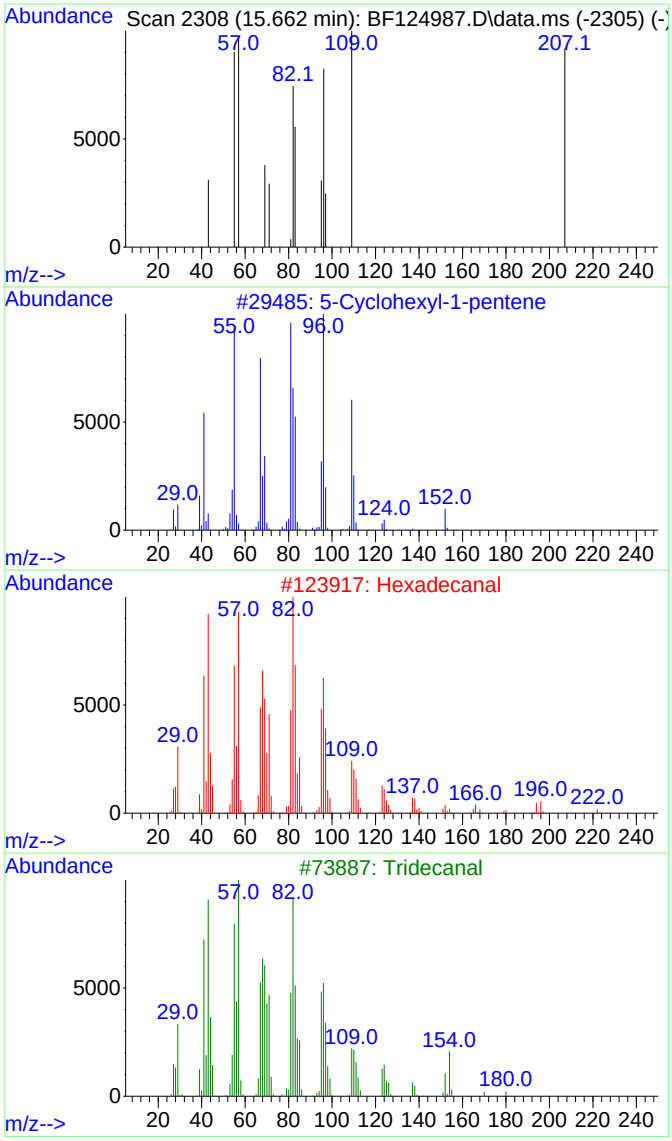
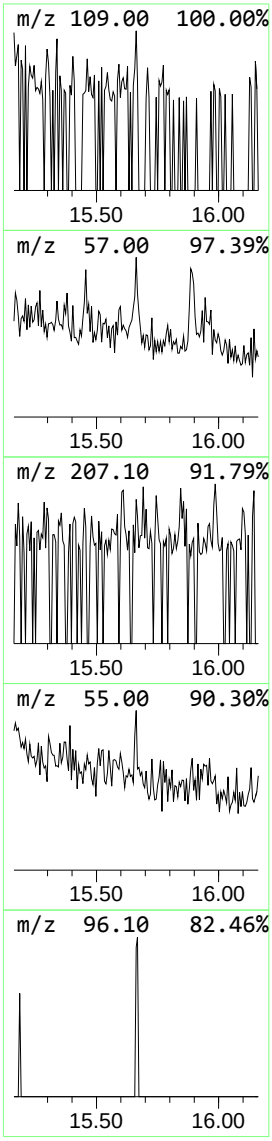
Peak Number 14 unknown15.662 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.662	6.07 ng	8205	Perylene-d12	15.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	43
2	Hexadecanal	240	C16H32O	000629-80-1	43
3	Tridecanal	198	C13H26O	010486-19-8	35
4	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	32
5	cis-1,2-Cyclododecanediol	200	C12H24O2	004422-05-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124987.D
Acq On : 7 Aug 2021 22:15
Operator : JU/CG
Sample : M3293-07 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2071

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
unknown9.574	9.574	2.8	ng	12344	3	9.869	87589	20.0
unknown9.616	9.616	4.4	ng	19366	3	9.869	87589	20.0
unknown9.733	9.733	2.1	ng	9136	3	9.869	87589	20.0
unknown9.774	9.774	3.6	ng	15629	3	9.869	87589	20.0
unknown10.039	10.039	3.8	ng	16605	3	9.869	87589	20.0
unknown10.121	10.121	3.7	ng	16157	3	9.869	87589	20.0
unknown10.186	10.186	4.4	ng	19153	3	9.869	87589	20.0
unknown10.210	10.210	4.8	ng	20986	3	9.869	87589	20.0
unknown10.274	10.274	9.7	ng	42454	3	9.869	87589	20.0
Octadecane, 2,6...	10.798	14.4	ng	118076	4	11.368	163523	20.0
Hexadecane, 2-m...	11.274	20.0	ng	163523	4	11.368	163523	20.0
unknown14.898	14.898	7.4	ng	10052	6	15.456	27017	20.0
Heptafluorobuty...	15.121	9.4	ng	12770	6	15.456	27017	20.0
unknown15.662	15.662	6.1	ng	8205	6	15.456	27017	20.0