LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050421\
Data File : BF123816.D
Acq On : 4 May 2021 19:20
Operator : JU/CG
Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-2

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-BF042721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123816.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.992	491	494	504	rVB	210913	251140	4.33%	0.566%
2	5.416	562	566	578	rBV	4521146	4121595	71.12%	9.286%
3	6.081	675	679	682	rBV	2355442	1966217	33.93%	4.430%
4	6.245	704	707	710	rVB	188203	160589	2.77%	0.362%
5	6.434	735	739	747	rBV	4400457	4296663	74.14%	9.680%
6	6.504	747	751	754	rVB	2459153	1991590	34.37%	4.487%
7	6.798	798	801	804	rBV	1788902	1315358	22.70%	2.964%
8	6.869	809	813	819	rBV	221592	401568	6.93%	0.905%
9	7.363	892	897	900	rBV	3273318	2817911	48.62%	6.349%
10	8.022	1006	1009	1016	rVB	402643	294599	5.08%	0.664%
11	8.080	1016	1019	1022	rBV	1934295	1679849	28.99%	3.785%
12	9.163	1199	1203	1206	rBV	5497828	4418897	76.25%	9.956%
13	9.498	1256	1260	1263	rBV	208926	169583	2.93%	0.382%
14	9.839	1315	1318	1321	rVB	2198031	1713406	29.57%	3.860%
15	10.627	1448	1452	1455	rBV	3167929	2609411	45.03%	5.879%
16	11.069	1524	1527	1531	rBV	2436573	2059887	35.54%	4.641%
17	11.227	1550	1554	1561	rBV	173335	206419	3.56%	0.465%
18	11.321	1567	1570	1574	rBV	1730003	1608066	27.75%	3.623%
19	11.386	1578	1581	1584	rVB	168265	190834	3.29%	0.430%
20	11.786	1647	1649	1652	rBV2	187045	232546	4.01%	0.524%
21	11.863	1659	1662	1664	rBV2	256976	270522	4.67%	0.609%
22	11.892	1664	1667	1669	rBV	422678	418759	7.23%	0.943%
23	11.921	1669	1672	1675	rVV	1110432	942410	16.26%	2.123%
24	12.004	1684	1686	1689	rBV2	459117	393177	6.78%	0.886%
25	12.039	1690	1692	1694	rVV	303309	268192	4.63%	0.604%
26	12.316	1737	1739	1744	rBV2	571325	926442	15.99%	2.087%
27	12.921	1839	1842	1849	rBV2	4210246	5795358	100.00%	13.057%
28	13.474	1934	1936	1939	rVB	3524234	2864086	49.42%	6.453%

Sum of corrected areas: 44385074

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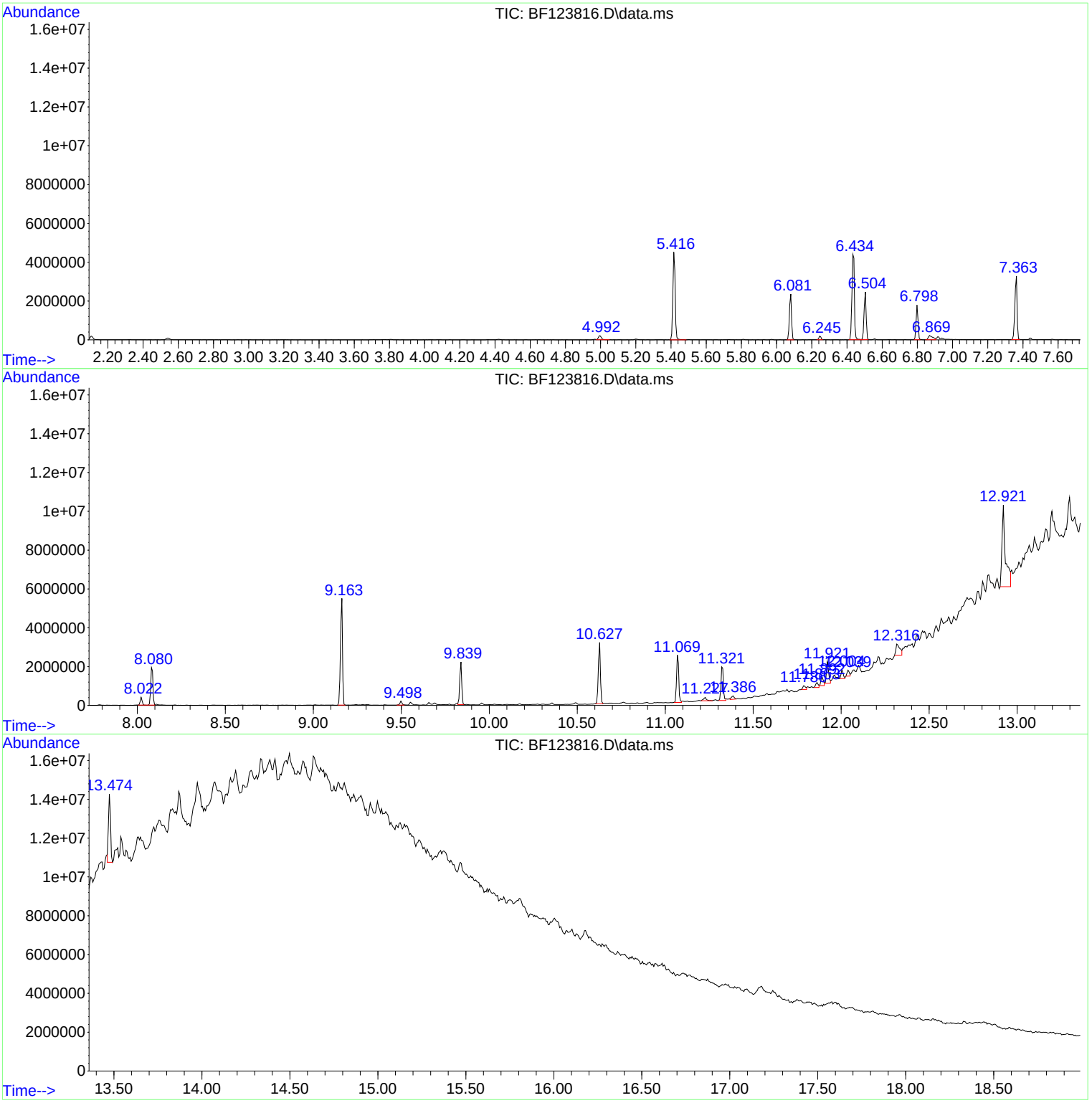
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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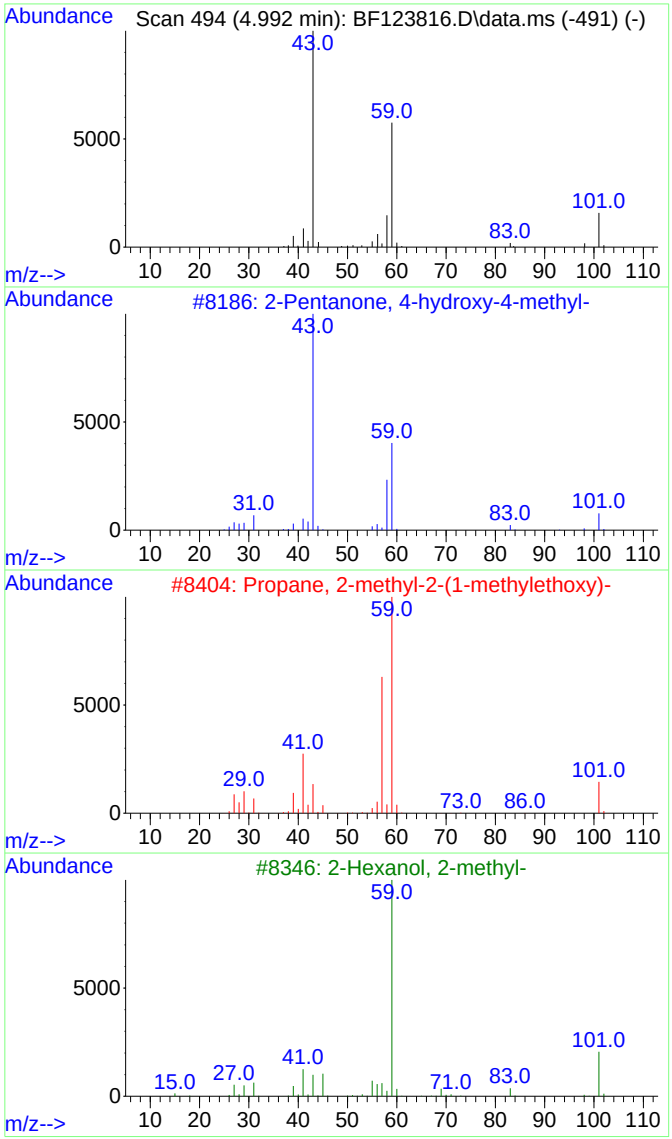
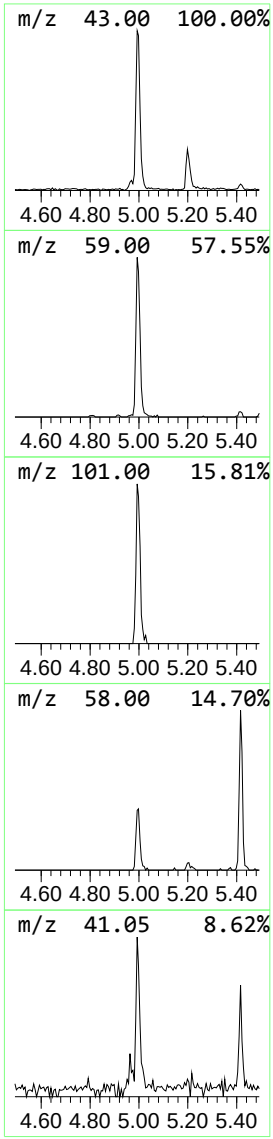
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	3.82 ng	251140	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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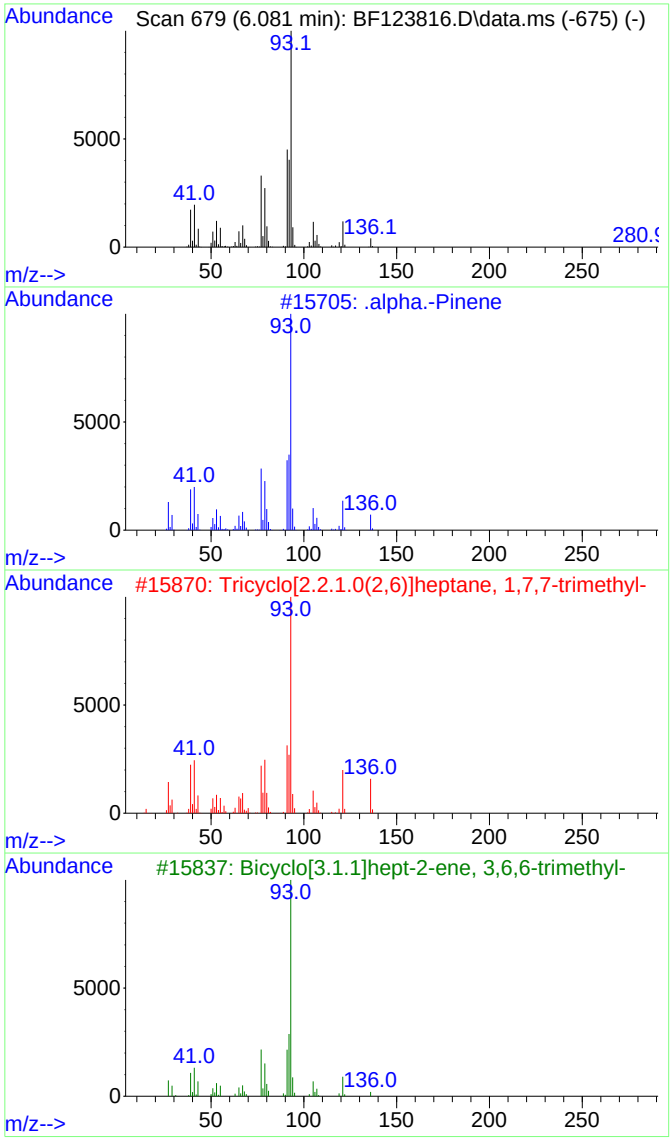
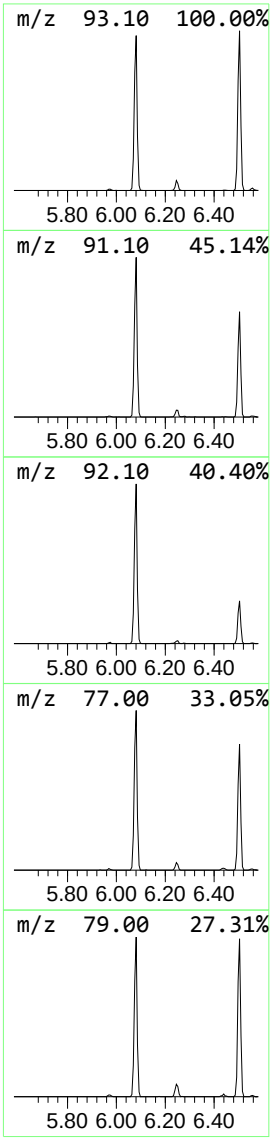
Peak Number 2 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.081	29.90 ng	1966220	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4	3-Carene	136	C10H16	013466-78-9	87
5	(+)-3-Carene	136	C10H16	000498-15-7	87





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Operator : JU/CG
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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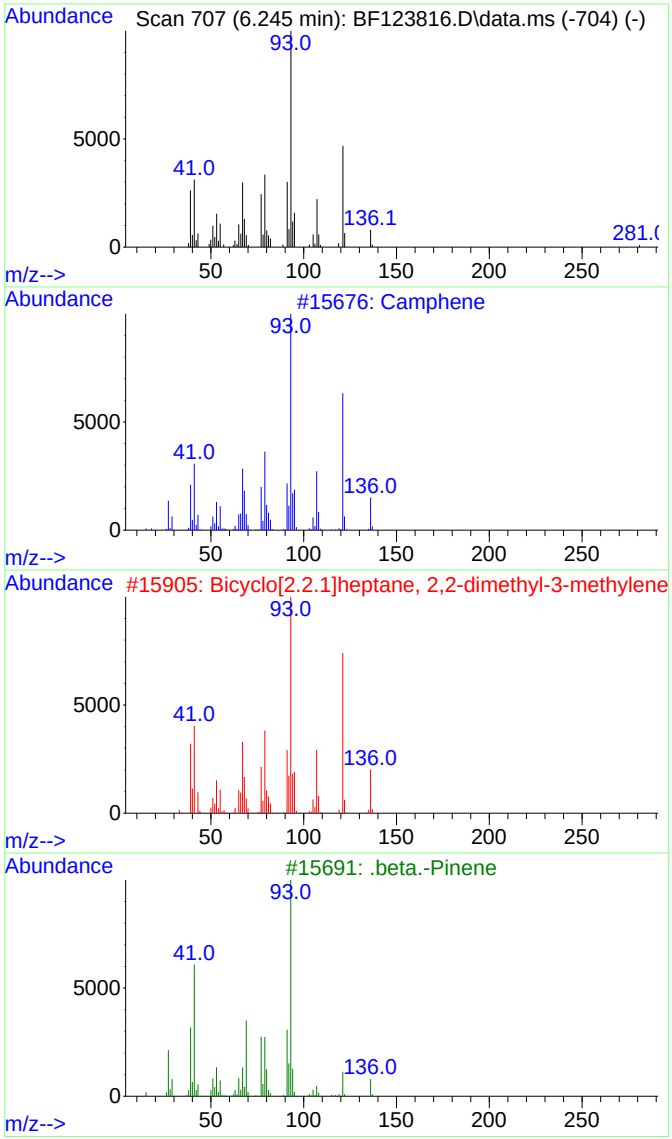
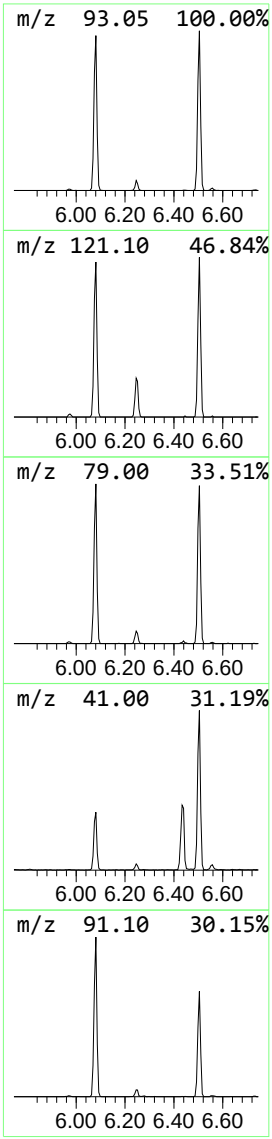
Peak Number 3 Camphene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	2.44 ng	160589	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphene	136	C10H16	000079-92-5	95
2	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	83
3	.beta.-Pinene	136	C10H16	000127-91-3	72
4	(+)-4-Carene	136	C10H16	029050-33-7	68
5	.beta.-Phellandrene	136	C10H16	000555-10-2	60





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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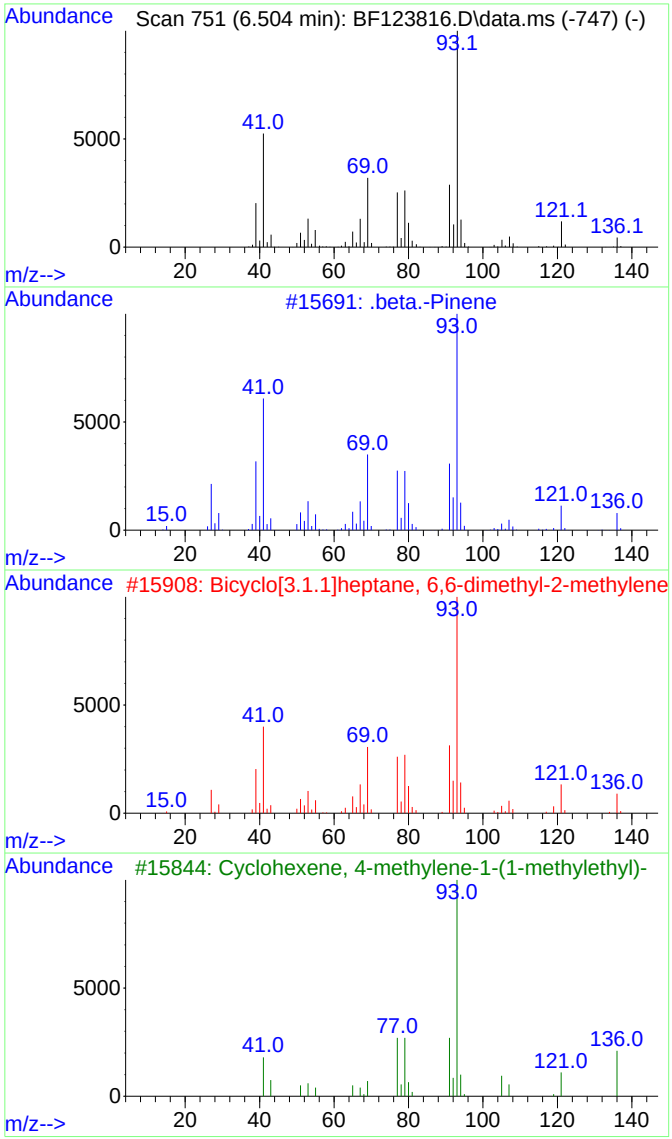
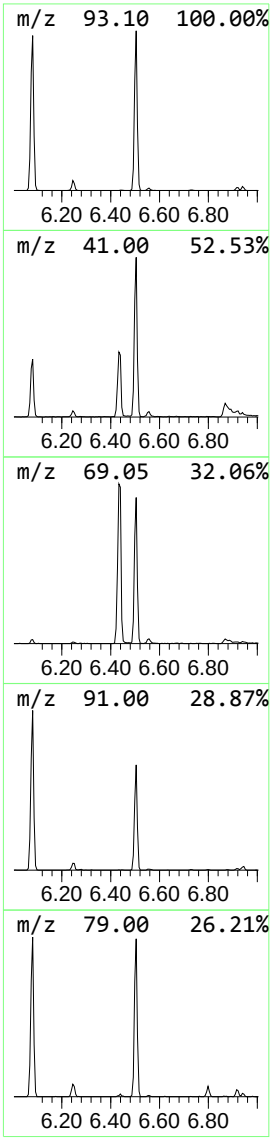
Peak Number 4 .beta.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.504	30.28 ng	1991590	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	94
2	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
3	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	87
4	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	86
5	.alpha.-Pinene	136	C10H16	000080-56-8	83





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Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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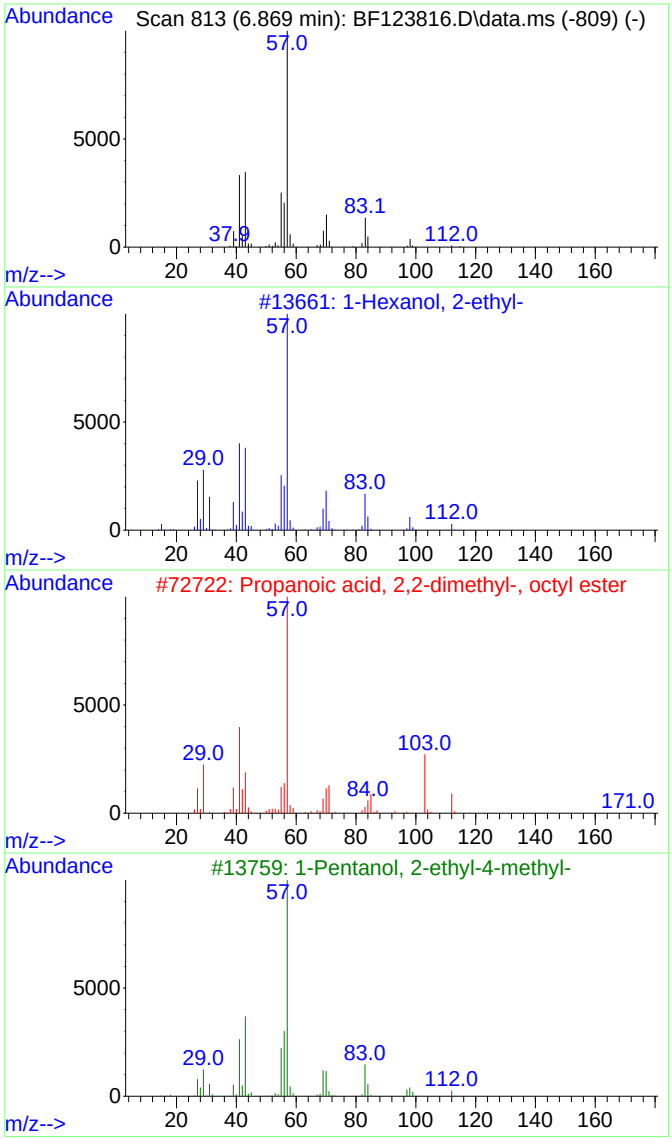
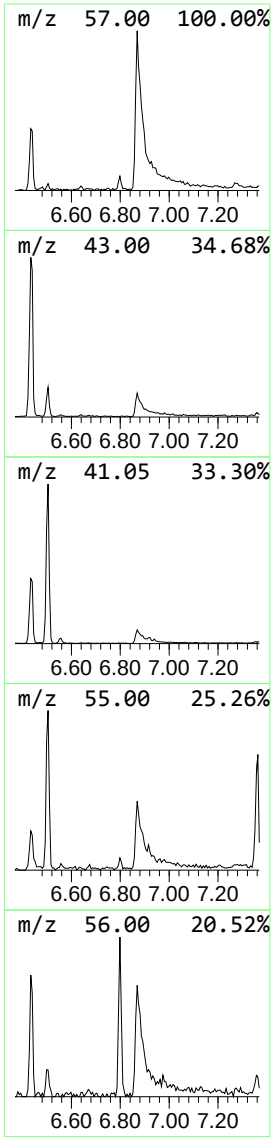
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.869	6.11 ng	401568	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	45
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
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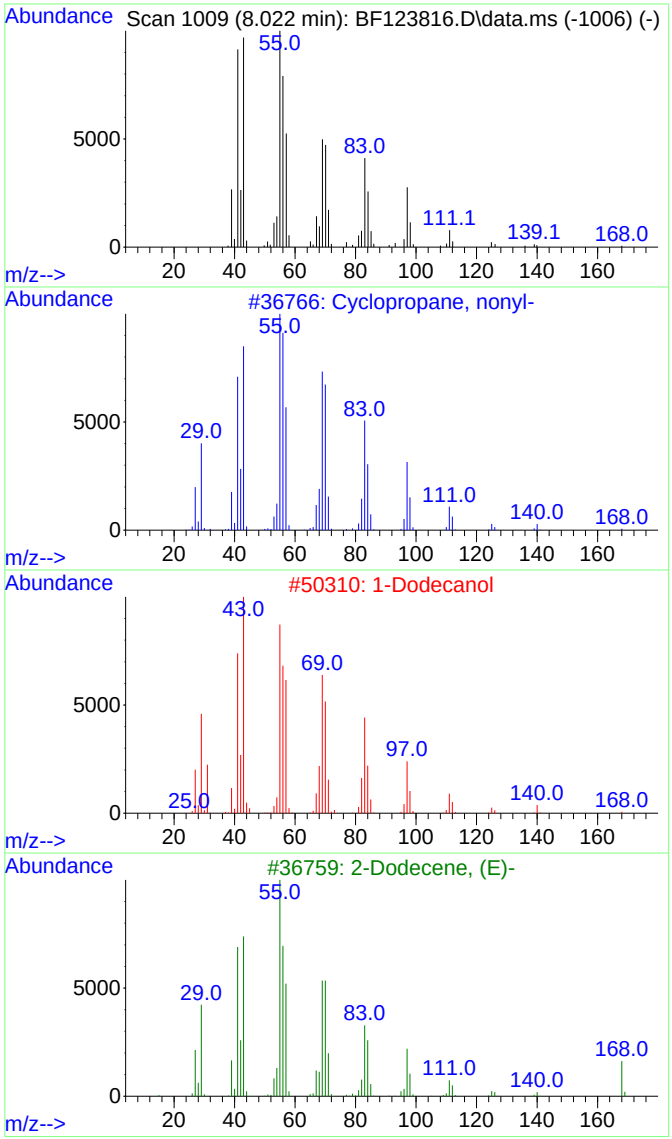
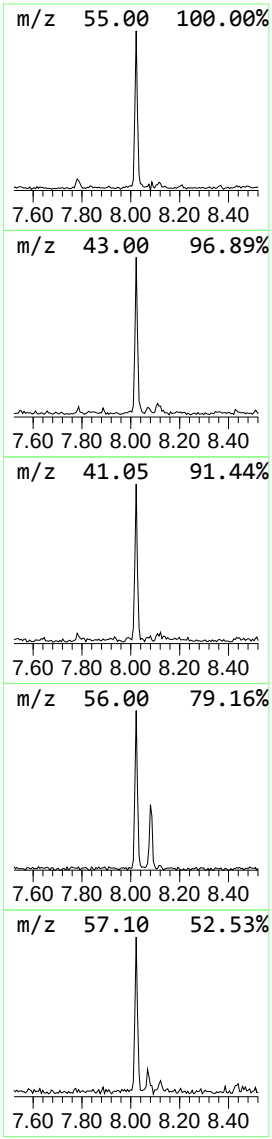
Peak Number 6 Cyclopropane, nonyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	3.51 ng	294599	Naphthalene-d8	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, nonyl-	168	C12H24	074663-85-7	94
2	1-Dodecanol	186	C12H26O	000112-53-8	90
3	2-Dodecene, (E)-	168	C12H24	007206-13-5	90
4	4-Dodecene	168	C12H24	002030-84-4	90
5	2-Dodecene, (Z)-	168	C12H24	007206-26-0	86





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Instrument :
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TIC Library : C:\DATABASE\NIST11.L
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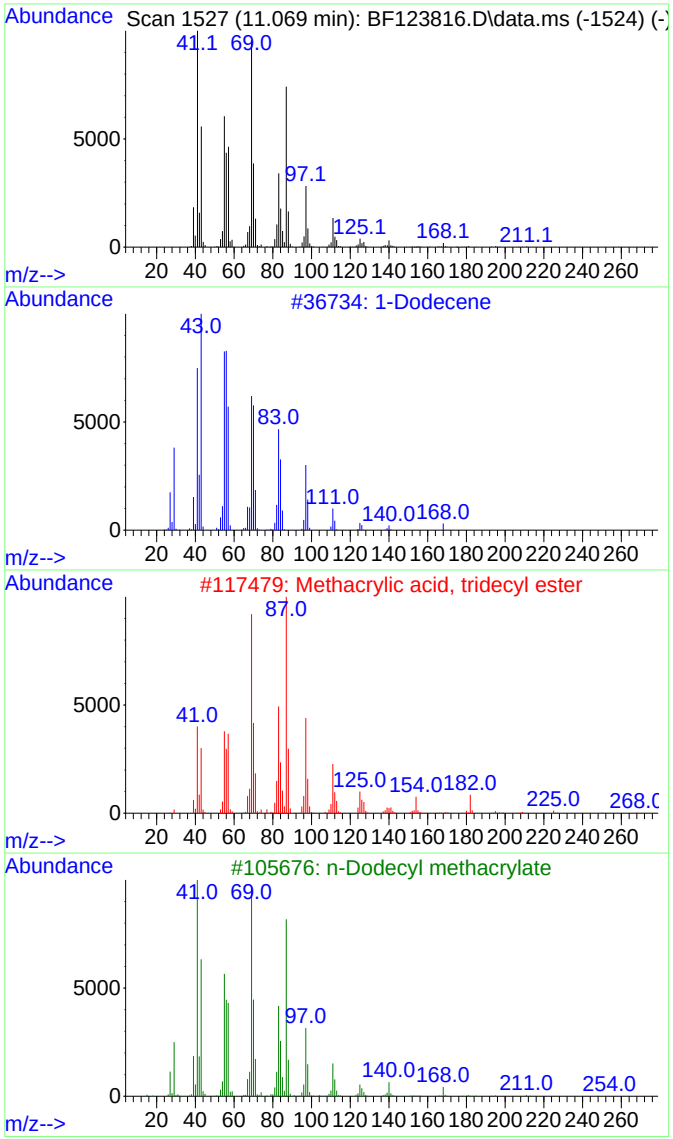
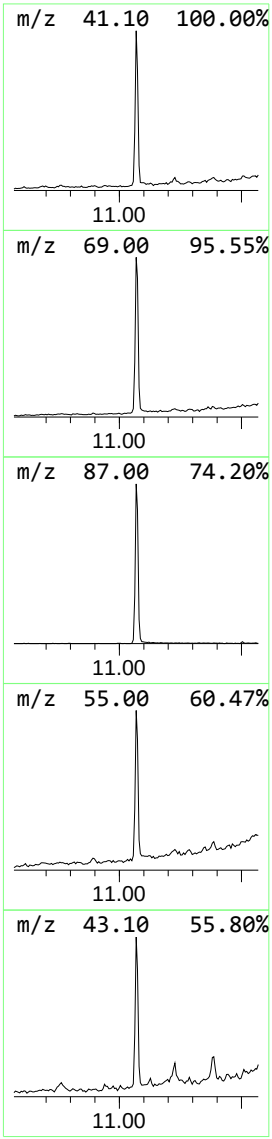
Peak Number 7 1-Dodecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	25.62 ng	2059890	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecene	168	C12H24	000112-41-4	93
2	Methacrylic acid, tridecyl ester	268	C17H32O2	1000340-28-9	91
3	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
4	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	87
5	Cyclododecane	168	C12H24	000294-62-2	83





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Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-2

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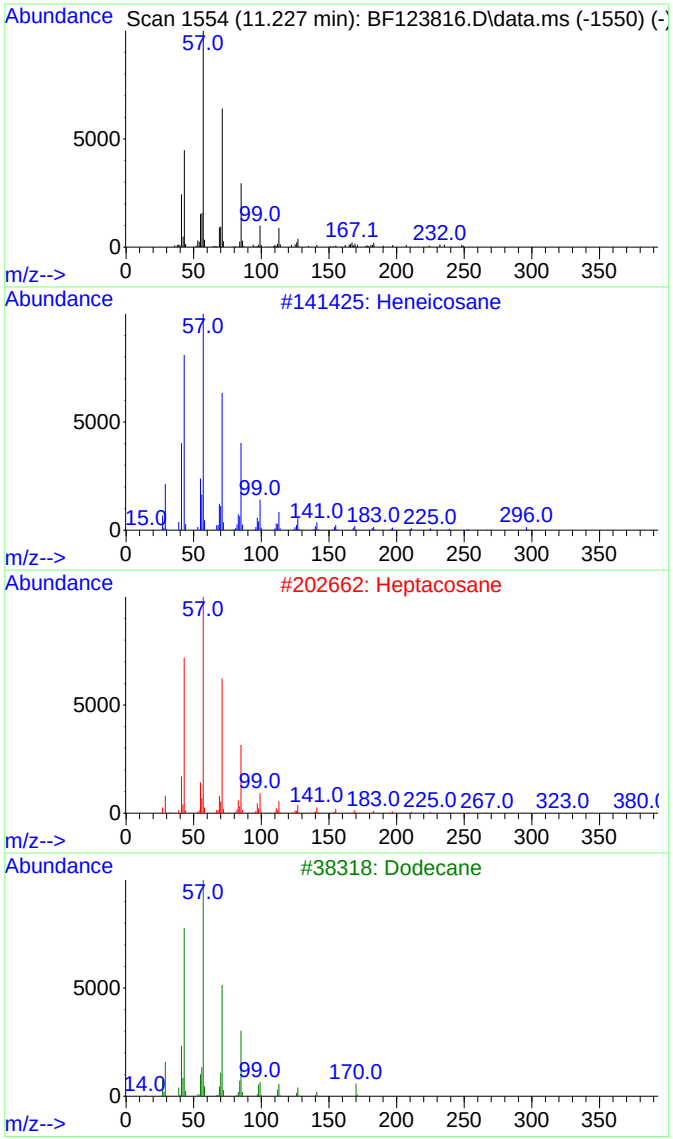
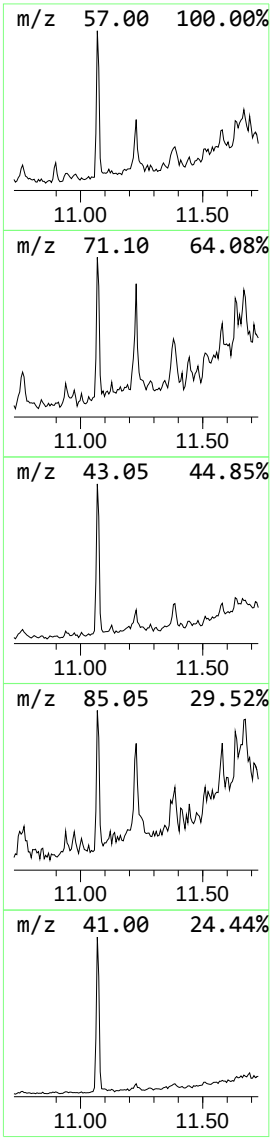
Peak Number 8 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.227	2.57 ng	206419	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Heptacosane	380	C27H56	000593-49-7	78
3	Dodecane	170	C12H26	000112-40-3	78
4	Eicosane	282	C20H42	000112-95-8	78
5	Hexadecane	226	C16H34	000544-76-3	72





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TIC Library : C:\DATABASE\NIST11.L
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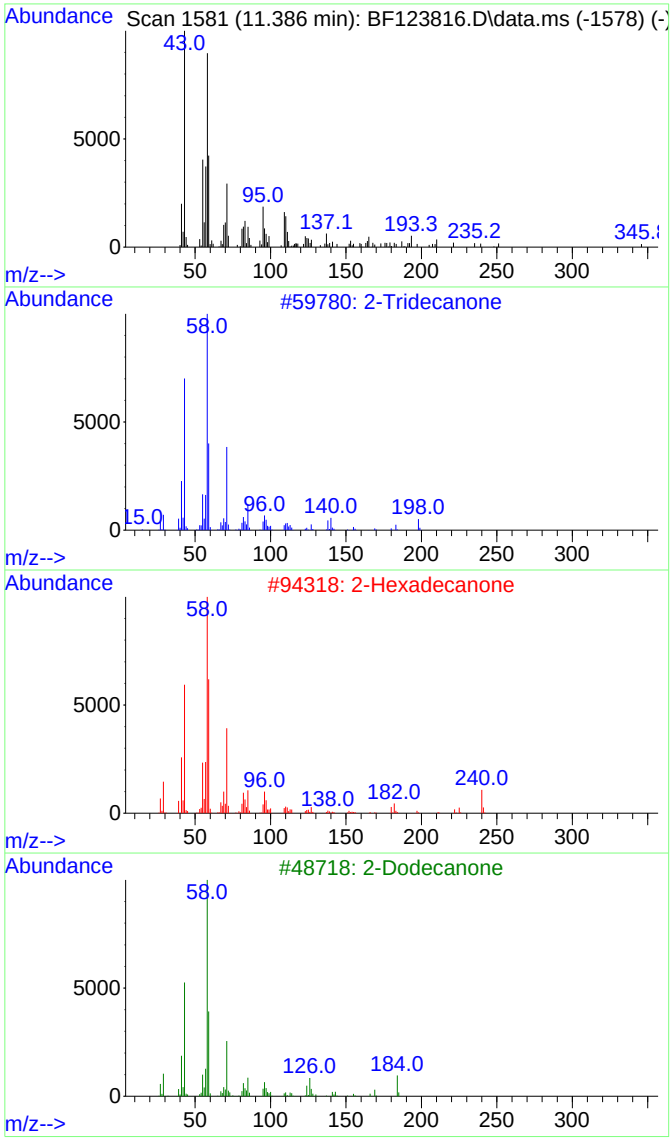
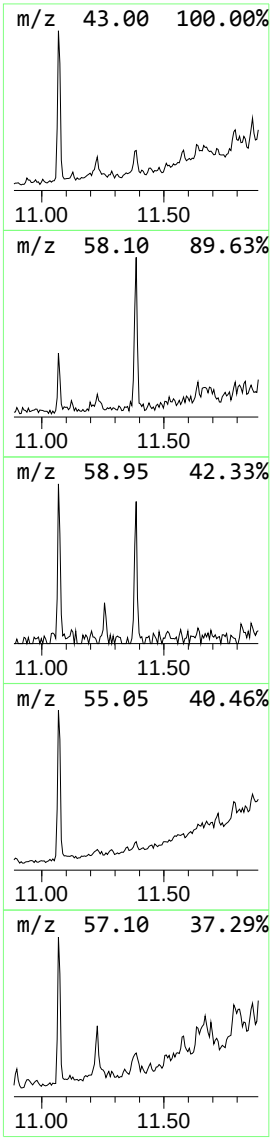
Peak Number 9 2-Tridecanone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.386	2.37 ng	190834	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecanone	198	C13H26O	000593-08-8	64
2	2-Hexadecanone	240	C16H32O	018787-63-8	64
3	2-Dodecanone	184	C12H24O	006175-49-1	64
4	2-Pentadecanone, 6,10,14-trimethyl-	268	C18H36O	000502-69-2	53
5	2-Tetradecanone	212	C14H28O	002345-27-9	53





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Instrument : BNA_F
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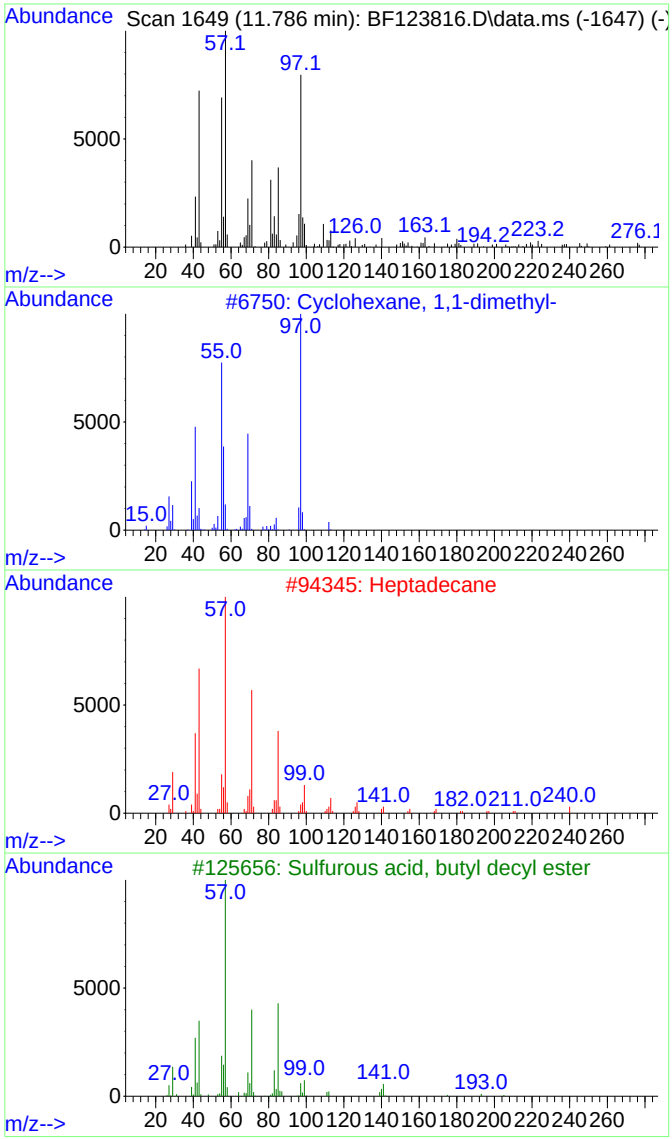
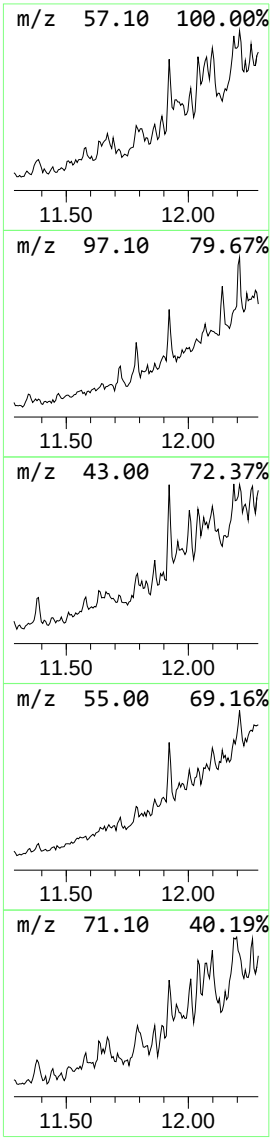
Peak Number 10 unknown11.786 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	2.89 ng	232546	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	41
2	Heptadecane	240	C17H36	000629-78-7	38
3	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	38
4	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	38
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	38





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Data File : BF123816.D
Acq On : 4 May 2021 19:20
Operator : JU/CG
Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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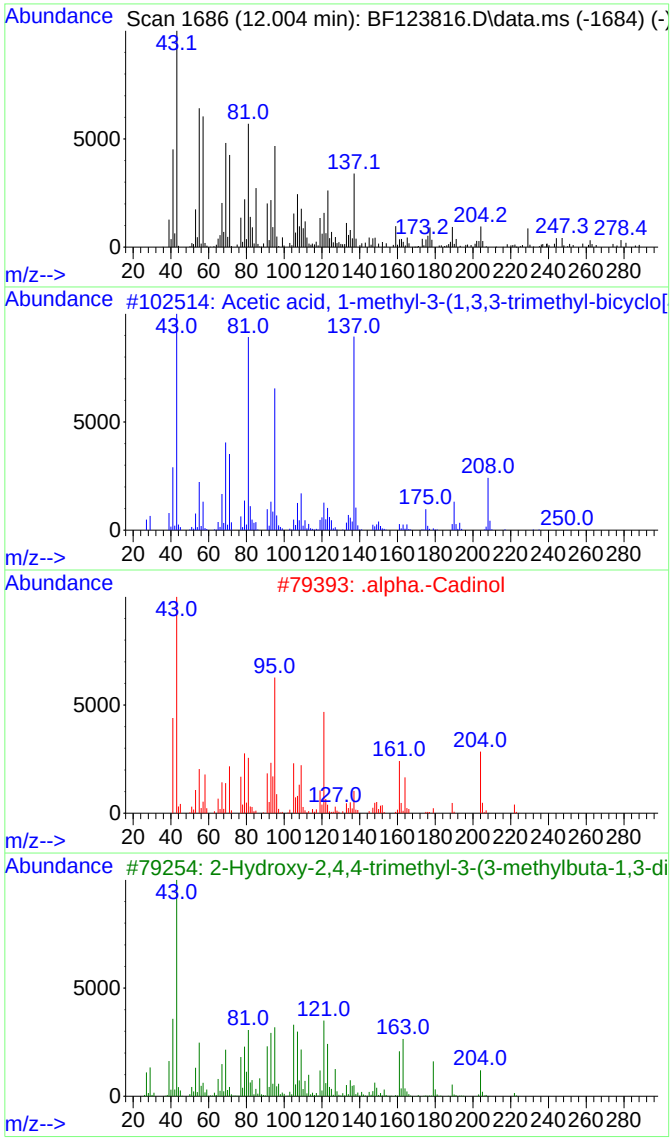
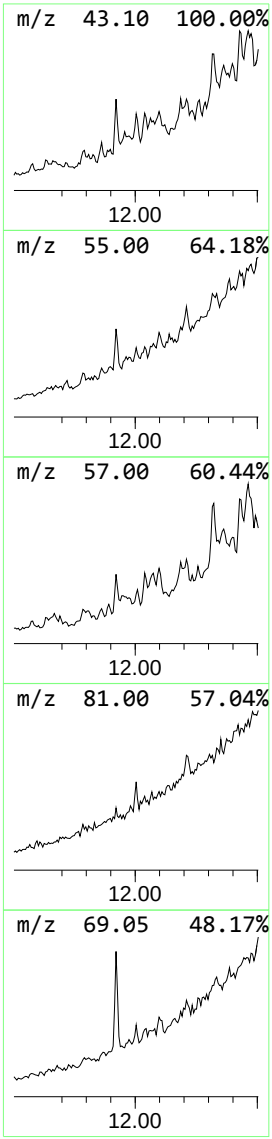
Peak Number 11 unknown12.004 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	4.89 ng	393177	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1-methyl-3-(1,3,3-t...	250	C16H26O2	1000192-22-3	35
2	.alpha.-Cadinol	222	C15H26O	000481-34-5	30
3	2-Hydroxy-2,4,4-trimethyl-3-(3-m...	222	C14H22O2	1000191-17-4	30
4	14-Oxatricyclo[9..2.1.0(1,10)]te...	262	C18H30O	1000193-06-8	25
5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	18





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Operator : JU/CG
Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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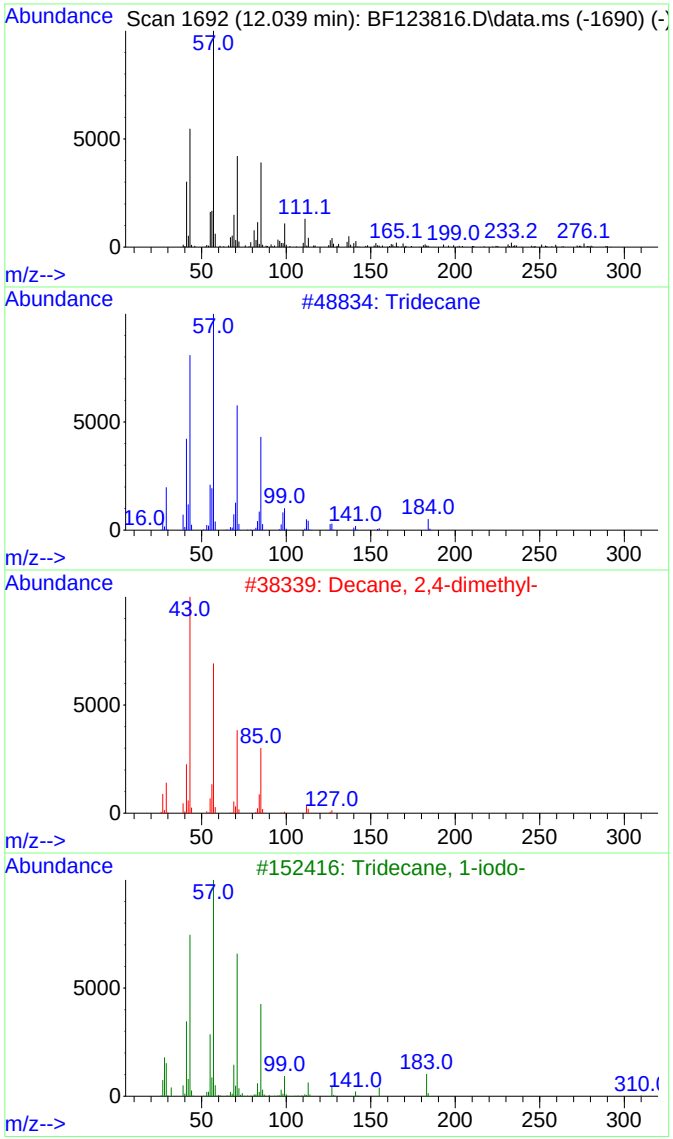
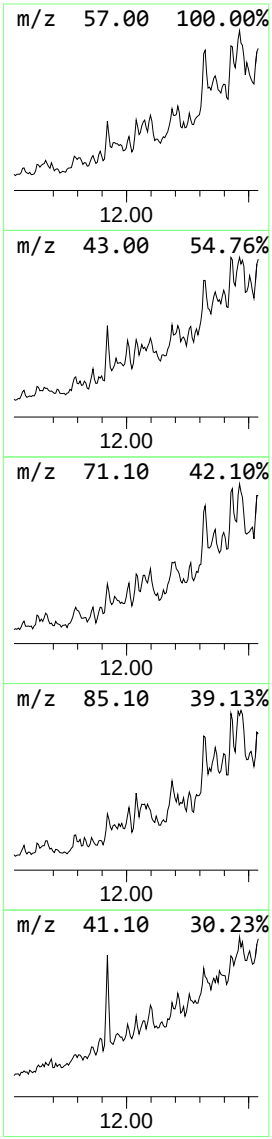
Peak Number 12 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	3.34 ng	268192	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	64
2	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	59
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	59
4	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	49
5	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	43





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Acq On : 4 May 2021 19:20
Operator : JU/CG
Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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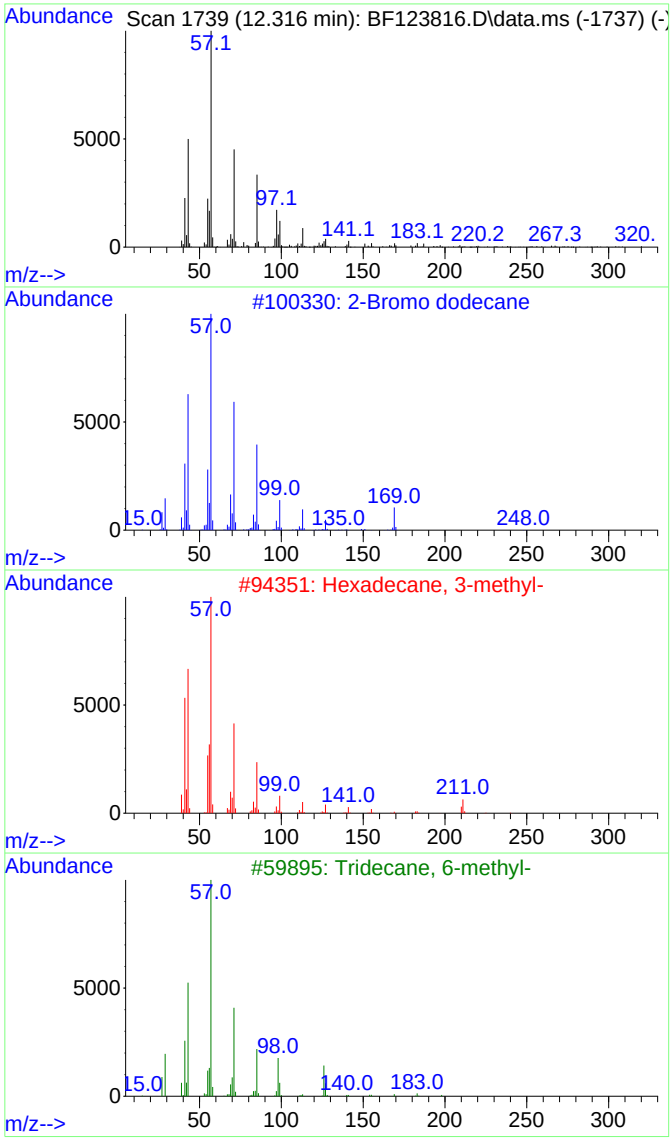
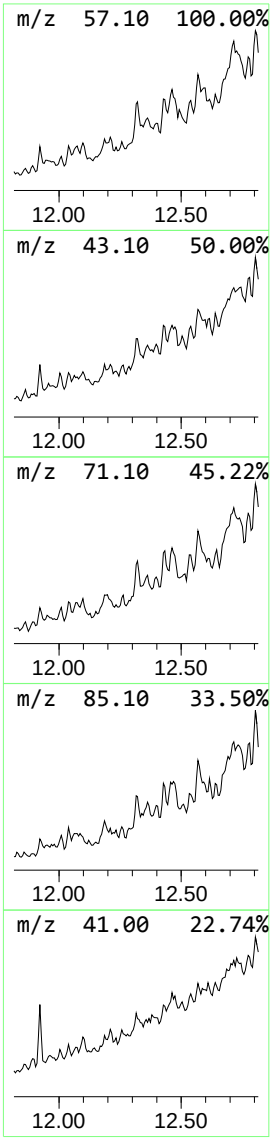
Peak Number 13 2-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.316	11.52 ng	926442	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
2	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	74
3	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
4	Octadecane	254	C18H38	000593-45-3	72
5	Pentadecane	212	C15H32	000629-62-9	72





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Data File : BF123816.D
Acq On : 4 May 2021 19:20
Operator : JU/CG
Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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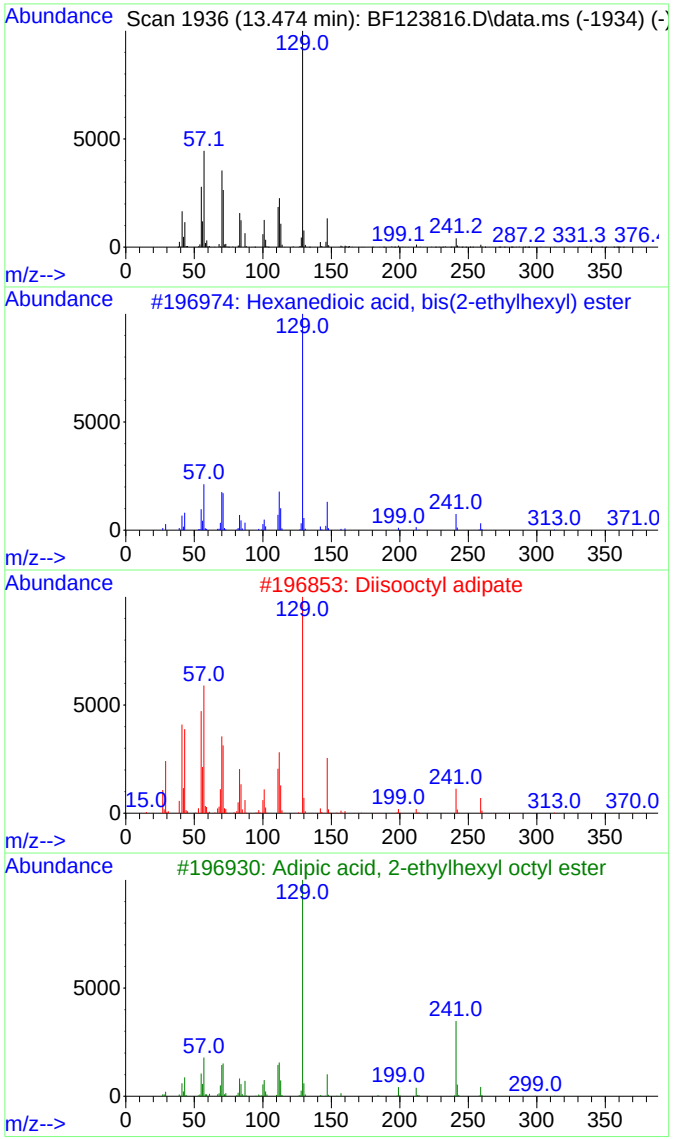
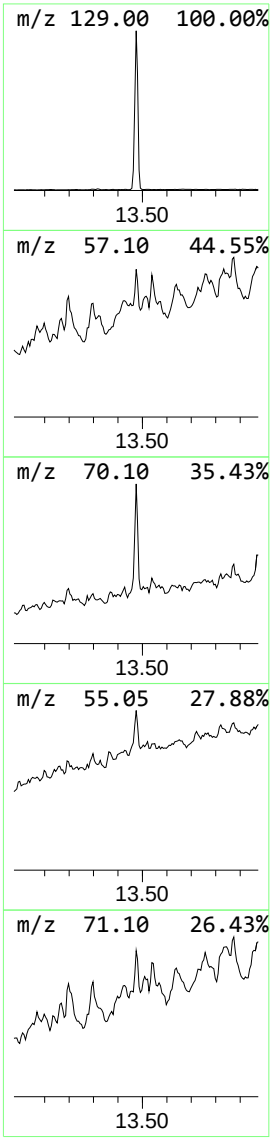
Peak Number 14 Hexanedioic acid, bis(2-eth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	20.00 ng	2864090	Chrysene-d12	13.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Diisooctyl adipate	370	C22H42O4	001330-86-5	90
3	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	86
4	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68
5	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050421\
Data File : BF123816.D
Acq On : 4 May 2021 19:20
Operator : JU/CG
Sample : M2252-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STONE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.992	3.8	ng	251140	1	6.798	1315360	20.0
.alpha.-Pinene	6.081	29.9	ng	1966220	1	6.798	1315360	20.0
Camphene	6.245	2.4	ng	160589	1	6.798	1315360	20.0
.beta.-Pinene	6.504	30.3	ng	1991590	1	6.798	1315360	20.0
1-Hexanol, 2-et...	6.869	6.1	ng	401568	1	6.798	1315360	20.0
Cyclopropane, n...	8.022	3.5	ng	294599	2	8.080	1679850	20.0
1-Dodecene	11.069	25.6	ng	2059890	4	11.322	1608070	20.0
Heneicosane	11.227	2.6	ng	206419	4	11.322	1608070	20.0
2-Tridecanone	11.386	2.4	ng	190834	4	11.322	1608070	20.0
unknown11.786	11.786	2.9	ng	232546	4	11.322	1608070	20.0
unknown12.004	12.004	4.9	ng	393177	4	11.322	1608070	20.0
Tridecane	12.039	3.3	ng	268192	4	11.322	1608070	20.0
2-Bromo dodecane	12.316	11.5	ng	926442	4	11.322	1608070	20.0
Hexanedioic aci...	13.474	20.0	ng	2864090	5	13.986	2864090	20.0